Optimal Designs of Two-Level Factorials when $N \equiv 1$ and $2 \pmod 4$ under a Baseline Parameterization

by

Kunasekaran Nirmalkanna
B.Sc. (Hons.), University of Colombo, 2011

A Project Submitted in Partial Fulfillment
of the Requirements for the Degree of

Master of Science

in the
Department of Statistics & Actuarial Science
Faculty of Science

SIMON FRASER UNIVERSITY
Summer 2014

APPROVAL

Name: Kunasekaran Nirmalkanna

Degree: Master of Science

Title of Project: Optimal Designs of Two-Level Factorials when $N \equiv 1$ and $2 \pmod 4$ under a Baseline Parameterization

Examining Committee: Dr. Tim Swartz,
Professor,
Chair

Dr. Boxin Tang,
Professor, Senior Supervisor

Dr. Thomas M. Loughin,
Professor, Supervisor

Dr. Jiguo Cao,
Professor, Internal Examiner

Date Approved: August 18th, 2014

Partial Copyright Licence

Abstract

This work considers two-level factorial designs under a baseline parameterization where the two levels are denoted by 0 and 1. Orthogonal parameterization is commonly used in two-level factorial designs. But in some cases the baseline parameterization is natural. When only main effects are of interest, such designs are equivalent to biased spring balance weighing designs. Commonly, we assume that the interactions are negligible, but if this is not the case then these non-negligible interactions will bias the main effect estimates. We review the minimum aberration criterion under the baseline parameterization, which is to be used to compare the sizes of the bias among different designs.

We define a design as optimal if it has the minimum bias among most efficient designs. Optimal designs for $N \equiv 0 \pmod 4$, where N is the run size, were discussed by Mukerjee & Tang (2011). We continue this line of study by investigating optimal designs for the cases $N \equiv 1$ and $2 \pmod 4$. Searching for an optimal design among all possible designs is computationally very expensive, except for small N and m, where m is the number of factors. Cheng's (2014) results are used to narrow down the search domain. We have done a complete search for small N and m. We have found that one can directly use Cheng's (2014) theorem to find an optimal design for the case $N \equiv 1 \pmod 4$. But for the case $N \equiv 2 \pmod 4$, a small modification is required.

Acknowledgments

I am forever grateful for having the opportunity to work under the supervision of Dr. Boxin Tang. I will always cherish the memories of working with you and learning from you throughout my time at SFU. Thank you for your all support sir. Many thanks to Dr. Tom Loughin and Dr. Jiguo Cao for agreeing to be in my committee and providing great feedback on this project.

Specially, I would like to thank Dr. Boxin Tang and Dr. Tim Swartz for giving me the wonderful opportunity to pursue a Masters Degree at SFU. I would like to express my gratitude to all the professors at SFU who taught me how to think statistically. I would also like to thank Saidka, Kelly and Charlene for their help.

Last but not least I would like to thank my wife Ananthika. Her unconditional love and invaluable support has led me to achieve this success.

Contents

List of Tables

Chapter 1

Introduction

Fractional factorials are popular among practitioners because of their run size economy. This study considers two-level factorial designs. Fisher and Yates started doing study on the two-level factorial and fractional factorials and up to now those designs have been extensively studied. The study of optimal fractional factorial designs under the minimum aberration and related model robustness criteria has received significant attention over the last two decades. The most common approach to analyzing data from a regular two-level fractional factorial design is to estimate the effects using orthogonal parameterization. In orthogonal parameterization, main effects and interaction effects are a set of orthogonal contrasts as described by Box, Hunter and Hunter (2005). Another approach, which is less common but more natural, is the so called baseline parameterization. If there is a null state or baseline level for each factor, then the baseline parameterization is natural.

When we estimate the parameters, we prefer the estimates which give the minimum mean squared error. The mean squared error is the sum of two components, the variance and the squared bias. If a two-level fractional factorial design is an orthogonal array, then it minimizes the variances of the main effect estimates. This is true for both orthogonal and baseline parameterization. The minimum aberration criterion can be used to minimize the bias of the main effect estimates due to active interaction effects. This study defines an optimal design as a design which has a minimum bias among the designs which have minimum variance in estimating parameters.

In 2011, Mukerjee and Tang developed a theory of minimum aberration for two-level factorials under a baseline parameterization. They derived general results for minimum aberration designs for $N = 4t$, $m = 4t-1$ and $m = 4t-2$, where N is the run size and m is the number of factors. Minimum aberration designs for $m \leq 4t-3$ are obtained up to $N = 16$ by complete search. Such results for

$N = 20$ are available in Li, Miller and Tang (2014). The results of Mukerjee and Tang (2011) and Li et al. (2014) are restricted to the run sizes that are multiples of 4. This project continues this line of study by investigating optimal designs for the cases $N = 1$ and $2 \pmod 4$.

For example, if we want an optimal design for $N = 9$ and $m = 7$ then there exist many possible estimable designs. Searching for an optimal design among them is computationally very expensive. Cheng's (2014) theory is used here to narrow down the search domain. It says that by adding one and two specific runs to an orthogonal array one can obtain the most efficient design.

Cheng's theorem for $N \equiv 1 \pmod 4$ states that adding an all-one run or all-zero run to an orthogonal array gives a most efficient design. By complete search, we found that the global optimal design can be obtained by adding an all-zero run to a particular orthogonal array. Cheng's theorem for $N \equiv 2 \pmod 4$ says that adding an all-one run and a run with $m/2$ or $(m-1)/2$ ones to an orthogonal array gives the most efficient design where m is even or odd respectively. Level switched forms of these two runs also give the same result. In our study, the level switched case gives better designs. But, in some cases, by allowing level switches in the columns of those two runs, one can obtain the global optimal designs.

The rest of this project is organized as follows. In Chapter 2, we give an overview of orthogonal and baseline parameterizations, and the existing criteria of optimal designs. Our algorithms for searching optimal designs are discussed in detail in Chapter 3. Some optimal designs are also presented in this chapter. Finally, in Chapter 4, we give brief concluding remarks.

Chapter 2

Optimal Factorials under a Baseline Parameterization

Consider a two-level full factorial design with 3 factors. We use this example to explain how the main and interaction effects are defined under two rather different parameterizations.

Table 2.1: Two-level factorial design with 3 factors with their means

Factor 1	Factor 2	Factor 3	Response Mean
Low	Low	Low	μ_1
Low	Low	High	μ_2
Low	High	Low	μ_3
Low	High	High	μ_4
High	Low	Low	μ_5
High	Low	High	μ_6
High	High	Low	μ_7
High	High	High	μ_8

If we want to estimate the main and interaction effects of explanatory variables, simply we can fit a multiple regression model and then draw conclusions. Consider a linear model with m explanatory variables,

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_m X_m + \epsilon,$$
$$E(\epsilon) = 0 \text{ and } V(\epsilon) = \sigma^2 I.$$

The model can be re-written in matrix form as, $Y = X\boldsymbol{\beta} + \epsilon$, where $\boldsymbol{\beta} = (\beta_0, \beta_1, \cdots, \beta_m)^T$ and $X = \left(1 \vdots X_1 \vdots X_2 \vdots \cdots \vdots X_m\right)$. Then the least square estimate of $\boldsymbol{\beta}$ is $\hat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T Y$.

2.1 Orthogonal Parameterization

For the example in Table 2.1, usually people assign -1 to the low level and 1 to the high level. This is the so called orthogonal parameterization. The model matrix is defined in Table 2.2.

