Contributions to Factorial Designs and Space-Filling Designs

by

Guanzhou Chen

M.Sc., University of Chicago, 2018
B.Sc., Beijing Normal University, 2016

Thesis Submitted in Partial Fulfillment of the
Requirements for the Degree of
Doctor of Philosophy

in the
Department of Statistics and Actuarial Science
Faculty of Science

SIMON FRASER UNIVERSITY
Summer 2023

Declaration of Committee

Name: **Guanzhou Chen**

Degree: **Doctor of Philosophy**

Thesis title: **Contributions to Factorial Designs and Space-Filling Designs**

Committee:

Chair: Liangliang Wang
Associate Professor, Statistics and Actuarial Science

Boxin Tang
Supervisor
Professor, Statistics and Actuarial Science

Richard Lockhart
Committee Member
Professor, Statistics and Actuarial Science

Jiguo Cao
Examiner
Professor, Statistics and Actuarial Science

Hongquan Xu
External Examiner
Professor, Statistics
University of California, Los Angeles

Abstract

In physical and computer experiments, factorial designs and space-filling designs are frequently employed to explore the relationship between several input factors and a response variable. Several new developments for these designs are documented in this thesis.

Generalized resolution, projectivity, and hidden projection property are useful measures to evaluate a factorial design, especially when only a few factors are believed to be active a priori. In this thesis, we substantially expand existing theoretical results on these topics by examining designs from Paley's constructions of Hadamard matrices. Next, we study two-level factorial experiments where the two levels are symmetrical for some factors but asymmetrical for other factors. A mixed parametrization of factorial effects is proposed for such situations. For robust estimation of main effects, we introduce two minimum aberration criteria and provide theoretical and algorithmic constructions of optimal and nearly optimal designs under these criteria.

Space-filling designs based on orthogonal arrays are attractive for computer experiments. However, it's not very clear how they perform under other space-filling criteria. In this thesis, we justify the use of these designs under a broad class of space-filling criteria including those of distance, orthogonality and discrepancy. Based on the theoretical results, we investigate various constructions of space-filling orthogonal array-based designs. Finally, we develop a construction method of space-filling designs using nonregular designs. Designs obtained this way have very flexible run sizes as compared to those constructed from regular designs.

Keywords: Baseline parametrization; mappable nearly orthogonal array; minimum aberration; non-empty-cell design; orthogonal array; strong orthogonal array

Dedication

To my parents

Acknowledgements

Words cannot express my appreciation to my supervisor, Professor Boxin Tang, who provided me with extraordinary guidance throughout my doctoral studies. I learned so much from his broad knowledge and deep insights, and am especially grateful for his criticisms which allow me to realize my weaknesses and improve myself. Without his instruction this thesis would not have been possible.

I am thankful to Professors Jiguo Cao, Richard Lockhart, Liangliang Wang and Hongquan Xu for serving as my committee members and reading the thesis carefully. Their constructive suggestions have greatly improved the thesis.

I would like to express my deep gratitude to Professor Yuanzhen He at Beijing Normal University for believing in my potential and encouraging me to pursue further studies at SFU.

I also want to thank all my friends for their help and companionship during my PhD studies. Many thanks to Angela, Boyi, Charlie, Cheng-Yu, Chenlu, Chi-Kuang, Chunhong, Grace, Guohua, Guoyao, Ken, Lulu, Shifan, Tianxing, Wendy, Xingyu and Xuekun. I'm particularly grateful to Zhujun for her support and encouragement.

Finally, I would like to thank all the faculty and staff members in the Department of Statistics and Actuarial Science at SFU for creating a nice environment for me to study and research.

Table of Contents

List of Tables

List of Figures

Chapter 1

Introduction

Statistical methods are ubiquitous and indispensable in modern science. Typically, a statistical investigation of a scientific problem consists of five steps (MacKay and Oldford, 2000): (i) specifying the problem, (ii) planning research, (iii) collecting data, (iv) analyzing data and (v) drawing conclusions. To be successful in this process, data should be carefully collected in step (iii). A good set of data provides insights into the problem as well as benefits for modelling and data analysis; on the other hand, useful conclusions can hardly be drawn from a dataset that is of poor quality or otherwise irrelevant to the problem of concern.

Experimental design is a branch of statistics that studies the collection of data through experimentation. Humans have a long history of acquiring knowledge from experiments, but statistical principles for designing experiments only came into being around 100 years ago due to Sir R. A. Fisher at the Rothamsted Experimental Station (Fisher, 1926). Over 100 years of evolution, the subject of experimental design has grown into a full-fledged research field with abundant theory and diverse applications.

The development of the subject can be roughly divided into three stages (Wu, 2015). The early use of experimental designs centered around agricultural applications, which gave rise to several major subbranches such as block designs, factorial designs and crossover designs (Fisher, 1935; Yates, 1936; Cochran, 1939). After the Second World War, the focus of the subject gradually shifted to industrial experiments and quality improvement; examples of significant progresses include the response surface methodology (Box and Wilson, 1951) and robust parameter design (Taguchi, 1986). In the late 20th century, computers gave birth to virtual computer experiments which are becoming increasingly popular nowadays (Sacks et al., 1989).

This thesis is devoted to design strategies for two classes of experiments, namely, factorial experiments and computer experiments. We split this chapter into two sections to introduce the two topics and outline contributions of the thesis.

1.1 Factorial experiments and orthogonal arrays

People have long been curious about the causal effects of several input factors over a response variable. Problems of this kind can be explored by factorial experiments in which effects of all the input factors are studied simultaneously. Factorial experiments were first advocated by Fisher and Yates as opposed to traditional one-factor-at-a-time experiments, because they are more efficient and also allow interactions among factors to be investigated (Cochran and Cox, 1957; Cox, 1958).

In a factorial experiment, the number of level combinations grows geometrically as the number of factors increases, and soon goes beyond that permitted by resources. This was realized by Finney (1945) who introduced fractional replications to address the issue. Around the same time, Plackett and Burman (1946) also proposed some highly fractionated factorial designs for main effects estimation. The designs studied by Finney and Plackett and Burman all belong to a general class of designs called orthogonal arrays (Rao, 1947).

Orthogonal arrays are elegant mathematical structures. As fractional factorial designs, they are the most widely-used in practice, because they provide optimal estimation of lower-order factorial effects when higher-order ones are negligible (Cheng, 1980). Since there are many orthogonal arrays for given numbers of runs and factors, many criteria have been developed for design selection. Among them the most popular ones are the resolution (Box and Hunter, 1961) and minimum aberration criterion (Fries and Hunter, 1980), which were extended to the generalized resolution and the minimum G- and G_2-aberration criteria for general two-level orthogonal arrays (Deng and Tang, 1999; Tang and Deng, 1999), and to the generalized minimum aberration criterion for multilevel orthogonal arrays (Xu and Wu, 2001).

There are two classes of orthogonal arrays known as regular designs and nonregular designs. As compared with regular designs, nonregular designs have flexible run sizes and are attractive in terms of generalized resolution, projectivity (Box and Tyssedal, 1996) and hidden projection property (Wang and Wu, 1995). The criterion of generalized resolution aims at eliminating the most severe aliasing among the important lower-order effects, while the properties of projectivity and hidden projection evaluate a design by looking at its projections onto low-dimensions. In Chapter 2, we conduct a comprehensive study on these topics by examining three classes of designs that are obtained from Paley's two constructions of Hadamard matrices. In terms of generalized resolution, we complete the study of Shi and Tang (2023) on strength-two designs by adding results on strength-three designs. In terms of projectivty and hidden projection property, our results substantially expand those of Cheng (1995, 1998) and Bulutoglu and Cheng (2003). For the purpose of practical applications, we conduct an extensive search of minimum G-aberration designs from those with maximum generalized resolutions and results are obtained for strength-two designs with 36, 44, 48, 52, 60, 64, 96 and 128 runs and strength-three designs with 72, 88 and 120 runs. A paper containing these results has been submitted to *Electronic Journal of Statistics* and is under the second round of review after some minor revision.

The next problem investigated in this thesis concerns the parametrization of factorial effects for two-level factorial experiments. The most commonly used factorial effects are those given by the orthogonal parametrization (Box and Hunter, 1961). While such a parametrization is appropriate for experiments where the two levels of each factor are symmetrical, the baseline parametrization is well suited for experiments where the two levels of each factor are asymmetrical and one level, called a baseline level, is more important than the other (Mukerjee and Tang, 2012). Chapter 3 considers a general situation where some factors have a baseline level while others do not. A mixed parametrization of factorial effects is proposed and its connection with the existing parametrizations is established. Under this new parametrization, we show that orthogonal arrays continue to be optimal for estimating main effects, and then put forward two minimum aberration criteria for further design selection. Both theoretical and algorithmic constructions of minimum aberration designs are examined and useful designs are obtained. The results of this chapter have been submitted for publication.

1.2 Computer experiments and space-filling designs

Physical experiments can sometimes be too expensive or even impractical to implement. With the advancement of computing science, computer experiments are playing an important role as alternatives to physical experiments in modern experimentation.

In a computer experiment, a simulator is often employed to simulate a physical process, where the simulator refers to computer codes described by, for example, complex differential equations. To examine the relationship between input factors and a response, a set of design points for input factors is selected to feed into the simulator and then the responses are recorded. Based on these data, experimenters hope to build a cheap surrogate model for the simulator because the simulation is often time-consuming. The design of computer experiments concerns how to select design points so that information can be efficiently collected (Fang et al., 2006; Santner et al., 2018).

Most of the simulators are deterministic; that is, the same sets of input values always yield the same outputs. In addition, prior knowledge on the relationship between the input factors and the response is seldom available. These features render space-filling designs most useful for computer experiments. Broadly speaking, a space-filling design is a design that scatters its points in the design region in some uniform fashion. Justifications for the use of such designs can be found in Box and Draper (1959), Sacks and Ylvisaker (1984) and Vazquez and Bect (2011).

Space-filling designs can be evaluated by numerous space-filling criteria such as those of distance (Johnson et al., 1990), orthogonality (Owen, 1994) and discrepancy (Fang et al., 2000), but theoretical constructions of optimal designs under these criteria are challenging. On the other hand, space-filling designs based on orthogonal arrays (Tang, 1993) are attractive for they can easily be generated with desirable low-dimensional stratification properties. However, it is not very clear how they behave and how to construct good such designs under other space-filling criteria. In Chapter 4, we justify orthogonal array-based designs under a broad class of space-filling criteria, which include commonly used distance-, orthogonality- and discrepancy-based measures. To identify designs with even better space-filling properties, we partition orthogonal array-based designs into classes by allowable level permutations and show that the average performance of each class of designs is determined by two types of stratifications, with one of them being achieved by strong orthogonal arrays of strength 2+ (He et al., 2018). Based on these results, we investigate various new and existing constructions of space-filling orthogonal array-based designs, including some strong orthogonal arrays of strength 2+ and mappable nearly orthogonal arrays (Mukerjee et al., 2014). The results of this chapter have been published in *The Annals of Statistics* (Chen and Tang, 2022a).

The results of Chapter 4 show that strong orthogonal arrays of strength 2+ are appealing because of their space-filling properties in two-dimensions. Most of previous work on strong orthogonal arrays of strength 2+ focuses on the use of regular designs. In Chapter 5, we develop a method of constructing space-filling designs using nonregular designs. Designs so constructed have very flexible run sizes compared to those constructed from regular designs. Apart from some theoretical results, computer searches are conducted to find space-filling designs using two-level nonregular designs of up to 40 runs and three-level nonregular designs of 27 and 54 runs. The results of the chapter have been published in *Journal of Statistical Planning and Inference* (Chen and Tang, 2022b).

Chapter 2

Nonregular Designs from Paley's Hadamard Matrices: Generalized Resolution, Projectivity and Hidden Projection Property

2.1 Introduction

Two-level orthogonal arrays are a very useful class of fractional factorial designs for the planning of factorial experiments, especially for those studies that involve a large number of factors. They can be classified into regular designs and nonregular designs. Regular designs are easy to construct and have simple aliasing structures, but their run sizes are limited to powers of two. By comparison, nonregular designs allow for more flexible run sizes and also enjoy better statistical properties in terms of generalized resolution (Deng and Tang, 1999), projectivity (Box and Tyssedal, 1996), and hidden projection property (Wang and Wu, 1995). We refer to Xu et al. (2009) for an excellent review on nonregular designs.

Shi and Tang (2018, 2023) investigated the theoretical construction of nonregular designs with maximum generalized resolutions. Except for a special case, their results focus on orthogonal arrays of strength two. Prior to Shi and Tang (2018, 2023), finding designs with maximum generalized resolution is largely computational; see, for example, Schoen and Mee (2012) and Schoen et al. (2017).

Among all the factors investigated in an experiment, very often only a few of them are active. It is therefore important to examine the properties of a design when projected onto low dimensions. One way to characterize the projection properties of a design is through the concept of projectivity (Box and Tyssedal, 1996). A design is said to have projectivity h if its projection design onto any h factors contains all possible level combinations. For an orthogonal array of strength t, the existing results can only be used to determine whether or not it has projectivity $t+1$ (Cheng, 1995; Box and Tyssedal, 1996).

The hidden projection property of a design provides another way of evaluating its projection designs if only the main effects and two-factor interactions are of interest (Wang and Wu, 1995). A design is said to have the hidden projection property for h factors if its projection design onto any h factors allows estimation of all main effects and all two-factor interactions. Cheng (1995) showed that a strength-two orthogonal array has the hidden projection property for 4 factors if it does not have defining words of length 3 or 4. Cheng (1998) further established that if a strength-three array does not have any defining word of length 4, it has the hidden projection property for 5 factors. Bulutoglu and Cheng (2003) later proved that Paley designs with more than 8 runs do not have any defining words of length 3 or 4, thereby showing that Paley designs have the hidden projection property for 4 factors and their foldovers have the hidden projection property for 5 factors.

In this chapter, we conduct a comprehensive study on three classes of designs from Paley's Hadamard matrices (Paley, 1933) in terms of generalized resolution, projectivity and hidden projection property. The three classes of designs are denoted by P_n, $\tilde{P}_{2n}$ and Q_{2n} with their precise definitions to be given later in the chapter. For now, it suffices to say that P_n is a saturated orthogonal array of strength two obtained from Paley's first construction of Hadamard matrix, $\tilde{P}_{2n}$ is the foldover of P_n, and Q_{2n} is an orthogonal array of strength two obtained by judiciously selecting n columns from Paley's second construction of Hadamard matrix of order $2n$.

Shi and Tang (2023) examined theoretical construction of designs with maximum generalized resolutions with a focus on orthogonal arrays of strength two, and showed in particular that P_n and Q_{2n} and their subdesigns have maximum generalized resolutions. We complete their investigations by showing that $\tilde{P}_{2n}$ and many of its subdesigns, all of which are orthogonal arrays of strength three, also have maximum generalized resolutions.

More importantly, we provide a general investigation of all three classes of designs, P_n, $\tilde{P}_{2n}$ and Q_{2n} into their projectivity and hidden projection property for h factors. From Cheng (1995, 1998) and Bulutoglu and Cheng (2003), we can draw conclusions on the projectivity of P_n and Q_{2n} for $h = 3$ and of $\tilde{P}_{2n}$ for $h = 4$, and on the hidden projection property of P_n and Q_{2n} for $h = 4$ and of $\tilde{P}_{2n}$ for $h = 5$. As will be seen in Section 2.3, our results substantially expand these existing results of Cheng (1995, 1998) and Bulutoglu and Cheng (2003).

For practical purposes, we also study the selection problem using the minimum G-aberration criterion from the designs with maximum generalized resolutions. Besides our main focus, which is the design selection from P_n, $\tilde{P}_{2n}$ and Q_{2n}, we also consider those designs with maximum generalized resolutions obtained by Shi and Tang (2023) using tensor product construction. We tabulate our findings for strength-two designs with 36, 44, 48, 52, 60, 64, 96 and 128 runs and strength-three designs with 72, 88 and 120 runs.

The remainder of the chapter is organized as follows. Section 2.2 of the chapter introduces necessary notation and reviews some background. Section 2.3 studies strength-three orthogonal arrays with maximum generalized resolutions, and examines the projectivity and hidden projection property of three classes of designs P_n, $\tilde{P}_{2n}$ and Q_{2n}. Section 2.4 looks into the design selection problem using the minimum G-aberration criterion. The proofs are postponed to Section 2.5 and the chapter is concluded with a discussion in Section 2.6.

2.2 Notation and background

A two-level orthogonal array of N runs, m factors and strength t, denoted by $\mathrm{OA}(N, 2^m, t)$, is an $N \times m$ matrix of ± 1 such that in any of its $N \times t$ submatrix, the 2^t possible level combinations occur equally often. Such an array can be characterized by its J-characteristics. Suppose $D = (d_{ij})$ is an $\mathrm{OA}(N, 2^m, t)$. Given a set $\mathbf{u} \subseteq \mathbb{Z}_m = \{1, \ldots, m\}$, the J-characteristic of the columns of D indexed by $\mathbf{u}$ is defined as $J_{\mathbf{u}}(D) = \sum_{i=1}^{N} \prod_{j \in \mathbf{u}} d_{ij}$. Clearly, we have $J_{\mathbf{u}}(D) = 0$ if $|\mathbf{u}| \leq t$, where $|\mathbf{u}|$ is the cardinality of $\mathbf{u}$. In addition, we note that $|J_{\mathbf{u}}(D)|$ can only take values of $\{N, N-8, \ldots, N-8\lfloor N/8 \rfloor\}$ for $|\mathbf{u}| = 3, 4$ when $t = 2$, and

$\{N, N-16, \ldots, N-16\lfloor N/16 \rfloor\}$ for $|\mathbf{u}| = 4$ when $t = 3$, where $\lfloor \cdot \rfloor$ is the floor function; see, for example, Lemma 3 of Stufken and Tang (2007).

Let r be the smallest integer such that $\max_{|\mathbf{u}|=r} |J_{\mathbf{u}}(D)| > 0$. The generalized resolution of D is defined as $r + 1 - \max_{|\mathbf{u}|=r} |J_{\mathbf{u}}(D)|/N$ (Deng and Tang, 1999). When $N/2 < m \leq N-1$, we have $r = 3$. Shi and Tang (2023) derived the following lower bound on $\max_{|\mathbf{u}|=3} |J_{\mathbf{u}}(D)|$.