Table 2.2: Two-level factorial design with 3 factors under orthogonal parameterization

Response Mean (Y)	**Model Matrix** (X)							
	Intercept	**Main effects**			**2-FI**			**3-FI**
		F1	**F2**	**F3**	**F1*F2**	**F1*F3**	**F2*F3**	**F1*F2*F3**
μ_1	1	-1	-1	-1	1	1	1	-1
μ_2	1	-1	-1	1	1	-1	-1	1
μ_3	1	-1	1	-1	-1	1	-1	1
μ_4	1	-1	1	1	-1	-1	1	-1
μ_5	1	1	-1	-1	-1	-1	1	1
μ_6	1	1	-1	1	-1	1	-1	-1
μ_7	1	1	1	-1	1	-1	-1	-1
μ_8	1	1	1	1	1	1	1	1

* FI = Factor Interaction effect

The interaction columns are products of the corresponding main effect columns. Then we have that $\boldsymbol{\beta} = (X^T X)^{-1} X^T \boldsymbol{\mu}$ where $\boldsymbol{\mu} = (\mu_1, \mu_2, \cdots, \mu_8)^T$, ie,

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_{12} \\ \beta_{13} \\ \beta_{23} \\ \beta_{123} \end{pmatrix} = \begin{pmatrix} ^1/_8 & ^1/_8 & ^1/_8 & ^1/_8 & ^1/_8 & ^1/_8 & ^1/_8 & ^1/_8 \\ -^1/_8 & -^1/_8 & -^1/_8 & -^1/_8 & ^1/_8 & ^1/_8 & ^1/_8 & ^1/_8 \\ -^1/_8 & -^1/_8 & ^1/_8 & ^1/_8 & -^1/_8 & -^1/_8 & ^1/_8 & ^1/_8 \\ -^1/_8 & ^1/_8 & -^1/_8 & ^1/_8 & -^1/_8 & ^1/_8 & -^1/_8 & ^1/_8 \\ ^1/_8 & ^1/_8 & -^1/_8 & -^1/_8 & -^1/_8 & -^1/_8 & ^1/_8 & ^1/_8 \\ ^1/_8 & -^1/_8 & ^1/_8 & -^1/_8 & -^1/_8 & ^1/_8 & -^1/_8 & ^1/_8 \\ ^1/_8 & -^1/_8 & -^1/_8 & ^1/_8 & ^1/_8 & -^1/_8 & -^1/_8 & ^1/_8 \\ -^1/_8 & ^1/_8 & ^1/_8 & -^1/_8 & ^1/_8 & -^1/_8 & -^1/_8 & ^1/_8 \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \\ \mu_6 \\ \mu_7 \\ \mu_8 \end{pmatrix}.$$

Under this orthogonal parameterization, the intercept term of the linear model is the grand mean of all the responses.

- The intercept is

$$\beta_0 = \frac{\mu_1 + \mu_2 + \mu_3 + \mu_4 + \mu_5 + \mu_6 + \mu_7 + \mu_8}{8}.$$

In what follows, we note that the coefficients are not the effect of factors (Box, Hunter and Hunter, 2005). Rather the effects are twice the corresponding coefficients.

- Main Effect of F1 is

$$2\beta_1 = \frac{(\mu_8 - \mu_4) + (\mu_7 - \mu_3) + (\mu_6 - \mu_2) + (\mu_5 - \mu_1)}{4},$$

- Main Effect of F2 is

$$2\beta_2 = \frac{(\mu_8 - \mu_6) + (\mu_7 - \mu_5) + (\mu_4 - \mu_2) + (\mu_3 - \mu_1)}{4} \text{ and}$$

- Main Effect of F3 is

$$2\beta_3 = \frac{(\mu_8 - \mu_7) + (\mu_6 - \mu_5) + (\mu_4 - \mu_3) + (\mu_2 - \mu_1)}{4}.$$

Now, consider the interaction effect of factor 1 and factor 2. It is the difference between the effects of factor 2 when factor 1 is held at the low and high levels.

- Interaction Effect of F1 & F2 is

$$2\beta_{12} = \frac{\{(\mu_8 - \mu_6) + (\mu_7 - \mu_5)\} - \{(\mu_4 - \mu_2) + (\mu_3 - \mu_1)\}}{4},$$

- Interaction Effect of F1 & F3 is

$$2\beta_{13} = \frac{\{(\mu_8 - \mu_7) + (\mu_6 - \mu_5)\} - \{(\mu_4 - \mu_3) + (\mu_2 - \mu_1)\}}{4} \text{ and}$$

- Interaction Effect of F2 & F3 is

$$2\beta_{23} = \frac{\{(\mu_8 - \mu_7) + (\mu_4 - \mu_3)\} - \{(\mu_6 - \mu_5) + (\mu_2 - \mu_1)\}}{4}.$$

The interaction among factors 1,2 and 3 is the difference between the interaction effects of factor 2 and 3 when factor 1 is held at the low and high levels.

- Interaction Effect of F1, F2 & F3 is

$$2\beta_{123} = \frac{\{(\mu_8 - \mu_7) - (\mu_6 - \mu_5)\} - \{(\mu_4 - \mu_3) - (\mu_2 - \mu_1)\}}{4}.$$

These effects are the contrasts of treatment means and are mutually orthogonal. This is the reason why it is named as the orthogonal parameterization.

2.2 Baseline Parameterization

In the baseline parameterization, the low and high levels are denoted by 0 and 1, respectively. Then the model matrix becomes that in Table 2.3.

Table 2.3: Two-level factorial design with 3 factors under baseline parameterization

Response Mean (Y)	**Model Matrix** (X)							
	Intercept	**Main effects**			**2-FI**			**3-FI**
		F1	**F2**	**F3**	**F1*F2**	**F1*F3**	**F2*F3**	**F1*F2*F3**
μ_1	1	0	0	0	0	0	0	0
μ_2	1	0	0	1	0	0	0	0
μ_3	1	0	1	0	0	0	0	0
μ_4	1	0	1	1	0	0	1	0
μ_5	1	1	0	0	0	0	0	0
μ_6	1	1	0	1	0	1	0	0
μ_7	1	1	1	0	1	0	0	0
μ_8	1	1	1	1	1	1	1	1

* FI = Factor Interaction effect

Here also the interaction columns are products of the corresponding main effect columns. The linear model becomes

$$Y = X\boldsymbol{\theta} + \epsilon, \quad \text{where } \boldsymbol{\theta} = (\theta_0, \theta_1, \theta_2, \theta_3, \theta_{12}, \theta_{13}, \theta_{23}, \theta_{123})^T.$$

For convenience, we use $\boldsymbol{\theta}$ instead of $\boldsymbol{\beta}$ to represent baseline effects. We have $\boldsymbol{\theta} = (X^TX)^{-1}X^T\boldsymbol{\mu}$ where $\boldsymbol{\mu} = (\mu_1, \mu_2, \cdots, \mu_8)^T$. We obtain

$$\boldsymbol{\theta} = \begin{pmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_{12} \\ \theta_{13} \\ \theta_{23} \\ \theta_{123} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & -1 & 0 & 1 & 0 \\ 1 & -1 & 0 & 0 & -1 & 1 & 0 & 0 \\ 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \\ \mu_6 \\ \mu_7 \\ \mu_8 \end{pmatrix}.$$

Therefore,

$$\theta_0 = \mu_1.$$

The change in the responses when the level of any factor changes from low level to high level while others remain in low levels, is the main effect of that factor. Consider μ_1 and μ_5. In these two cases, factors 2 and 3 are in low levels but factor 1 has different levels. Therefore, the difference between these two means is then the main effect of factor 1. More precisely,

- Main Effect of F1 : $\theta_1 = \mu_5 - \mu_1$.

For the other two factors, we have

- Main Effect of F2 : $\theta_2 = \mu_3 - \mu_1$ and
- Main Effect of F3 : $\theta_3 = \mu_2 - \mu_1$.

Similarly, we have

- Interaction Effect of F1 & F2 : $\theta_{12} = \mu_7 - \mu_1 - (\theta_1 + \theta_2) = \mu_7 + \mu_1 - \mu_5 - \mu_3$,
- Interaction Effect of F1 & F3 : $\theta_{13} = \mu_6 - \mu_1 - (\theta_1 + \theta_3) = \mu_6 + \mu_1 - \mu_5 - \mu_2$,
- Interaction Effect of F2 & F3 : $\theta_{23} = \mu_4 - \mu_1 - (\theta_2 + \theta_3) = \mu_4 + \mu_1 - \mu_2 - \mu_3$ and
- Interaction Effect of F1, F2 & F3 :

$$\theta_{123} = \mu_8 - \mu_1 - (\theta_1 + \theta_2 + \theta_3 + \theta_{12} + \theta_{13} + \theta_{23}) = \mu_8 + \mu_5 + \mu_3 + \mu_2 - \mu_7 - \mu_6 - \mu_4 - \mu_1.$$

The main and interaction effects are still contrasts of the treatment means, but these contrasts are not mutually orthogonal, unlike those under the orthogonal parameterization.

So far we have discussed the orthogonal and baseline parameterizations and the difference between them. In the orthogonal parameterization, we cannot interpret the significant main effect directly in the presence of significant interaction effects. But in the baseline parameterization, it does not have that problem.

2.3 Efficient Designs

For now, we assume that the interactions are negligible. The least square estimate of $\boldsymbol{\theta}$ (i.e. $\hat{\boldsymbol{\theta}}$) is $(X^TX)^{-1}X^TY$, where X is a matrix with only the intercept column and the main effects columns. The variance of the estimate ($V(\hat{\boldsymbol{\theta}})$) is $(X^TX)^{-1}\sigma^2$. If we want to minimize the variance of the estimate then we need to minimize $(X^TX)^{-1}$ or maximize X^TX. This matrix X^TX is also known as the information matrix. There are several criteria such as A-criterion and D-criterion, which are useful to compare the efficiency of two or more designs. Low variance means high efficiency and vise versa. Let's see how to compute those criteria.

- ***A*-criterion:** Calculate the *trace* of $\left(X^T X\right)^{-1}$. If it has the minimum value, then the corresponding design is an A-optimal design.
- ***D*-criterion:** Calculate the *determinant* of $\left(X^T X\right)^{-1}$. If it has the minimum value, then the corresponding design is a D-optimal design.

For example, let's consider a model matrix X with 10 runs and 4 two-level factors,

$$X = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 \end{pmatrix}, (X^T X)^{-1} = \begin{pmatrix} 0.381 & -0.143 & -0.143 & -0.167 & -0.167 \\ -0.143 & 0.429 & -0.071 & 0 & 0 \\ -0.143 & -0.071 & 0.429 & 0 & 0 \\ -0.167 & 0 & 0 & 0.417 & -0.083 \\ -0.167 & 0 & 0 & -0.083 & 0.417 \end{pmatrix},$$

We obtain

$$A\text{-criterion} : trace((X^T X)^{-1}) = 2.07143 \text{ and}$$
$$D\text{-criterion} : |(X^T X)^{-1}| = 0.00298.$$

The A-criterion and D-criterion consider the model matrix which includes intercept column and the design matrix. In screening experiments, the intercept term is of little interest. Therefore, after calculating the $(X^T X)^{-1}$, we can simply ignore the first column and the first row which correspond to the intercept term. We are led to considering the following criteria.

- **A_s-criterion:** Calculate the $\left(X^T X\right)^{-1}$ matrix. Remove the first row and first column and calculate the *trace* of the resulting matrix. If this has the minimum value, then the corresponding design is an A_s-optimal design.

- **D_s-criterion:** Calculate the $\left(X^TX\right)^{-1}$ matrix. Remove the first row and first column and calculate the *determinant* of the resulting matrix. If this has the minimum value, then the corresponding design is a D_s-optimal design.

In our example,

$$(X^TX)^{-1} = \left(\begin{array}{r|rrrr} 0.381 & -0.143 & -0.143 & -0.167 & -0.167 \\ \hline -0.143 & 0.429 & -0.071 & 0 & 0 \\ -0.143 & -0.071 & 0.429 & 0 & 0 \\ -0.167 & 0 & 0 & 0.417 & -0.083 \\ -0.167 & 0 & 0 & -0.083 & 0.417 \end{array}\right)$$

$$= \left(\begin{array}{r|cccc} 0.381 & -0.143 & -0.143 & -0.167 & -0.167 \\ \hline -0.143 & & & & \\ -0.143 & & M & & \\ -0.167 & & & & \\ -0.167 & & & & \end{array}\right),$$

We have

A_s-criterion : $trace(M)$ = 1.690476 and

D_s-criterion : $|M|$ = 0.029762.

2.4 Minimum Aberration Designs

If interaction effects are not negligible, the parameter estimates for main effects are biased. Let's discuss the ways for evaluating the bias for a given design.

For the example in Section 2.3, let's define $\gamma_0 = \theta_0$, $\boldsymbol{\gamma}_1 = (\theta_1, \theta_2, \theta_3, \theta_4)^T$, $\boldsymbol{\gamma}_2 = (\theta_{12}, \theta_{13}, \theta_{14}, \theta_{23}, \theta_{24}, \theta_{34})^T$, $\boldsymbol{\gamma}_3 = (\theta_{123}, \theta_{124}, \theta_{134}, \theta_{234})^T$, $\gamma_4 = \theta_{1234}$. where γ_0 is the intercept term, γ_1 is the vector of all main effects, γ_2 is the vector of all two-factor interaction effects, γ_3 is the vector of all three-factor interaction effects and γ_4 is the four-factor interaction effect under a baseline parameterization.

The linear model can be rewritten as,

$$Y = W_0\gamma_0 + W_1\gamma_1 + W_2\gamma_2 + W_3\gamma_3 + W_4\gamma_4 + \epsilon \tag{2.1}$$

where,

$$W_0 = \begin{pmatrix} 1\\1\\1\\1\\1\\1\\1\\1\\1\\1 \end{pmatrix}, W_1 = \begin{pmatrix} 0&0&0&0\\0&0&1&1\\0&1&0&1\\0&1&1&0\\1&0&0&1\\1&0&1&0\\1&1&0&0\\1&1&1&1\\0&0&0&0\\0&0&1&1 \end{pmatrix}, W_2 = \begin{pmatrix} 0&0&0&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&1&0&0&0&0\\1&0&0&0&0&0\\1&1&1&1&1&1\\0&0&0&0&0&0\\0&0&0&0&0&1 \end{pmatrix}, W_3 = \begin{pmatrix} 0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\\1&1&1&1\\0&0&0&0\\0&0&0&0 \end{pmatrix}, W_4 = \begin{pmatrix} 0\\0\\0\\0\\0\\0\\0\\1\\0\\0 \end{pmatrix}.$$

Suppose the interactions are ignored. Then the fitted model is

$$Y = W_0\gamma_0 + W_1\gamma_1 + \epsilon. \tag{2.2}$$

Let $\boldsymbol{\theta}$ be $(\gamma_0, \gamma_1^T)^T$ and X be $(W_0 \vdots W_1)$. Then the estimate $\hat{\boldsymbol{\theta}}$ is $(X^TX)^{-1}X^TY$. If the interactions are non-negligible and the true model is (2.1), then $E(\hat{\boldsymbol{\theta}})$ is $(X^TX)^{-1}X^TE(Y) = (X^TX)^{-1}X^T(X\boldsymbol{\theta} + W_2\gamma_2 + W_3\gamma_3 + W_4\gamma_4)$ and therefore

$$E(\hat{\boldsymbol{\theta}}) = \boldsymbol{\theta} + ((X^TX)^{-1}X^TW_2)\gamma_2 + ((X^TX)^{-1}X^TW_3)\gamma_3 + ((X^TX)^{-1}X^TW_4)\gamma_4. \tag{2.3}$$

Here, $((X^TX)^{-1}X^TW_2)\gamma_2$ is the bias component which is added to main effect's estimation due to two-factor interactions, $((X^TX)^{-1}X^TW_3)\gamma_3$ is due to three-factor interactions and $((X^TX)^{-1}$ $X^TW_4)\gamma_4$ is due to four-factor interaction.