Lemma 2.1. *Suppose D is an OA$(N, 2^m, 2)$ with $N/2 < m \leq N-1$. Then $\max_{|\mathbf{u}|=3} |J_{\mathbf{u}}(D)| \geq N - 8\lfloor (N/8)(1-\xi^{1/2}) \rfloor$, where $\xi = (2m-N)/((m-1)(m-2))$.*

To distinguish designs with the same generalized resolution, Deng and Tang (1999) further proposed the minimum G-aberration criterion as a refinement. This criterion sequentially minimizes $F_1(N), \ldots, F_1(0), F_2(N), \ldots, F_2(0), \ldots, F_m(N), \ldots, F_m(0)$, where $F_k(l)$ is the frequency of $\mathbf{u}$'s such that $|\mathbf{u}| = k$ and $|J_{\mathbf{u}}(D)| = l$ for $k = 1, \ldots, m$ and $l = 0, \ldots, N$. For theoretical convenience, Tang and Deng (1999) introduced the criterion of minimum G_2-aberration, which aims to sequentially minimize the entries of $(A_1(D), \ldots, A_m(D))$ where $A_k(D) = \sum_{|\mathbf{u}|=k} |J_{\mathbf{u}}(D)/N|^2$.

Orthogonal arrays can be constructed from Hadamard matrices. A Hadamard matrix of order N is an $N \times N$ matrix H of ± 1 satisfying $H^T H = N I_N$, where I_N is the identity matrix of order N. Given a Hadamard matrix of order N, we can normalize one column by switching the signs of rows such that this column contains all ones, and then obtain an OA$(N, 2^{N-1}, 2)$ by dropping this normalized column.

Two constructions of Hadamard matrices were proposed by Paley (1933). Suppose s is a prime or prime power. Denote the Galois field of order s by $GF(s) = \{\alpha_1, \ldots, \alpha_s\}$ and define the function χ over $GF(s)$ such that $\chi(\alpha) = 0$ if $\alpha = 0$, $\chi(\alpha) = 1$ if $\alpha = \beta^2$ for some nonzero $\beta \in GF(s)$, and $\chi(\alpha) = -1$ otherwise. Let K be the $s \times s$ matrix with its (i,j)th entry being $\chi(\alpha_i - \alpha_j)$. Then Paley's first construction works if $s = 4l + 3$ for some integer l and leads to following Hadamard matrix of order $n = s + 1$:

$$H = \begin{bmatrix} 1 & -\mathbf{1}_s^T \\ \mathbf{1}_s & K + I_s \end{bmatrix}, \tag{2.1}$$

where $\mathbf{1}_s$ is a column vector of s ones. The OA$(n, 2^{n-1}, 2)$ obtained by removing the first column of H in (2.1) is called a Paley design and is denoted by P_n hereafter. A sharp upper bound on $\max_{|\mathbf{u}|=3,4} |J_{\mathbf{u}}(P_n)|$ was established by Shi and Tang (2018).

Lemma 2.2. *We have* $\max_{|\mathbf{u}|=3,4} |J_{\mathbf{u}}(P_n)| \leq U_P(n) = n - 8\lceil n/8 - (n-1)^{1/2}/4 - 1/2 \rceil$, *where* $\lceil \cdot \rceil$ *is the ceiling function.*

Using Lemma 2.2 together with Lemma 2.1, Shi and Tang (2023) obtained many designs with maximum generalized resolutions by dropping columns from P_n for $n = 12$, 20, 24, 28, 32, 44, 60, 72 and 80. Paley's second construction applies to the case $s = 4l + 1$ for some integer l, and yields a Hadamard matrix H of order $2n = 2s + 2$, as displayed in (2.2).

$$H = \begin{bmatrix} 1 & \mathbf{1}_s^T & -1 & \mathbf{1}_s^T \\ \mathbf{1}_s & K + I_s & \mathbf{1}_s & K - I_s \\ -1 & \mathbf{1}_s^T & -1 & -\mathbf{1}_s^T \\ \mathbf{1}_s & K - I_s & -\mathbf{1}_s & -K - I_s \end{bmatrix}, \qquad Q_{2n} = \begin{bmatrix} -1 & \mathbf{1}_s^T \\ \mathbf{1}_s & K - I_s \\ 1 & \mathbf{1}_s^T \\ -\mathbf{1}_s & -K - I_s \end{bmatrix}. \tag{2.2}$$

By multiplying the $(s+2)$th row of H in (2.2) by -1 and then removing the first $s + 1$ columns, Shi and Tang (2023) obtained the design Q_{2n} in (2.2). Shi and Tang (2023) proved that Q_{2n} achieves the minimum possible $\max_{|\mathbf{u}|=3} |J_{\mathbf{u}}(D)|$ value, as given in the next lemma.

Lemma 2.3. *The design* Q_{2n} *in* (2.2) *is an* $OA(2n, 2^n, 2)$ *with* $\max_{|\mathbf{u}|=3} |J_{\mathbf{u}}(Q_{2n})| = 4$.

2.3 Main results

2.3.1 Strength-3 arrays with maximum generalized resolutions

Lemma 2.1 provides a lower bound on $\max_{|\mathbf{u}|=3} |J_{\mathbf{u}}(D)|$ for orthogonal arrays of strength 2. We establish a similar lower bound on $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(D)|$ for strength-3 arrays.

Theorem 2.1. *Suppose D is an $OA(N, 2^m, 3)$ with $N/3 \leq m \leq N/2$. Then*

$$\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(D)| \geq N - 16 \left\lfloor (N/16)(1 - \zeta^{1/2}) \right\rfloor,$$

where

$$\zeta = \frac{4m^3 - 3m^2N + mN^2 - 3mN + 4m - N^3/8 + 3N^2/4 - N}{m(m-1)(m-2)(m-3)}.$$

Based on Theorem 2.1, some designs can be shown to have maximum generalized resolutions. For a Paley design P_n, consider its foldover design

$$\tilde{P}_{2n} = \begin{bmatrix} \mathbf{1}_n & P_n \\ -\mathbf{1}_n & -P_n \end{bmatrix}.$$

Clearly, $\tilde{P}_{2n}$ is an OA$(2n, 2^n, 3)$. Since $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(\tilde{P}_{2n})| = 2\max_{|\mathbf{u}|=3,4} |J_{\mathbf{u}}(P_n)|$, a sharp upper bound on $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(\tilde{P}_{2n})|$ follows directly from Lemma 2.2:

$$\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(\tilde{P}_{2n})| \leq 2U_P(n) = 2n - 16\lceil n/8 - (n-1)^{1/2}/4 - 1/2\rceil. \tag{2.3}$$

This shows that design $\tilde{P}_{2n}$ has a large generalized resolution as the upper bound $2U_P(n)$ on $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(\tilde{P}_{2n})|$ is in the order of $O(n^{1/2})$. Some of the $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(\tilde{P}_{2n})|$ values and the corresponding lower bounds obtained in Theorem 2.1 are given in Table 2.1 for small run sizes. Comparing the upper bound in (2.3) with the lower bound in Theorem 2.1, we deduce the next result.

Corollary 2.1. *Designs obtained by selecting any m columns from $\tilde{P}_{2n}$ have the maximum generalized resolutions for $2n = 24, 40, 48, 56, 64, 88, 120, 144, 160$ and $2n/3 \leq m \leq n$.*

We note that the special cases given by $m = n$ in Corollary 2.1 were previously obtained in Shi and Tang (2018).

Remark 2.1. *Shi and Tang (2018) found by computer search two Hadamard matrices H of order 36 with $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(H)| = 12$. Folding over any of these two Hadamard matrices by $[H^T \; -H^T]^T$ and then selecting any m columns, we obtain OA$(72, 2^m, 3)$s with the maximum generalized resolutions for $24 \leq m \leq 36$ by an application of Theorem 2.1.*

Table 2.1: Some values of $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(\tilde{P}_{2n})|$ and the corresponding lower bounds.

run size $2n$	24	40	48	56	64	88	96	120	136	144	160	168	208
$\max_{\lvert\mathbf{u}\rvert=4} \lvert J_{\mathbf{u}}(\tilde{P}_{2n})\rvert$	8	24	16	24	16	24	32	24	40	32	32	40	48
Lower bounds	8	24	16	24	16	24	16	24	24	32	32	24	32

2.3.2 Projectivities of P_n, $\tilde{P}_{2n}$ and Q_{2n}

Cheng (1995) pointed out that the projection of an OA$(N, 2^m, t)$, say D, onto $t+1$ factors indexed by $\mathbf{u}$ has $(N - |J_{\mathbf{u}}(D)|)/2^{t+1}$ copies of the full factorial plus $|J_{\mathbf{u}}(D)|/2^t$ copies of a half replicate of the full factorial. This settles projections of P_n, $\tilde{P}_{2n}$ and Q_{2n} onto 3, 4, and 3 factors, respectively. In this subsection, we investigate the projections of these designs onto more factors. A result from Tang (2001) is useful here. We describe it next.