Let $C_2 = (X^TX)^{-1}X^TW_2$, $C_3 = (X^TX)^{-1}X^TW_3$, $C_4 = (X^TX)^{-1}X^TW_4$. In order to minimize the bias, C_2, C_3 and C_4 should be minimized. Since C_2, C_3 and C_4 are in matrix form, we should consider a size measure for matrix $\|C\|^2 (= trace(C^TC))$. Usually k-factor interaction effects are more important than (k+1)-factor interaction effects. Thus, it is desirable to sequentially minimize $\|C_2\|^2$, $\|C_3\|^2$ and $\|C_4\|^2$, when comparing different designs.

In our example,

$$C_2 = ((X^TX)^{-1}X^TW_2) = \begin{pmatrix} -0.143 & -0.167 & -0.167 & -0.167 & -0.167 & -0.143 \\ 0.429 & 0.500 & 0.500 & 0 & 0 & -0.071 \\ 0.429 & 0 & 0 & 0.500 & 0.500 & -0.071 \\ 0 & 0.417 & -0.083 & 0.417 & -0.083 & 0.500 \\ 0 & -0.083 & 0.417 & -0.083 & 0.417 & 0.500 \end{pmatrix},$$

$$\|C_2\|^2 = trace(C_2^TC_2) = 2.751701.$$

Similarly $\|C_3\|^2 = 0.8163265$ and $\|C_4\|^2 = 0.2040816$. In C_2, the first row corresponds to the intercept and other rows correspond to the main effects. When only main effects are of interest, then first row can be ignored. In this situation, bias measurement can be redefined as,

$$K_p = \|Cs_p\|^2 = trace(Cs_p^TCs_p)$$

where Cs_p is a matrix obtained by removing the first row of C_p. In our example,

$$Cs_2 = \begin{pmatrix} 0.429 & 0.500 & 0.500 & 0 & 0 & -0.071 \\ 0.429 & 0 & 0 & 0.500 & 0.500 & -0.071 \\ 0 & 0.417 & -0.083 & 0.417 & -0.083 & 0.500 \\ 0 & -0.083 & 0.417 & -0.083 & 0.417 & 0.500 \end{pmatrix},$$

$$K_2 = \|Cs_2\|^2 = trace(Cs_2^TCs_2) = 2.599773.$$

Similarly $K_3 = 0.5895692$ and $K_4 = 0.1473923$. Hereafter, in this study, if a design sequentially minimizes K_2, K_3 and so on, then it is called a minimum aberration design. For orthogonal arrays, exact expressions for these K values are available in Mukerjee and Tang (2011).

2.5 Optimal Design

We define a design as optimal if it has the minimum bias among highly efficient designs.

Definition 1: *If a design sequentially minimizes A_s (or D_s), K_2, K_3..., then it is optimal .*

This is essentially the same as the definition for a minimum aberration design in Mukerjee and Tang (2011). The difference is, here in addition, it compares the criterion values of the efficiency. Mukerjee and Tang (2011) only considers orthogonal arrays, which are most efficient among all designs. Therefore, our definition can be regarded as a general version for all possible run sizes.

For example, let's consider 8 different two-level factorials with 6 runs and 3 factors. All of them contain 4×3 orthogonal arrays and those are highlighted. The first four designs have the same orthogonal array and the rest have another one. For the convenience, all the orthogonal arrays are aligned in the first four rows in all designs. Now, let's try to identify the optimal design among them according to the definition.

$$d_1 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{1} & \mathbf{0} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, d_2 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{1} & \mathbf{0} \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}, d_3 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{1} & \mathbf{0} \\ 0 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix}, d_4 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{1} & \mathbf{0} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$d_5 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{1} & \mathbf{1} & \mathbf{1} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, d_6 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{1} & \mathbf{1} & \mathbf{1} \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}, d_7 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{1} & \mathbf{1} & \mathbf{1} \\ 0 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix}, d_8 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{1} & \mathbf{1} & \mathbf{1} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

To identify the optimal one, we need to calculate A_s (or D_s), K_2 and K_3. Because, our main interest is on all main effects, not the intercept term. All such values for 8 designs are provided in Table 2.4.

Table 2.4: Example of Finding an Optimal Design

Design	**Efficiency**		**Bias**	
	D_s	A_s	K_2	K_3
d_1	0.500	2.500	2.250	0.000
d_2	0.500	2.500	1.667	0.000
d_3	0.375	2.250	2.250	0.000
$\boldsymbol{d_4}$	**0.375**	**2.250**	**1.312**	**0.000**
d_5	0.500	2.500	1.000	0.333
d_6	0.500	2.500	2.250	0.750
d_7	0.375	2.250	1.312	0.375
d_8	0.375	2.250	2.250	0.750

Designs d_3, d_4, d_7 and d_8 have minimum D_s and A_s values. Therefore, these are more efficient than others. Design d_5 has the minimum bias but it has less efficiency. Finally, d_4 sequentially minimizes A_s (or D_s), K_2 and K_3. Therefore, it is the optimal design among all 8 designs. Optimal designs for general $N \equiv 1$ and $2 \pmod 4$ are discussed in the next chapter.

Chapter 3

Optimal Designs

This chapter investigates optimal designs when the number of runs is in the form of $N \equiv 1$ and $2 \pmod 4$. As defined in the previous chapter, an optimal design should have the minimum bias among the designs which have the maximum efficiency.

Cheng (2014) proved that for the case $N \equiv 1 \pmod 4$, by adding one specific run to an orthogonal array, one can find the most efficient design. Similar results for the case $N \equiv 2 \pmod 4$ are also available in that paper. One result says that adding an all-one or all-zero run to an orthogonal array gives the most efficient design for the case $N \equiv 1 \pmod 4$. Another result states that adding all-one run and a run with $m/2$ ones when m is even (or $(m-1)/2$ ones when m is odd) or adding all-zero run and a run with $m/2$ zeros when m is even (or $(m-1)/2$ zeros when m is odd), to an orthogonal array gives the most efficient design for the case $N \equiv 2 \pmod 4$.

For convenience, let's define the optimality for two situations. Consider an orthogonal array and by adding all possible runs, one at a time, we can find the optimal one. Such a design is called a local optimal design. From a particular orthogonal array, there may exist one or more local optimal designs. Now suppose we consider all possible orthogonal arrays for fixed N and m. For each of them, we can find a local optimum. Among all local optimal designs, the best one is defined as the global optimal design. Similarly, we can use these definitions in the case of $N \equiv 2 \pmod 4$.

In the example in the previous chapter, d_1, d_2, d_3 and d_4 are obtained from one orthogonal array and d_5, d_6, d_7 and d_8 are from another. Designs d_4 and d_7 are the local optimal designs and d_4 is the global optimal design.

3.1 $N \equiv 1 \pmod 4$ case

According to Definition 1 in Chapter 2, an efficient design should have the minimum A_s or D_s. When we consider A_s and D_s criteria, adding any one run to an orthogonal array gives an efficient design. These designs are not equally biased but we can always find one local optimal design. Some orthogonal arrays give the same results because they are isomorphic to each other. Isomorphisms under orthogonal and baseline parameterization are not the same. A very good explanation and the definitions for the isomorphic designs are available in Mukerjee and Tang (2011).

Definition 2: *Two orthogonal arrays are combinatorially isomorphic if one can be obtained from the other by row and column permutations as well as renaming of symbols in one or more columns.*

Combinatorially isomorphic designs give the same result under orthogonal parameterization. But this is not true under baseline parameterization, because switching the symbols in any one or more columns gives different results.

Definition 3: *Two designs are isomorphic if one design can be obtained from the other by row and column permutations.*

We use $OA(N, m, 2, 2)$ to denote a two-level orthogonal array of N runs and m factors with strength two, where strength two means that the four level combinations of 0 and 1 occur with the same frequency for every two columns.

3.1.1 Method

An optimal design under a baseline parameterization is defined as the design that sequentially minimizes K_2, K_3,... among the designs that minimize the A_s (or D_s) criterion. Thus, if we collect all the non-isomorphic designs under Definition 3, by adding all possible single runs we can sequentially compare their A_s (or D_s), K_2, K_3,... and then obtain the optimal design for the case $N \equiv 1 \pmod 4$.

For any given N and m, where $N \equiv 1 \pmod 4$, suppose that we can list all the combinatorially non-isomorphic $OA(N-1, m, 2, 2)$'s with symbols 0 and 1. Such arrays can be obtained using the algorithm proposed in Schoen, Eendebak and Nguyen (2009). Suppose there are p such arrays. Each of these arrays can generate 2^m arrays by interchanging symbols in none, or any one or more of the m columns. Thus, we can assure that $p \times 2^m$ (say q) arrays contain all possible $(N-1) \times m$ non-isomorphic orthogonal arrays under Definition 3. For each of these q arrays, add any possible one run. In this way, we can create a design matrix with m columns and N rows. This will generate $q \times 2^m$ (say r) design matrices, because there are 2^m possible runs that can be added to an orthogonal array. For all such r design matrices, calculate the A_s (or D_s) values and find the designs which have minimum A_s (or D_s). Say there are g such efficient designs. For each of g such designs, by calculating and comparing the K_2, K_3,... values we can find the optimal designs.

The following is a detailed description of our algorithm of complete search.

- **STEP I :** List all the combinatorially non-isomorphic $OA(N-1, m, 2, 2)$'s for given N and m using the symbols 1 and 0, and denote the total number of such arrays as p.
- **STEP II :** For each of the p arrays, generate the $\binom{m}{0}$ array with no interchange of symbols of 0 and 1, $\binom{m}{1}$ arrays with interchanging symbols in any one of the m columns, $\binom{m}{2}$ arrays with interchanging symbols in any two columns, ..., and $\binom{m}{m}$ array with interchanging symbols in all m columns. Thus, it generates 2^m arrays for each of the p arrays, thus $p \times 2^m$ (say q) arrays in total.
- **STEP III :** Add all possible runs, one at a time. It will produce $r = q \times 2^m$ design matrices.
- **STEP IV :** Compute A_s (or D_s) for each of the r design matrices. Find the ones with minimum A_s (or D_s), and suppose that there are g such matrices.
- **STEP V :** For each of the g design matrices, compute the sequence K_2, K_3.... Find the arrays that sequentially minimize K_2, K_3.... and hence the optimal designs under the baseline parameterization.

3.1.2 Results

Adding any one run to an orthogonal array gives the same A_s value. This is also true for the D_s criterion. Thus we have $r = g$ in the algorithm. Among those r designs, some designs have the same sequence of K values. To illustrate, let us look at the results for $N = 9$ and $m = 6$ in Table 3.1.

In this case, there is only one (8×6) combinatorially non-isomorphic orthogonal array. Therefore, according to the algorithm $q = 1 \times 2^6 = 64$. Those 64 arrays contain all possible non-isomorphic orthogonal arrays according to Definition 3. We have $r = g = q \times 2^6 = 4096$. These 4096 designs

Table 3.1: Results from the algorithm for $N = 9$ and $m = 6$

Pattern	Frequency	D_s	A_s	K_2	K_3	K_4	K_5	K_6
1	8	0.0094	2.8000	8.2400	4.9733	2.5000	1.0000	0.1667
2	48	0.0094	2.8000	8.8400	5.4267	1.5867	0.1667	0.0000
3	48	0.0094	2.8000	9.2800	6.3867	2.1700	0.2900	0.0000
4	48	0.0094	2.8000	9.3467	7.2933	4.3500	1.7400	0.2900
5	24	0.0094	2.8000	9.4400	4.8933	0.8467	0.0000	0.0000
6	96	0.0094	2.8000	9.4400	6.5733	2.3900	0.3767	0.0000
7	192	0.0094	2.8000	9.6133	6.9067	2.4667	0.3600	0.0000
8	192	0.0094	2.8000	9.6800	6.3733	2.1500	0.2900	0.0000
9	48	0.0094	2.8000	9.8800	5.5733	1.0433	0.0000	0.0000
10	96	0.0094	2.8000	9.9467	5.5333	1.0600	0.0000	0.0000
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
41	24	0.0094	2.8000	10.6400	8.9200	5.2600	2.0400	0.3400
42	48	0.0094	2.8000	10.6533	7.8933	2.8867	0.4267	0.0000
43	48	0.0094	2.8000	10.6800	8.8400	4.9500	1.7400	0.2500
44	8	0.0094	2.8000	10.7200	9.8267	6.4000	2.5600	0.4267
45	192	0.0094	2.8000	10.8800	7.7867	2.6900	0.3767	0.0000
46	192	0.0094	2.8000	10.9467	8.3067	3.0467	0.4467	0.0000
47	48	0.0094	2.8000	11.2133	7.0667	1.6700	0.1067	0.0000
48	48	0.0094	2.8000	11.2400	8.4133	3.0400	0.4467	0.0000
49	48	0.0094	2.8000	11.2800	9.5467	4.3033	1.0233	0.1067
50	8	0.0094	2.8000	11.8400	8.2533	2.7800	0.6400	0.1067

have only 50 distinct sequences of A_s (or D_s) and K values. In Table 3.1, results are presented in the order from the best to worst designs. Pattern 1 is the best one and there exist 8 optimal designs. Pattern 50 is the worst case and the corresponding eight designs are the worst in terms of optimality.

For large N and m, r becomes extremely large. Calculating all the sequences of K values takes a large amount of time, but our algorithm ignores the unnecessary calculations and thus saves a lot of computing time.

Our results show that adding an all-zero run to an orthogonal array gives the global optimal design, although this is not true for every orthogonal array. For different N and m, such orthogonal arrays need some specifications. These are provided in Tables 3.2 and 3.3.