For any $\mathbf{s} \subseteq \mathbb{Z}_m$, let $\mathbf{r_s}$ be an m-dimensional row vector with its jth entry being 1 if $j \in \mathbf{s}$, and -1 otherwise for $j = 1, \ldots, m$. Define a matrix $\mathbf{C}$ as

$$\mathbf{C} = \left[\mathbf{r}_{\emptyset}^T, \mathbf{r}_{\{1\}}^T, \mathbf{r}_{\{2\}}^T, \mathbf{r}_{\{1,2\}}^T, \mathbf{r}_{\{3\}}^T, \mathbf{r}_{\{1,3\}}^T, \mathbf{r}_{\{2,3\}}^T, \mathbf{r}_{\{1,2,3\}}^T, \mathbf{r}_{\{4\}}^T, \ldots, \mathbf{r}_{\{1,2,\ldots,m\}}^T\right]^T.$$

Clearly, $\mathbf{C}$ contains all possible level combinations for m factors as rows. For $\mathbf{u} \subseteq \mathbb{Z}_m$, let $\mathbf{h_u}$ denote the Hadamard product of all the columns of $\mathbf{C}$ indexed by $\mathbf{u}$ and define

$$\mathbf{H} = \left[\mathbf{h}_{\emptyset}, \mathbf{h}_{\{1\}}, \mathbf{h}_{\{2\}}, \mathbf{h}_{\{1,2\}}, \mathbf{h}_{\{3\}}, \mathbf{h}_{\{1,3\}}, \mathbf{h}_{\{2,3\}}, \mathbf{h}_{\{1,2,3\}}, \mathbf{h}_{\{4\}}, \ldots, \mathbf{h}_{\{1,2,\ldots,m\}}\right],$$

where $\mathbf{h}_{\emptyset}$ is a column of all ones. Then the result of Tang (2001) can be stated as follows.

Lemma 2.4. *Suppose D is an OA$(N, 2^m, t)$. Let $N_{\mathbf{s}}$ be the frequency that $\mathbf{r_s}$ occurs in D for $\mathbf{s} \subseteq \mathbb{Z}_m$. Then $N_{\mathbf{s}} = 2^{-m} \sum_{\mathbf{u} \subseteq \mathbb{Z}_m} h_{\mathbf{su}} J_{\mathbf{u}}(D)$, where $h_{\mathbf{su}}$ is the element on the $\mathbf{s}$th row and $\mathbf{u}$th column of $\mathbf{H}$.*

Lemma 2.4 reveals that any design, up to row permutations, is uniquely determined by its J-characteristics. This enables us to study the projections of a design D onto k factors through $J_{\mathbf{u}}(D)$ for $|\mathbf{u}| \leq k$.

Proposition 2.1. *The projection of P_n (respectively, $\tilde{P}_{2n}$) onto any 4 (respectively, 5) factors has at least $\lceil n/16 - 5U_P(n)/16 \rceil$ copies of the full factorial.*

Proposition 2.1 indicates that the number of full factorials contained in any four-factor projection of P_n, or five-factor projection of $\tilde{P}_{2n}$, is approximately $n/16$ for large n, since $U_P(n)$ is of order $O(n^{1/2})$. A design is said to have projectivity h if its projection onto any h factors contains at least one full factorial. Using Proposition 2.1, one can check that P_n

(respectively, $\tilde{P}_{2n}$) has projectivity 4 (respectively, 5) when $n \geq 108$. Next, we examine the projections of Q_{2n} onto 4 and 5 factors, for which we need the following knowledge on $|J_{\mathbf{u}}(Q_{2n})|$ for $|\mathbf{u}| = 4$ and 5.

Lemma 2.5. *We have that* $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(Q_{2n})| \leq U_Q(2n) = 2n - 8\lceil n/4 - (n-1)^{1/2}/2 \rceil$ *and that* $|J_{\mathbf{u}}(Q_{2n})|$ *is either 0 or 8 for* $|\mathbf{u}| = 5$.

Remark 2.2. *The bound* $U_Q(2n)$ *for* Q_{2n} *appears quite sharp. We have checked that the bound is attained by all* $2n = 2s+2 < 600$ *with* s *being a prime power and all* $2n = 2s+2 < 5000$ *with* s *being a prime. We also see that* $U_Q(2n)$ *is asymptotically equivalent to the bound* $2U_P(n)$ *for* $\tilde{P}_{2n}$. *This is because the inequalities* (2.4) *in the proof of Lemma 2.5 hold no matter whether* $s \equiv 1 \pmod 4$ *or* $s \equiv 3 \pmod 4$, *and are therefore an intrinsic property of the matrix* K *in* (2.1) *and* (2.2). *We note that this property has been used to construct definitive screening designs by Wang et al. (2022b) recently.*

Lemma 2.5 allows us to study the projections of Q_{2n} onto 4 and 5 factors.

Proposition 2.2. *The projection of* Q_{2n} *onto any 4 (respectively, 5) factors has at least* $\lceil n/8 - U_Q(2n)/16 - 1 \rceil$ *(respectively,* $\lceil n/16 - U_Q(2n)/8 - 6/5 \rceil$*) copies of the full factorial.*

The proof of Proposition 2.2 is similar to that of Proposition 2.1 and thus omitted. It follows immediately that Q_{2n} has projectivity 4 when the run size $2n \geq 36$, and projectivity 5 when the run size $2n \geq 196$.

We now use a computer to take a closer look at the projections of P_n, $\tilde{P}_{2n}$ and Q_{2n} for small run sizes. For a design D with N runs, we denote by $f_k(l)$ the proportion of k-factor projections of D that contains l full factorials, and summarize the k-factor projection properties of D by the vector

$$\mathrm{PV}_k(D) = (f_k(0), f_k(1), \ldots, f_k(\lfloor N/2^k \rfloor)).$$

The vectors $\mathrm{PV}_4(P_n)$, $\mathrm{PV}_4(Q_{2n})$ and $\mathrm{PV}_5(Q_{2n})$ are displayed in Tables 2.2 and 2.3. The vectors $\mathrm{PV}_5(\tilde{P}_{2n})$ are omitted because we find $\mathrm{PV}_4(P_n) = \mathrm{PV}_5(\tilde{P}_{2n})$ for all $n < 108$. We conjecture this relationship holds for all n, though we cannot prove it for the moment.

Table 2.2: The four-factor projections of P_n for $n < 108$.

n	$\mathrm{PV}_4(P_n) = (f_4(0), f_4(1), \ldots, f_4(\lfloor n/16 \rfloor))$
20	$(100\%, 0)$
24	$(57.1\%, 42.9\%)$
28	$(50.0\%, 50.0\%)$
32	$(39.4\%, 59.1\%, 1.4\%)$
44	$(7.3\%, 67.1\%, 25.6\%)$
48	$(6.1\%, 51.5\%, 42.4\%, 0)$
60	$(0.4\%, 24.4\%, 65.8\%, 9.4\%)$
68	$(0, 10.1\%, 56.7\%, 33.2\%, 0)$
72	$(0, 6.4\%, 43.7\%, 44.8\%, 5.1\%)$
80	$(0, 2.1\%, 29.9\%, 53.7\%, 14.4\%, 0)$
84	$(0, 0.9\%, 18.5\%, 63.9\%, 16.7\%, 0)$
104	$(0, 0.2\%, 1.2\%, 22.0\%, 55.3\%, 20.2\%, 1.2\%)$

Table 2.3: The four- and five-factor projections of Q_{2n} for $2n < 196$.

$2n$	$\mathrm{PV}_4(Q_{2n}) = (f_4(0), f_4(1), \ldots, f_4(\lfloor n/8 \rfloor))$	$\mathrm{PV}_5(Q_{2n}) = (f_5(0), f_5(1), \ldots, f_5(\lfloor n/16 \rfloor))$
20	$(100\%, 0)$	100%
28	$(27.3\%, 72.7\%)$	100%
36	$(0, 100\%, 0)$	$(100\%, 0)$
52	$(0, 8.7\%, 91.3\%, 0)$	$(90.0\%, 10.0\%)$
60	$(0, 0, 55.6\%, 44.4\%)$	$(76.6\%, 23.3\%)$
76	$(0, 0, 0, 57.1\%, 42.9\%)$	$(39.1\%, 57.2\%, 3.7\%)$
84	$(0, 0, 0, 23.1\%, 76.9\%, 0)$	$(22.9\%, 76.3\%, 7.7\%)$
100	$(0, 0, 0, 0, 31.9\%, 68.1\%, 0)$	$(7.7\%, 65.2\%, 27.0\%, 0)$
108	$(0, 0, 0, 0, 5.9\%, 70.6, 23.5\%)$	$(4.5\%, 65.8\%, 29.7\%, 0)$
124	$(0, 0, 0, 0, 0, 13.6\%, 45.8\%, 40.7\%)$	$(1.9\%, 32.4\%, 59.8\%, 5.9\%)$
148	$(0, 0, 0, 0, 0, 0, 0, 45.1\%, 54.9\%, 0)$	$(0.1\%, 8.9\%, 59.4\%, 30.4\%, 1.1\%)$
164	$(0, 0, 0, 0, 0, 0, 0, 1.2\%, 53.2\%, 45.6\%, 0)$	$(0.4\%, 0.3\%, 42.9\%, 45.8\%, 10.4\%, 0)$
180	$(0, 0, 0, 0, 0, 0, 0, 0, 6.9\%, 37.9\%, 55.2\%, 0)$	$(0, 0.1\%, 22.4\%, 58.5\%, 18.3\%, 0.6\%)$

Table 2.3 suggests that the bound $\lceil n/8 - U_Q(2n)/16 - 1 \rceil$ on the number of full factorials in 4-factor projections of Q_{2n} is sharp as it is attained by all run sizes less than 196. More importantly, combining the computational results in Tables 2.2 and 2.3 and theoretical results in Propositions 2.1 and 2.2, we know exactly when designs P_n, $\tilde{P}_{2n}$ and Q_{2n} have projectivities 4 or 5. This we summarize as Theorem 2.2.