Table 3.2: Required orthogonal arrays for optimal designs for $N = 5$ and 9

N	m	$(N-1) \times m$ OA containing	Sequential Minimums				Example (Column numbers)
			D_s	A_s	K_2	K_3	
5	2	There is only one OA	0.7143	1.7143	0.3673	-	1, 2 in Z_4
5	3	an all-one run	0.6250	2.6250	1.2656	0.4219	Z_4
9	2	There is only one OA	0.2045	0.9091	0.4132	-	1, 2 in Z_8
9	3	an all-one run and an all-zero run	0.0938	1.3750	1.2656	0.1302	1, 2, 4 in Z_8
9	4	an all-one run and an all-zero run	0.0433	1.8462	2.5740	0.5917	1, 2, 4, 7 in Z_8
9	5	an all-one run	0.0201	2.3214	5.1071	2.3980	1, 2, 3, 4, 5 in Z_8
9	6	an all-one run	0.0094	2.8000	8.2400	4.9733	1, 2, 3, 4, 5, 6 in Z_8
9	7	an all-one run	0.0044	3.2813	12.3867	8.9141	Z_8

$$Z_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}, \quad Z_8 = \begin{pmatrix} 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

For example, a global optimal design with 9 runs and 6 factors is,

$$\begin{matrix} \\ \\ \\ 8 \times 6 \text{ OA} \\ \\ \\ \\ \\ \textbf{Added run} \end{matrix} \begin{pmatrix} 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}.$$

The sequence of A_s, K_2, K_3, K_4, K_5 and K_6 is 2.8000, 8.2400, 4.9733, 2.5000, 1.0000 and 0.1667.

Table 3.3: Required orthogonal arrays for optimal designs for $N = 13$

N	**m**	$(N-1) \times m$ **OA containing**	**Sequential Minimums**				**Example (Columns in Z_{12})**
			D_s	A_s	K_2	K_3	
13	2	There is only one OA	0.096296	0.622222	0.436	-	1, 2
13	3	2 all-one run and an all-zero run	0.030093	0.937500	1.307	0.255	1, 2, 3
13	4	2 all-one runs	0.009441	1.254902	2.607	1.206	1, 2, 3, 4
13	5	2 all-one runs	0.002972	1.574074	4.321	3.361	1, 2, 3, 4, 5
13	6	an all-one run	0.000939	1.894737	7.487	5.317	1, 2, 3, 4 ,5, 6
13	7	an all-one run	0.000297	2.216667	11.311	8.968	1, 2, 3, 4, 5, 6, 7
13	8	an all-one run	0.000094	2.539683	15.802	14.996	1, 2, 3, 4, 5, 6, 7, 8
13	9	an all-one run	0.000030	2.863636	21.376	23.198	1, 2, 3, 4, 5, 6, 7, 8, 9
13	10	an all-one run	0.000010	3.188406	27.845	34.820	1, 2, 3, 4, 5, 6, 7, 8, 9, 10
13	11	an all-one run	0.000003	3.513889	35.425	50.194	All

$$Z_{12} = \begin{pmatrix} 0&0&0&1&1&1&0&1&1&0&0 \\ 0&0&1&0&1&1&1&0&0&0&1 \\ 0&0&1&1&0&0&1&1&0&1&0 \\ 0&1&0&0&1&0&1&0&1&1&0 \\ 0&1&0&1&0&1&0&0&0&1&1 \\ 0&1&1&0&0&0&0&1&1&0&1 \\ 1&0&0&0&1&0&0&1&0&1&1 \\ 1&0&0&1&0&0&1&0&1&0&1 \\ 1&0&1&0&0&1&0&0&1&1&0 \\ 1&1&0&0&0&1&1&1&0&0&0 \\ 1&1&1&1&1&0&0&0&0&0&0 \\ 1&1&1&1&1&1&1&1&1&1&1 \end{pmatrix}.$$

3.2 $N \equiv 2 \pmod 4$ case

This section discusses the search for optimal designs where the number of runs is in the form of $N \equiv 2 \pmod 4$ such as $N = 6, 10, 14, 18$. As proved in Cheng (2014), adding two specific runs to an orthogonal array gives a most efficient design. There are some other choices of two runs that also give the same A_s and D_s values as Cheng's runs. Different orthogonal arrays give different local optimal designs when adding two runs. Therefore, we need to check all possible orthogonal arrays like we did in the previous case.

3.2.1 Method

For given N and m, suppose we are able to list all the combinatorially non-isomorphic $OA(N-2, m, 2, 2)$'s with symbols 0 and 1. Let's say there are p such arrays. Each of these arrays can generate 2^m arrays by interchanging symbols in none, or any one or more of the m columns. Thus, $p \times 2^m$ (say q) arrays contain all possible $(N-2) \times m$ non-isomorphic orthogonal arrays under Definition 3. For each of these q arrays, consider adding all possible two runs. Now we can create a design matrix with m columns and N rows where $N \equiv 2 \pmod 4$. This will generate $q \times \left\{ \binom{2^m}{2} + 2^m \right\}$ (say r) design matrices, because there are $\binom{2^m}{2}$ possible pairs of two different runs and 2^m possibilities if the same run is used twice. For all such r design matrices, calculate the A_s (or D_s) values and find the designs which have the minimum A_s (or D_s). Say there are g such efficient designs. By calculating and comparing the K_2, K_3,... values for these g designs, we can find the optimal designs.

The following is a detailed description of our algorithm of complete search.

- **STEP I :** List all the combinatorially non-isomorphic $OA(N-2, m, 2, 2)$s for given N and m using the symbols 1 and 0, and denote the total number of such arrays as p.
- **STEP II :** For each of the p arrays, generate the $\binom{m}{0}$ array with no interchange of symbols of 0 and 1, $\binom{m}{1}$ arrays with interchanging symbols in any one of the m columns, $\binom{m}{2}$ arrays with interchanging symbols in any two columns, ..., and $\binom{m}{m}$ array with interchanging symbols in all m columns. Therefore, we generate 2^m arrays for each of the p arrays, thus $q \times 2^m$ arrays in total.
- **STEP III :** Add two runs in all possible ways. It will produce $q \times \left\{\binom{2^m}{2} + 2^m\right\}$ arrays, and denote the total number of such arrays as r.
- **STEP IV :** Compute A_s (or D_s) for each of the r arrays. Find the arrays with minimum A_s (or D_s), and suppose there are g such arrays.
- **STEP V :** For each of the g arrays, compute the sequence K_2, K_3... Find the arrays that sequentially minimize K_2, K_3.... and hence the optimal designs under the baseline parameterization.

In the algorithm, among those r designs, some designs have the same sequence of values for all relevant criteria. To illustrate, the results for $N = 10$ and $m = 6$ are provided in Table 3.4.

According to the complete search algorithm $q = 1 \times 2^6 = 64$, $r = q \times \left\{\binom{2^6}{2} + 2^6\right\} = 64 \times 2080 = 133120$ and if we skip the STEP IV then there will be 133120 designs. These designs have only 412 distinct sequences of criteria values. In Table 3.4, results are presented in the order from the best to worst designs. Pattern 1 is the best and there exist 128 global optimal designs. Pattern 412 is the worst case and those 8 are the worst designs in terms of optimality. The patterns from 382 to 412 have 4096 designs and these worst designs are obtained by adding two identical runs. Not only for this case, for all cases we have checked so far, the worst designs in terms of efficiency are always those from adding the same run twice to an orthogonal array. Therefore, hereafter adding the same run twice can be skipped in the algorithm.