Theorem 2.2. *The design P_n (respectively, $\tilde{P}_{2n}$) has projectivity 4 (respectively, 5) when $n \geq 68$. The design Q_{2n} has projectivity 4 when $2n \geq 36$, and projectivity 5 when $2n \geq 180$.*

2.3.3 Hidden projection properties of P_n, $\tilde{P}_{2n}$ and Q_{2n}

An orthogonal array is said to have the hidden projection property for h factors if in its projection onto any h factors, all the main effects and two-factor interactions are estimable under the assumption that higher-order interactions are negligible.

Bulutoglu and Cheng (2003) showed that P_n does not have defining words of lengths three or four as long as $n \geq 12$ and thus has the hidden projection property for 4 factors by a result of Cheng (1995). It is also easy to deduce, according to Cheng (1998), that $\tilde{P}_{2n}$ has the hidden projection property for 5 factors as long as the run size $2n$ is at least 24. In this subsection, we show that even better hidden projection properties can be achieved by P_n, $\tilde{P}_{2n}$ and also Q_{2n} for moderate n.

Lemma 2.6. *The design P_n (respectively, $\tilde{P}_{2n}$) has the hidden projection property for h (respectively, $h+1$) factors if $n > (h-1)(h-2)U_P(n)/2$. The design Q_{2n} has the hidden projection property for h factors if $2n > 4(h-2) + (h-2)(h-3)U_Q(2n)/2$.*

Lemma 2.6 guarantees that P_n (respectively, $\tilde{P}_{2n}$) has the hidden projection property for 5 (respectively, 6) factors when $n = 132$, 140, 152 and $n \geq 168$, and that Q_{2n} has the hidden projection property for 5 factors when $2n \geq 76$, and for 6 factors when $2n \geq 300$. We then proceed with a computer study of those cases not covered by Lemma 2.6. Combining our computational findings with Lemma 2.6, we obtain Theorem 2.3.

Theorem 2.3. *The design P_n (respectively, $\tilde{P}_{2n}$) has the hidden projection property for 5 (respectively, 6) factors when $n \geq 28$. The design Q_{2n} has the hidden projection property for 5 factors when $2n \geq 28$, and for 6 factors when $2n = 28$ and $2n \geq 52$.*

Table 2.4: Some values of $h_{\max}(P_n)$, $h_{\max}(\tilde{P}_{2n})$ and $h_{\max}(Q_{2n})$.

n	20	24	28	32	44	48	60	68	72	80	84
$h_{\max}(P_n)$	4	4	5	6	8	7	≥ 7	≥ 7	≥ 7	≥ 6	≥ 6
$h_{\max}(\tilde{P}_{2n})$	5	5	6	7	9	8	≥ 8	≥ 8	≥ 8	≥ 7	≥ 7
$2n$	20	28	36	52	60	76	84	100	108	124	148
$h_{\max}(Q_{2n})$	4	6	5	6	7	7	≥ 8	≥ 8	≥ 8	≥ 7	≥ 7

For a design D, let $h_{\max}(D)$ be the largest integer h such that D has the hidden projection property for h factors. We obtain the following computational results on $h_{\max}(P_n)$, $h_{\max}(\tilde{P}_{2n})$ and $h_{\max}(Q_{2n})$ as displayed in Table 2.4, which strengthen the general theoretical results in Theorem 2.3 for many cases.

When $n \geq 60$ for P_n, $\tilde{P}_{2n}$ and $2n \geq 84$ for Q_{2n}, we only provide a lower bound for $h_{\max}$ as the computation becomes too heavy to handle. Nonetheless, we can still see a trend that better hidden projection properties can be achieved by designs with larger run sizes. This is expected because, by Lemma 2.6, $h_{\max}$ should be in the order of $O(n^{1/4})$.

2.4 Design selection by minimum G-aberration

The generalized resolution, as a design selection criterion, only looks at the most severe aliasing among factorial effects. A more general design selection criterion is that of minimum G-aberration. This section is devoted to finding minimum G-aberration designs from those with maximum generalized resolutions. Our focus is on design selection from the three classes of designs P_n, $\tilde{P}_{2n}$ and Q_{2n}. Also considered are some designs by tensor product construction from Shi and Tang (2023). In our computer search, we use J-characteristics for up to four factors, as done by most authors.

A brief review on designs with minimum G-aberration is necessary. Specifically, such OA$(N, 2^m, t)$s are already available for $N = 12$, 16, 20 and $m \leq N - 1$ (Sun et al., 2008); $N = 24$ and $m \leq 23$, $N = 28$ and $m \leq 14$, $N = 36$ and $m \leq 18$ (Schoen et al., 2017); $N = 32$, 40 and 48 and $m \leq N/2$ (Schoen and Mee, 2012). Recently, Vazquez and Xu (2019); Vazquez et al. (2019, 2022) algorithmically studied some strength-3 designs with larger run sizes. It should be noted that Schoen et al. (2017); Vazquez et al. (2022, 2019) have examined strength-2 designs from projections of P_{32}, strength-3 designs from projections of $\tilde{P}_{56}$ and $\tilde{P}_{64}$, respectively.

2.4.1 Designs from Paley's constructions

The orthogonal arrays in this subsection come from Paley's constructions of Hadamard matrices, except for those with 36 and 72 runs, which are from the two Hadamard matrices of order 36 in Remark 2.1.

We first consider Hadamard matrices from Paley's first construction as well as the two of order 36. Given a Hadamard matrix of order n, we first randomly select a submatrix with m columns, then obtain an $\mathrm{OA}(n, 2^{m-1}, 2)$ by normalizing and removing a randomly selected column, and an $\mathrm{OA}(2n, 2^m, 3)$ by folding over the submatrix. The procedure is repeated 200,000 times and the designs with minimum G-aberrations are selected. A complete search is done when $\binom{n}{m}$ is less than 200,000. We apply this approach to Paley's first Hadamard matrices of order 44, 60 and the two Hadamard matrices of 36. It should also be mentioned that the strength-2 designs of 44 and 60 runs obtained this way may not be subdesigns of P_{44} and P_{60}, since the normalized column need not be the first column of the Hadamard matrix. We present the search results for strength-2 orthogonal arrays of $n = 36$, 44 and 60 runs in Table 2.5 and strength-3 orthogonal arrays of $2n = 72$, 88 and 120 runs in Table 2.6. Details of all the designs in this chapter are available upon request.

For these projection designs the $|J_{\mathbf{u}}|$'s can only take two values, thus the criteria of minimum G- and G_2-aberration are equivalent. Let E be the complement of an $\mathrm{OA}(n, m, 2, 2)$, say D, in an $\mathrm{OA}(n, n-1, 2, 2)$. Then the complementary design theory (Tang and Deng, 1999) states that the sequential minimization of $A_3(D)$ and $A_4(D)$ can be done by sequentially maximizing $A_3(E)$ and minimizing $A_4(E)$, where the latter is much faster when $m > n/2$. In addition, when $|J_{\mathbf{u}}(E)|$ can only be 4 or 12, we have $A_3(E) \leq \binom{n-1-m}{3}(12/n)^2$ and $A_4(E) \geq \binom{n-1-m}{4}(4/n)^2$. Similar bounds can also be derived for strength-3 designs. These simple bounds enable us to identify the best projection designs when the search is incomplete. In Tables 2.5 and 2.6, we mark a value or a vector by an asterisk if it is minimized or sequentially minimized among all projections, respectively.

Table 2.5: Strength-2 designs of 36, 44 and 60 runs.