Table 3.4: Complete set of result for $N = 10$ and $m = 6$

Pattern	Frequency	D_s	A_s	K_2	K_3	K_4	K_5	K_6
1	128	0.0056	2.5982	7.7659	4.4882	1.3416	0.1667	0.0000
2	32	0.0056	2.5982	8.2452	4.9716	2.5004	1.0002	0.1667
3	192	0.0056	2.5982	8.2717	4.9692	2.5004	1.0002	0.1667
4	384	0.0056	2.5982	8.5217	5.1370	1.5359	0.1667	0.0000
5	96	0.0056	2.5982	8.7452	5.3795	1.7518	0.2487	0.0000
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
178	192	0.0056	2.6071	11.2143	7.0657	1.6598	0.1033	0.0000
179	192	0.0056	2.6071	11.2602	7.7506	2.6677	0.6199	0.1033
180	96	0.0058	2.6111	7.7840	4.7685	2.5000	1.0000	0.1667
181	192	0.0058	2.6111	8.0062	4.9861	1.4923	0.1667	0.0000
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
327	48	0.0058	2.6389	11.0216	7.5108	2.4390	0.5370	0.0895
328	48	0.0058	2.6389	11.0525	9.2238	4.0617	0.9167	0.0895
329	48	0.0063	2.6500	7.6700	4.5850	2.2875	0.9150	0.1525
330	48	0.0063	2.6500	8.0700	5.0150	1.4675	0.1525	0.0000
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
380	48	0.0063	2.7000	10.8800	7.9200	2.7900	0.4000	0.0000
381	8	0.0063	2.7000	11.2800	7.2600	2.0400	0.3600	0.0600
382	8	0.0071	2.7273	7.5868	3.8926	1.6736	0.6694	0.1116
383	48	0.0071	2.7273	8.4050	4.8843	1.3140	0.1116	0.0000
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
408	192	0.0071	2.7273	11.1983	8.8512	3.4174	0.5331	0.0000
409	48	0.0071	2.7273	11.5620	7.7190	2.0888	0.1983	0.0000
410	48	0.0071	2.7273	11.6529	10.6612	5.4153	1.5310	0.1983
411	48	0.0071	2.7273	11.6777	9.1157	3.4545	0.5331	0.0000
412	8	0.0071	2.7273	12.4959	9.6942	4.0785	1.1901	0.1983

Complete search can be done for up to $N = 14$ and $m = 7$, but for higher N and m it is computationally very expensive. Therefore, instead of checking all possible two runs, we only consider those two runs that lead to most efficient designs. Cheng's theory (2014) for $N \equiv 2 \pmod 4$ says that adding an all-zero run and a run with $m/2$ or $(m+1)/2$ ones to an orthogonal array gives an efficient design where m is even or odd respectively. Therefore, we can modify the complete search algorithm as follows:

Modified Complete Search

- **STEP I :** List all the combinatorially non-isomorphic $OA(N-2, m, 2, 2)$s for given N and m using the symbols 1 and 0, and denote the total number of such arrays as p.
- **STEP II :** For each of the p arrays, generate the $\binom{m}{0}$ array with no interchange of symbols of 0 and 1, $\binom{m}{1}$ arrays with interchanging symbols in any one of the m columns, $\binom{m}{2}$ arrays with interchanging symbols in any two columns, ..., and $\binom{m}{m}$ array with interchanging symbols in all m columns. Therefore, we generate 2^m arrays for each of the p arrays, thus $q \times 2^m$ arrays in total.
- **STEP III :** Add an all-zero run and a run with $m/2$ or $(m+1)/2$ ones where m is even or odd respectively. It will produce $q \times \binom{m}{m/2}$ or $q \times \binom{m}{(m+1)/2}$ number of $N \times m$ arrays, and denote the total number of such arrays as r.
- **STEP IV :** Compute A_s (or D_s) for each of the r arrays. Find the arrays with minimum A_s (or D_s), and suppose there are g such arrays.
- **STEP V :** For each of the g arrays, compute the sequence K_2, K_3... Find the arrays that sequentially minimize K_2, K_3... and hence the optimal designs under the baseline parameterization.

Somewhat surprisingly, from the complete search results, we found that there exist some situations where adding two runs which do not follow Cheng's structure gives better designs. They have the same A_s and D_s values as those from Cheng's structure, but different K values. Let's consider a matrix with two added runs. According to Cheng's structure, one row should have all zeros and another with half zeros. In some cases, by switching the levels in some columns of this added matrix, better designs can be obtained.

For example, consider two designs d_1 and d_2:

$$d_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{1} & \mathbf{1} & \mathbf{0} \end{pmatrix}, \qquad d_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} \end{pmatrix}.$$

Both designs have the same D_s and A_s values which equal 0.375 and 2.25 respectively. But they don't have the same K_2 value, d_1 has 2.25 and d_2 has 1.3125. According to our definition, d_2 is a better design. We can clearly see that d_2 does not follow Cheng's structure. For this reason, we have included an extra step in between step III and step IV, allowing symbol-switching in the columns of the added matrix.

3.2.2 Results

Optimal designs of $N = 6$ and 10 runs found by complete search are provided in Table 3.5. Optimal designs of $N = 14$ runs found by our method are provided in Table 3.6.

Table 3.5: Orthogonal arrays and two added runs, which give optimal designs for $N = 6$ and 10

N	**m**	**Required OA (Columns Numbers)**	**# of 1s in New**		**Sequential Minimums**			
			Run 1	**Run 2**	$\boldsymbol{D_s}$	$\boldsymbol{A_s}$	$\boldsymbol{K_2}$	$\boldsymbol{K_3}$
6	2	1, 2 in Z'_4	0	1	0.5000	1.4167	0.3611	-
6	3	Z'_4	1	1	0.3750	2.2500	1.3125	0.0000
10	2	1, 2 in Z'_8	0	1	0.1667	0.8167	0.4100	-
10	3	1, 2, 4 in Z'_8	0	2	0.0694	1.2500	1.3681	0.1181
10	4	1, 2, 4, 7 in Z'_8	0	2	0.0298	1.6905	2.5998	0.5896
10	5	1, 2, 3, 4, 5 in Z'_8	0	3	0.0128	2.1429	5.1429	2.3469
10	6	1, 2, 3, 4 ,5, 8 in Z'_8	1	2	0.0056	2.5982	7.7659	4.4882
10	7	1, 2, 3, 4, 5, 6, 7 in Z'_8	0	3	0.0024	3.0625	12.0469	8.8750

Note:
- All the new runs should be the symbol-switched form of existing runs in the OA
- 1s in the new runs shouldn't overlap in their columns

$$Z_4' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad Z_8' = \begin{pmatrix} 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}.$$

Table 3.6: Orthogonal arrays and two added runs, which give optimal designs for $N = 14$

N	**m**	**Required OA (Columns in Z_{12}')**	**# of 1s in New**		**Sequential Minimums**			
			Run 1	**Run 2**	$\boldsymbol{D_s}$	$\boldsymbol{A_s}$	$\boldsymbol{K_2}$	$\boldsymbol{K_3}$
14	2	1, 2	0	1	0.083333	0.5774	0.4337	-
14	3	1, 2, 12	1	1	0.024306	0.8750	1.3681	0.0833
14	4	1, 2, 3, 4	0	2	0.007202	1.1759	2.6746	1.2023
14	5	1, 2, 3, 4, 5	0	3	0.002134	1.4815	4.5062	3.3155
14	6	1, 2, 3, 4, 5, 6	0	3	0.000640	1.7889	7.3252	5.1050
14	7	1, 2, 3, 4, 13, 6, 14	2	2	0.000192	2.1000	11.0867	8.2378
14	8	1, 2, 3, 4, 13, 6, 14, 15	2	2	0.000058	2.4121	15.1343	14.0396
14	9	1, 2, 3, 4, 13, 6, 14, 8, 9	3	2	0.000018	2.7273	21.0413	22.2654
14	10	1, 2, 3, 4, 5, 6, 7, 8, 9, 10	0	5	0.000005	3.0429	26.8756	33.4284
14	11	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11	0	6	0.000002	3.3611	34.6181	49.2824

Note:

- All the new runs should be the symbol-switched form of existing runs in the OA
- 1s in the new runs shouldn't overlap in their columns

$$Z'_{12} = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \end{pmatrix}$$

We observe that the two additional runs are in the symbol-switched form of existing runs in the orthogonal array. Also, those two runs shouldn't have all ones in their columns. In Section 2.5, the example has 8 designs with $N = 6$ and $m = 3$. According to Table 3.5, the two added runs should have only one 1 in each row and both runs are symbol-switched form of existing runs. Both d_2 and d_4 satisfy these conditions, but in d_2, one of the columns in the added two runs has all-one entries. In other words, the ones in the added runs in d_2 are overlapping in their columns. Such an overlap does not give an optimal design.