$n \times m$	(A_3, A_4)	$(F_3(12), F_4(12))$	$n \times m$	(A_3, A_4)	$(F_3(12), F_4(12))$
36×19	$(26.6, 122.5)$	$(148, 756)$	36×26	$(76.5, 456.9)$	$(450, 2757)$
36×20	$(32.2, 150.4)$	$(184, 917)$	36×27	$(86.2, 536.5)$	$(507, 3238)$
36×21	$(37.7, 187.0)$	$(215, 1145)$	36×28	$(97.9, 622.7)$	$(582, 3745)$
36×22	$(44.1, 225.9)$	$(254, 1373)$	36×29	$(109.1^*, 722.6)$	$(648^*, 4347)$
36×23	$(50.7, 273.7)$	$(292, 1664)$	36×30	$(122.2^*, 831.7)$	$(730^*, 4995)$
36×24	$(59.5, 324.7)$	$(349, 1959)$	36×31	$(135.9^*, 953.9)$	$(814^*, 5725)$
36×25	$(67.7, 386.3)$	$(398, 2330)$	36×32	$(150.2, 1089.8)^*$	$(901, 6539)^*$
44×23	$(41.5, 216.9)$	$(407, 2174)$	44×32	$(120.0, 878.1)$	$(1195, 8786)$
44×24	$(47.7, 262.4)$	$(469, 2641)$	44×33	$(132.2, 999.5)$	$(1317, 10003)$
44×25	$(54.4, 311.5)$	$(536, 3130)$	44×34	$(145.2, 1131.5)$	$(1448, 11317)$
44×26	$(61.9, 365.0)$	$(611, 3652)$	44×35	$(159.0, 1277.4)$	$(1587, 12776)$
44×27	$(69.9, 430.5)$	$(691, 4317)$	44×36	$(173.7, 1437.2)$	$(1734, 14374)$
44×28	$(78.4, 501.0)$	$(777, 5019)$	44×37	$(189.1, 1611.3)$	$(1889, 16116)$
44×29	$(87.9, 582.0)$	$(872, 5834)$	44×38	$(205.5, 1800.5)$	$(2054, 18006)$
44×30	$(97.9, 670.5)$	$(973, 6715)$	44×39	$(222.8, 2006.2)$	$(2227, 20063)$
44×31	$(108.6, 767.8)$	$(1081, 7680)$	44×40	$(240.9, 2229.1)^*$	$(2409, 22291)^*$
60×31	$(77.2, 554.0)$	$(1610, 11647)$	60×44	$(231.3, 2382.9)$	$(4849, 50049)$
60×32	$(85.2, 631.4)$	$(1775, 13262)$	60×45	$(248.0, 2615.0)$	$(5201, 54923)$
60×33	$(94.1, 718.0)$	$(1964, 15078)$	60×46	$(265.4, 2863.7)$	$(5566, 60143)$
60×34	$(103.3, 813.9)$	$(2156, 17093)$	60×47	$(283.6, 3130.1)$	$(5948, 65739)$
60×35	$(113.0, 920.2)$	$(2360, 19336)$	60×48	$(302.7, 3414.5)$	$(6351, 71709)$
60×36	$(123.7, 1033.2)$	$(2586, 21697)$	60×49	$(322.5, 3717.9)$	$(6768, 78081)$
60×37	$(134.8, 1158.5)$	$(2820, 24327)$	60×50	$(343.2, 4041.0)$	$(7202, 84867)$
60×38	$(146.4, 1295.4)$	$(3062, 27206)$	60×51	$(364.9, 4384.8)$	$(7659, 92085)$
60×39	$(158.8, 1444.4)$	$(3323, 30343)$	60×52	$(387.3, 4750.1)$	$(8130, 99755)$
60×40	$(171.8, 1603.3)$	$(3597, 33670)$	60×53	$(410.7, 5137.6)$	$(8623, 107891)$
60×41	$(185.7, 1777.6)$	$(3889, 37337)$	60×54	$(435.0, 5548.5)$	$(9133, 116520)$
60×42	$(200.1, 1964.4)$	$(4193, 41258)$	60×55	$(460.2, 5983.5)^*$	$(9663, 125654)^*$
60×43	$(215.3, 2166.2)$	$(4514, 45497)$	60×56	$(486.3, 6443.7)^*$	$(10212, 135318)^*$

Table 2.6: Strength-3 designs of 72, 88 and 120 runs.

$2n \times m$	A_4	$F_4(24)$	$2n \times m$	A_4	$F_4(24)$	$2n \times m$	A_4	$F_4(24)$
72×9	2.8	13	72×17	70.2	413	72×25	381.9	2285
72×10	5.1	25	72×18	90.7	536	72×26	451.7	2705
72×11	8.5	45	72×19	115.5	685	72×27	530.8	3181
72×12	13.4	74	72×20	144.9	861	72×28	619.6	3714
72×13	20.0	113	72×21	179.4	1068	72×29	719.2	4313
72×14	28.5	163	72×22	219.8	1311	72×30	830.2*	4980*
72×15	39.4	228	72×23	266.7	1593	72×31	953.4*	5720*
72×16	53.2	311	72×24	320.4	1916	72×32	1089.7*	6538*
88×9	2.0	14	88×20	115.5	1142	88×31	765.7	7648
88×10	3.9	33	88×21	143.1	1416	88×32	875.6	8748
88×11	6.8	61	88×22	175.6	1741	88×33	996.8	9961
88×12	10.6	98	88×23	213.1	2116	88×34	1129.9	11293
88×13	15.7	148	88×24	256.5	2552	88×35	1276.0	12754
88×14	22.4	214	88×25	305.8	3044	88×36	1436.0	14357
88×15	31.2	302	88×26	362.0	3607	88×37	1610.4	16102
88×16	42.1	409	88×27	425.3	4239	88×38	1800.1*	18000*
88×17	55.3	539	88×28	497.1	4959	88×39	2006.0*	20060*
88×18	72.0	707	88×29	577.2	5762	88×40	2229.0*	22290*
88×19	91.8	904	88×30	666.4	6654			
120×9	1.6	29	120×25	218.6	4567	120×41	1774.2	37241
120×10	2.9	55	120×26	259.1	5418	120×42	1961.4	41172
120×11	4.7	92	120×27	304.3	6365	120×43	2162.8	45403
120×12	7.5	149	120×28	355.6	7443	120×44	2379.6	49957
120×13	11.2	227	120×29	413.0	8646	120×45	2612.0	54839
120×14	15.9	323	120×30	477.3	9998	120×46	2861.3	60075
120×15	22.0	449	120×31	548.3	11488	120×47	3127.9	65677
120×16	29.9	614	120×32	627.3	13148	120×48	3412.5	71654
120×17	39.5	813	120×33	714.3	14975	120×49	3716.1	78030
120×18	51.4	1062	120×34	810.4	16996	120×50	4039.6	84825
120×19	65.5	1359	120×35	915.3	19197	120×51	4383.6	92051
120×20	82.2	1707	120×36	1030.3	21613	120×52	4749.1	99727
120×21	101.9	2118	120×37	1155.6	24245	120×53	5137.0	107874
120×22	125.3	2611	120×38	1292.0	27111	120×54	5548.1*	116508*
120×23	152.2	3175	120×39	1439.9	30216	120×55	5983.4*	125650*
120×24	183.3	3826	120×40	1600.6	33592	120×56	6443.7*	135317*

Next we study designs from Q_{2n}'s with run sizes 52, 60 and 76 and search for those with minimum G-aberration. Although the minimum G_2-aberration criterion and complementary design theory cannot be applied to find such designs because $|J_{\mathbf{u}}(Q_{2n})|$ takes three values for $|\mathbf{u}| = 4$, we can still use the minimum G_e-aberration to accelerate the search as suggested by Ingram and Tang (2005). For a design D with N runs, the criterion of minimum G_e-aberration sequentially minimizes $A_{1,e}(D), \ldots, A_{m,e}(D)$ where $A_{k,e}(D) = \sum_{|\mathbf{u}|=k} |J_{\mathbf{u}}(D)/N|^e$ for some $e > 0$. It can be shown that for OA$(2n, 2^m, 2)$s studied here, the minimum G- and G_e-aberration criteria are equivalent if we take $e > \log \binom{m}{4} / \{\log(20) - \log(12)\}$. For each $2n \times m$, a complete search is done if $\binom{n}{m} < 200{,}000$ otherwise a total of 200,000 random subdesigns from Q_{2n} are compared then the best one is selected. The results are displayed in Table 2.7. We mark a value or a vector by an asterisk if it is minimized or sequentially minimized among all projections, respectively.

2.4.2 Designs from the tensor product method

Besides designs from Paley's constructions, Shi and Tang (2023) constructed some strength-2 orthogonal arrays with maximum generalized resolutions by the tensor product $D = H_{n_1} \otimes B$ for $n_1 = 2$ and 4, where $B = (b_1, \ldots, b_{m_2})$ is an OA$(n_2, 2^{m_2}, 2)$,

$$H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad \text{and} \quad H_4 = \begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}.$$

We provide some theoretical results to select such designs by the minimum G-aberration criterion. For convenience, we use again the equivalence of minimum G- and G_e-aberrations for large e and present our results in terms of the latter.

Proposition 2.3. *Suppose $D = H_{n_1} \otimes B$ for $n_1 = 2$ or 4.*

(i) For any $e > 0$, we have $A_{3,e}(D) = \gamma_1 A_{3,e}(B)$ and $A_{4,e}(D) = \gamma_2 A_{4,e}(B) + \gamma_3$, where γ_1, γ_2 and γ_3 are positive constants depending on H_{n_1} and e.

Table 2.7: Strength-2 designs of 52, 60 and 76 runs.

$2n \times m$	A_4	$F_4(20,12)$	$2n \times m$	A_4	$F_4(20,12)$	$2n \times m$	A_4	$F_4(20,12)$
52×4	0.01*	$(0,0)^*$	52×12	17.84	$(30,225)$	52×20	178.07	$(420,1896)$
52×5	0.08*	$(0,1)^*$	52×13	25.77	$(50,305)$	52×21	220.08*	$(520,2341)^*$
52×6	0.37	$(0,6)$	52×14	36.46	$(74,423)$	52×22	269.08*	$(636,2862)^*$
52×7	1.01	$(0,17)$	52×15	49.97	$(110,555)$	52×23	325.77*	$(770,3465)^*$
52×8	2.02	$(0,34)$	52×16	66.15	$(149,723)$	52×24	390.92*	$(924,4158)^*$
52×9	3.96	$(5,53)$	52×17	86.89	$(201,935)$	52×25	465.38*	$(1100,4950)^*$
52×10	6.92	$(9,93)$	52×18	112.02	$(260,1204)$			
52×11	11.89	$(20,150)$	52×19	142.32	$(334,1520)$			
60×5	0.02*	$(0,0)^*$	60×14	31.15	$(97,460)$	60×23	283.91	$(980,3938)$
60×6	0.28	$(0,6)$	60×15	41.80	$(135,600)$	60×24	340.88	$(1179,4722)$
60×7	0.80	$(0,18)$	60×16	57.44	$(188,824)$	60×25	405.91*	$(1405,5620)^*$
60×8	1.63	$(0,37)$	60×17	75.68	$(251,1078)$	60×26	479.85*	$(1661,6644)^*$
60×9	3.23	$(5,60)$	60×18	97.19	$(328,1367)$	60×27	563.33*	$(1950,7800)^*$
60×10	5.91	$(14,98)$	60×19	123.50	$(420,1729)$	60×28	657.22*	$(2275,9100)^*$
60×11	9.68	$(26,153)$	60×20	154.69	$(529,2158)$	60×29	762.38*	$(2639,10556)^*$
60×12	14.86	$(43,227)$	60×21	191.29	$(656,2664)$			
60×13	22.24	$(66,338)$	60×22	234.18	$(805,3257)$			
76×6	0.04*	$(0,0)^*$	76×17	58.80	$(514,814)$	76×28	522.71	$(4666,7030)$
76×7	0.47	$(2,11)$	76×18	75.62	$(660,1050)$	76×29	606.27	$(5417,8138)$
76×8	1.06	$(5,24)$	76×19	96.90	$(853,1329)$	76×30	699.85	$(6253,9396)$
76×9	2.32	$(17,38)$	76×20	122.14	$(1079,1669)$	76×31	803.95	$(7186,10787)$
76×10	4.11	$(33,60)$	76×21	150.89	$(1336,2053)$	76×32	918.94	$(8216,12324)$
76×11	7.23	$(60,105)$	76×22	185.18	$(1641,2519)$	76×33	1045.96	$(9352,14028)$
76×12	11.43	$(92,178)$	76×23	224.66	$(1999,3034)$	76×34	1185.53*	$(10600,15900)^*$
76×13	16.78	$(142,242)$	76×24	270.32	$(2405,3655)$	76×35	1338.53*	$(11968,17952)^*$
76×14	24.14	$(205,349)$	76×25	322.13	$(2868,4351)$	76×36	1505.84*	$(13464,20196)^*$
76×15	33.32	$(285,478)$	76×26	381.22	$(3399,5137)$	76×37	1688.37*	$(15096,22644)^*$
76×16	44.71	$(385,635)$	76×27	447.44	$(3996,6009)$			

Table 2.8: Strength-2 designs of 48 runs.

$N \times m$	A_3	$F_3(8)$	$N \times m$	A_3	$F_3(8)$	$N \times m$	A_3	$F_3(8)$
48×25	42.2	1520	48×32	99.6	3584	48×39	197.3	7104
48×26	48.9	1760	48×33	112.0	4032	48×40	213.3	7680
48×27	55.6	2000	48×34	124.4	4480	48×41	233.3	8400
48×28	62.2	2240	48×35	136.9	4928	48×42	253.3	9120
48×29	71.6	2576	48×36	149.3	5376	48×43	273.3	9840
48×30	80.9	2912	48×37	165.3	5952	48×44	293.3	10560
48×31	90.2	3248	48×38	181.3	6528			

(ii) Let $g(k) = \sum_{i<j} |J(b_i, b_j, b_k)/n_2|^e$ for $k = 1, \ldots, m_2$ and suppose $g(k_0) = \max_{1 \le k \le m_2} g(k)$. Then designs obtained by successively removing columns of $H_{n_1} \otimes b_{k_0}$ from D have minimum $A_{3,e}$ values among all projections of D.

With a sufficiently large e, part (i) of Proposition 2.3 implies that the G-aberration property of D is determined by that of B, and that it is preferable to use a B with minimum G-aberration. This is feasible as catalogues of designs with minimum or small G-aberration for small run sizes are readily available in Sun et al. (2008) and Schoen et al. (2017). After that, we apply part (ii) of Proposition 2.3 to delete columns from $H_{n_1} \otimes B$ to cover all cases. Following this procedure, we obtain the designs of 48, 64, 96 and 128 runs displayed in Tables 2.8 and 2.9. We note that when $m \le 56$ for 64-run designs, it is better to take $A = H_4$ and B as 16-run minimum G-aberration designs in Sun et al. (2008) than to take $A = H_2$ and B as the 32-run designs in Schoen et al. (2017).

2.5 Proofs

Proof of Theorem 2.1. Butler (2007) showed that for $N/3 \le m \le N/2$, any $\mathrm{OA}(N, 2^m, 3)$ can be written as $D = [V^T \; -V^T]^T$ where $V = [v_1, \ldots, v_m]$ is an $(N/2) \times m$ matrix of ± 1 with orthogonal columns. Clearly, we have $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(D)| = 2 \max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(V)|$. The rest of the proof is similar to that for Theorem 1 in Shi and Tang (2023). Let $n' = N/2$ and $m' = n' - m$. Then there exist real vectors $w_1, \ldots, w_{m'}$ such that $(n')^{-1/2}[v_1, \ldots, v_m, w_1, \ldots, w_{m'}]$ form an orthonormal basis for the n'-dimensional Euclidean space. We first consider the scenario

Table 2.9: Strength-2 designs of 64, 96 and 128 runs.

$N \times m$	A_3	$F_3(16)$	$N \times m$	A_3	$F_3(16)$	$N \times m$	A_3	$F_3(16)$
64×33	16.0	256	64×43	178.0	2848	64×53	376.0	6016
64×34	32.0	512	64×44	192.0	3072	64×54	400.0	6400
64×35	48.0	768	64×45	208.0	3328	64×55	424.0	6784
64×36	64.0	1024	64×46	224.0	3584	64×56	448.0	7168
64×37	92.0	1472	64×47	240.0	3840	64×57	477.9	7646
64×38	104.0	1664	64×48	256.0	4096	64×58	504.0	8064
64×39	116.0	1856	64×49	280.0	4480	64×59	532.0	8512
64×40	128.0	2048	64×50	304.0	4864	64×60	560.0	8960
64×41	150.0	2400	64×51	328.0	5248	64×61	590.0	9440
64×42	164.0	2624	64×52	352.0	5632	64×62	620.0	9920
96×49	124.0	4464	96×64	398.2	14336	96×79	821.3	29568
96×50	136.0	4896	96×65	427.1	15376	96×80	853.3	30720
96×51	148.0	5328	96×66	450.7	16224	96×81	904.0	32544
96×52	160.0	5760	96×67	474.2	17072	96×82	940.4	33856
96×53	191.1	6880	96×68	497.8	17920	96×83	976.9	35168
96×54	208.0	7488	96×69	522.7	18816	96×84	1013.3	36480
96×55	224.9	8096	96×70	547.6	19712	96×85	1053.3	37920
96×56	241.8	8704	96×71	572.4	20608	96×86	1093.3	39360
96×57	261.3	9408	96×72	597.3	21504	96×87	1133.3	40800
96×58	280.9	10112	96×73	634.7	22848	96×88	1173.3	42240
96×59	300.4	10816	96×74	664.9	23936	96×89	1217.3	43824
96×60	320.0	11520	96×75	695.1	25024	96×90	1261.3	45408
96×61	342.2	12320	96×76	725.3	26112	96×91	1305.3	46992
96×62	360.9	12992	96×77	757.3	27264	96×92	1349.3	48576
96×63	379.6	13664	96×78	789.3	28416			
128×65	310.5	19872	128×85	749.2	47952	128×105	1476.2	94480
128×66	327.0	20928	128×86	778.5	49824	128×106	1521.5	97376
128×67	343.5	21984	128×87	807.8	51696	128×107	1566.8	100272
128×68	360.0	23040	128×88	837.0	53568	128×108	1612.0	103168
128×69	379.8	24304	128×89	869.2	55632	128×109	1660.8	106288
128×70	398.5	25504	128×90	901.5	57696	128×110	1709.5	109408
128×71	417.2	26704	128×91	933.8	59760	128×111	1758.2	112528
128×72	436.0	27904	128×92	966.0	61824	128×112	1807.0	115648
128×73	457.0	29248	128×93	1001.5	64096	128×113	1859.2	118992
128×74	478.0	30592	128×94	1037.0	66368	128×114	1911.5	122336
128×75	499.0	31936	128×95	1072.5	68640	128×115	1963.8	125680
128×76	520.0	33280	128×96	1108.0	70912	128×116	2016.0	129024
128×77	544.5	34848	128×97	1147.5	73440	128×117	2072.0	132608
128×78	568.0	36352	128×98	1186.0	75904	128×118	2128.0	136192
128×79	591.5	37856	128×99	1224.5	78368	128×119	2184.0	139776
128×80	615.0	39360	128×100	1263.0	80832	128×120	2240.0	143360
128×81	642.0	41088	128×101	1304.8	83504	128×121	2300.0	147200
128×82	668.0	42752	128×102	1346.5	86176	128×122	2360.0	151040
128×83	694.0	44416	128×103	1388.2	88848	128×123	2420.0	154880
128×84	720.0	46080	128×104	1430.0	91520	128×124	2480.0	158720