Let's look at another example, Consider three designs

$$d_1^* = \begin{pmatrix} 0&0&0&1&0&0&0\\ 0&0&1&0&0&0&1\\ 0&0&1&1&1&1&1\\ 0&1&0&0&1&0&1\\ 0&1&0&1&0&1&0\\ 0&1&1&0&1&1&0\\ 1&0&0&0&1&0&0\\ 1&0&0&1&1&1&1\\ 1&0&1&0&0&1&0\\ 1&1&0&0&0&1&1\\ 1&1&1&1&0&0&1\\ 1&1&1&1&1&0&0\\ \mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}\\ \mathit{1}&\mathit{1}&\mathit{1}&\mathit{1}&\mathit{0}&\mathit{0}&\mathit{0} \end{pmatrix}, d_2^* = \begin{pmatrix} 0&0&0&1&0&0&0\\ 0&0&1&0&0&0&1\\ 0&0&1&1&1&1&1\\ 0&1&0&0&1&0&1\\ 0&1&0&1&0&1&0\\ 0&1&1&0&1&1&0\\ 1&0&0&0&1&0&0\\ 1&0&0&1&1&1&1\\ 1&0&1&0&0&1&0\\ 1&1&0&0&0&1&1\\ \mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{0}&\mathbf{0}&\mathbf{1}\\ \mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{0}&\mathbf{0}\\ \mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{1}&\mathit{1}&\mathit{0}\\ \mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{1}&\mathit{1} \end{pmatrix}, d_3^* = \begin{pmatrix} 0&0&0&1&0&0&0\\ 0&0&1&0&0&0&1\\ \mathbf{0}&\mathbf{0}&\mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{1}\\ 0&1&0&0&1&0&1\\ 0&1&0&1&0&1&0\\ 0&1&1&0&1&1&0\\ 1&0&0&0&1&0&0\\ 1&0&0&1&1&1&1\\ 1&0&1&0&0&1&0\\ 1&1&0&0&0&1&1\\ 1&1&1&1&0&0&1\\ \mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{1}&\mathbf{0}&\mathbf{0}\\ \mathit{1}&\mathit{1}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}\\ \mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{0}&\mathit{1}&\mathit{1} \end{pmatrix}.$$

Design	D_s	A_s	K_2	K_3	K_4	K_5	K_6	K_7
d_1^*	0.000192	2.100000	12.037	9.346	3.561	0.560	0.000	0.000
d_2^*	0.000200	2.111111	11.292	8.570	3.366	0.564	0.000	0.000
$\boldsymbol{d_3^*}$	**0.000192**	**2.100000**	**11.086**	**8.238**	**3.204**	**0.540**	**0.000**	**0.000**

Design d_1^* follows Cheng's structure, but others do not. Designs d_1^* and d_3^* have the same efficiency, which is the best efficiency, but d_1^* has a larger bias than d_3^*. According to Table 3.6, to get the optimal design with $N = 14$ and $m = 7$ we have to add 2 runs, each with only 2 ones to an (12×7) orthogonal array. These 2 runs should be symbol-switched form of already existing runs. Designs d_2^* and d_3^* satisfy the first condition. But d_2^* does not satisfy the condition that the ones in the new runs shouldn't overlap in their columns. Therefore, d_3^* is the optimal design, which satisfies all the conditions.

3.3 Discussion

In Mukerjee and Tang (2011), optimal designs for $N = 4, 8, 12$ and 16 are obtained. These designs are orthogonal arrays. In our study, we add one and two runs to orthogonal arrays to find optimal designs for $N \equiv 1$ and $2 \pmod 4$. We have obtained the results for $N = 5, 6, 9, 10, 13$ and 14 and these optimal designs need some specific orthogonal arrays with $N = 4, 8$ and 12. This section discusses the relationship between the orthogonal arrays in Mukerjee and Tang (2011) and those in the current study.

In our study, in general, it requires an orthogonal array with an all-one run to obtain the optimal designs for $N \equiv 1 \pmod 4$. In Mukerjee and Tang (2011), the orthogonal arrays do not have all-one runs. Instead, they have all-zero runs. Thus, by interchanging all the levels in the entire orthogonal array, we can obtain the orthogonal array the current study needs. One exception is when $N = 8$ and $m = 4$. This orthogonal array does not have an all-one run nor an all-zero run. By switching the levels in any one column, we can get the orthogonal array the current study requires.

For $N = 5, 9$ and 13, we do not need a separate table for the required orthogonal arrays. We can simply use the table from Mukerjee and Tang (2011). To get the optimal designs for such Ns, we need to follow these simple steps:

1. Obtain the required $(N-1) \times m$ orthogonal array from Mukerjee and Tang (2011),
2. If $N = 9$ and $m = 4$, then level-switch any one column in the orthogonal array,
3. Otherwise level-switch the entire orthogonal array and
4. Add an all-zero run.

This simple procedure may not work for $N = 17$. Because, the corresponding orthogonal arrays in Mukerjee and Tang (2011) do not have an all-one run nor an all-zero run. For $N \equiv 2 \pmod 4$, no simple relationship is observed between the orthogonal arrays in Mukerjee and Tang (2011) and those in our project.

Chapter 4

Concluding Remarks

In many applications, the baseline parameterization is more natural than the orthogonal parameterization. In this study, we have defined an optimal design by considering both the efficiency and the bias. To compare the efficiency between designs, we used modified A (or D) criterion which considers only the main effects. The bias on main effect estimates due to active interactions is evaluated using the minimum aberration criterion under the baseline parameterization.

In our searching algorithm we get the orthogonal arrays from combinatorially non-isomorphic orthogonal arrays by switching the levels in all possible combinations of columns. Many of these arrays may be isomorphic according to Definition 3. Isomorphic orthogonal arrays always give local optimal designs which have the same sequence of A_s (or D_s), K_2,K_3,... values. Therefore, if we can develop an algorithm to identify the non-isomorphic orthogonal arrays then we can drastically narrow down our search domain. This is a topic for future research. Another topic of practical importance is to examine how optimal designs for $N \equiv 3 \pmod 4$ runs can be obtained.

References

[1] BOX, G. E. P., HUNTER, J. S., AND HUNTER, W. G. *Statistics for experimenters: design, innovation, and discovery*. Wiley series in probability and statistics. Wiley-Interscience, 2005.

[2] CHENG, C. S. Optimal biased weighing designs and two-level main-effect plans. *Journal of Statistical Theory and Practice 8* (2014), 83–99.

[3] LI, P., MILLER, A., AND TANG, B. Algorithmic search for baseline minimum aberration designs. *Journal of Statistical Planning and Inference 149* (2014), 172–182.

[4] MUKERJEE, R., AND TANG, B. Optimal fractions of two-level factorials under a baseline parameterization. *Biometrika* (2011), 1–14.

[5] SCHOEN, E. D., EENDEBAK, P. T., AND NGUYEN, M. V. M. Complete enumeration of pure-level and mixed-level orthogonal arrays. *Journal of Combinatorial Designs* (2009), 123–140.