$m' \geq 4$. Note that

$$
\begin{aligned}
&\sum_{distinct\, i_1,i_2,i_3,i_4} J(v_{i_1}, v_{i_2}, v_{i_3}, v_{i_4})^2 \\
&= \sum_{distinct\, i_1,i_2,i_3} \left\{ (n')^2 - \sum_{i_4=1}^{m'} J(v_{i_1}, v_{i_2}, v_{i_3}, w_{i_4})^2 \right\} \\
&= m(m-1)(m-2)(n')^2 - \sum_{i_1 \neq i_2} \sum_{i_4=1}^{m'} \left\{ (n')^2 - \sum_{i_3 \neq i_4} J(v_{i_1}, v_{i_2}, w_{i_3}, w_{i_4})^2 \right\} \\
&= \{m(m-1)(m-2) - m(m-1)m'\}(n')^2 \\
&\quad + \sum_{i_1=1}^{m} \sum_{i_3 \neq i_4} \left\{ (n')^2 - \sum_{i_2 \neq i_3, i_4} J(v_{i_1}, w_{i_2}, w_{i_3}, w_{i_4})^2 \right\} \\
&= \{m(m-1)(m-2) - m(m-1)m' + mm'(m'-1) - m'(m'-1)(m'-2)\}(n')^2 \\
&\quad + \sum_{distinct\, i_1,i_2,i_3,i_4} J(w_{i_1}, w_{i_2}, w_{i_3}, w_{i_4})^2,
\end{aligned}
$$

where, for example, we use $J(v_{i_1}, v_{i_2}, v_{i_3}, v_{i_4})$ to denote the J-characteristics of columns v_{i_1}, v_{i_2}, v_{i_3} and v_{i_4}. Thus we have that $\sum_{distinct\, i_1,i_2,i_3,i_4} J(v_{i_1}, v_{i_2}, v_{i_3},\ v_{i_4})^2 \geq \{m(m-1)(m-2) - m(m-1)m' + mm'(m'-1) - m'(m'-1)(m'-2)\}(n')^2$. It can be easily verified that the equality holds for $m' \leq 3$. Therefore, $\max_{|\mathbf{u}|=4} J^2_{\mathbf{u}}(V) \geq \{m(m-1)(m-2) - m(m-1)m' + mm'(m'-1) - m'(m'-1)(m'-2)\}(n')^2/\{m(m-1)(m-2)(m-3)\}$. Note that $n' - \max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(V)|$ must be a multiple of 8 (Shi and Tang, 2018). The result follows by some tedious algebra. □

Proof of Proposition 2.1. Let D_0 be the projected design of P_n onto certain 4 factors. By Lemma 2.4, for any $\mathbf{s} \subseteq \mathbb{Z}_4$, the frequency of $\mathbf{r_s}$ occurs in D_0 is given by $N_{\mathbf{s}} = 2^{-4}\{n + \sum_{\emptyset \neq \mathbf{u} \subseteq \mathbb{Z}_4} h_{\mathbf{su}} J_{\mathbf{u}}(D_0)\}$. Recall that $J_{\mathbf{u}}(D_0) = 0$ for $|\mathbf{u}| = 1, 2$ and that $|J_{\mathbf{u}}(D_0)| \leq U_P(n)$ for $|\mathbf{u}| = 3, 4$. Then we have $N_{\mathbf{s}} \geq 2^{-4}\{n - 5U_P(n)\}$ since $h_{\mathbf{su}} = \pm 1$. The result on P_n follows by the fact that $N_{\mathbf{s}}$ must be an integer and that $\mathbf{s}$ is arbitrary. The proof for $\tilde{P}_{2n}$ can be done similarly by noting that $J_{\mathbf{u}}(\tilde{P}_{2n}) = 0$ for $|\mathbf{u}| \leq 3$ and $|\mathbf{u}| = 5$ and that $|J_{\mathbf{u}}(\tilde{P}_{2n})| \leq 2U_P(n)$ for $|\mathbf{u}| = 4$. □

Proof of Lemma 2.5. The arguments are similar to the proofs for Theorem 2.1 of Bulutoglu and Cheng (2003) and Theorem 5 of Shi and Tang (2023). For simplicity, we outline the proof for $|\mathbf{u}| = 4$ and omit that for $|\mathbf{u}| = 5$. Let's write $Q_{2n} = [q_0, q_1, \ldots, q_s]$, where $s = n - 1$. Then for any distinct integers $i_1, i_2, i_3, i_4 \in \{1, \ldots, s\}$, by some simple algebra we have $J(q_0, q_{i_1}, q_{i_2}, q_{i_3}) = 2\sum_{y\in GF(s)\setminus\{\alpha_{i_1},\alpha_{i_2},\alpha_{i_3}\}} \chi((y-\alpha_{i_1})(y-\alpha_{i_2})(y-\alpha_{i_3}))$ and $J(q_{i_1}, q_{i_2}, q_{i_3}, q_{i_4}) = 2\sum_{y\in GF(s)\setminus\{\alpha_{i_1},\alpha_{i_2},\alpha_{i_3},\alpha_{i_4}\}} \chi((y-\alpha_{i_1})(y-\alpha_{i_2})(y-\alpha_{i_3})(y-\alpha_{i_4})) + 2$. Let $N(s,k)$ be the number of solutions $(z,y) \in GF(s)\times GF(s)$ of $z^2 = \prod_{j=1}^{k}(y-\alpha_{i_j})$. Then we have $J(q_0, q_{i_1}, q_{i_2}, q_{i_3}) = 2N(s,3) - 2s$ and $J(q_{i_1}, q_{i_2}, q_{i_3}, q_{i_4}) = 2N(s,4) + 2 - 2s$. By a result of Hasse (1936) quoted by Stark (1973), we know that

$$|N(s,3) - s| \le 2s^{1/2} \quad \text{and} \quad |N(s,4) - s + 1| \le 2s^{1/2}, \tag{2.4}$$

from which it follows that $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(Q_{2n})| \le 4s^{1/2}$. The upper bound on $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(Q_{2n})|$ follows by noting that $(2n - |J_{\mathbf{u}}(Q_{2n})|)/8$ must be an integer. □

Proof of Lemma 2.6. Suppose X is a subdesign of P_n for h factors. Then the model matrix M for all the main effects and two-factor interactions of these h factors can be written as $M = [\mathbf{1}_n \; X \; Y]$, where Y is an $n\times\{h(h-1)/2\}$ matrix consisting of all the pairwise Hadamard products of columns of X. It can then be checked that in each row of the information matrix M^TM, there are at most $(h-1)(h-2)/2$ nonzero off-diagonal elements whose absolute values are all bounded above by $\max_{|\mathbf{u}|=3,4} |J_{\mathbf{u}}(P_n)| \le U_P(n)$. A square matrix $Z = (z_{ij})$ is said to be strictly diagonally dominant if $|z_{ii}| > \sum_{j\ne i} |z_{ij}|$ for all i; by Levy-Desplanques theorem, such a matrix must be nonsingular. Therefore, if $n > (h-1)(h-2)U_P(n)/2$, M^TM is strictly diagonally dominant and thus nonsingular. This completes the proof for P_n. The proofs for $\tilde{P}_{2n}$ and Q_{2n} are similar and thus omitted. □

Proof of Proposition 2.3. With a slight abuse of notation, write $H_{n_1} = [h_1, \ldots, h_{n_1}]$. Then invoking Lemma 2 of Tang (2006), we have

$$\begin{aligned} A_{3,e}(D) &= \sum_{distinct\,\{(i_1,i_2),(j_1,j_2),(k_1,k_2)\}} |J(h_{i_1}\otimes b_{i_2}, h_{j_1}\otimes b_{j_2}, h_{k_1}\otimes b_{k_2})/(n_1n_2)|^e \\ &= \sum_{1\le i_1,j_1,k_1\le n_1} \sum_{i_2<j_2<k_2} |J(h_{i_1}, h_{j_1}, h_{k_1})/n_1|^e |J(b_{i_2}, b_{j_2}, b_{k_2})/n_2|^e, \end{aligned}$$

since $J(b_{i_2}, b_{j_2}, b_{k_2}) = 0$ as long as i_2, j_2 and k_2 have common elements. Therefore $A_{3,e}(D) = \gamma_1 A_{3,e}(B)$ with $\gamma_1 = \sum_{1 \le i_1, j_1, k_1 \le n_1} |J(h_{i_1}, h_{j_1}, h_{k_1})/n_1|^e$. The proof for the result on $A_{4,e}(D)$ is similar. Part (ii) can be done by observing that at each time a column of $H \otimes b_{k_0}$ is removed, $A_{3,e}$ decreases by the same and also the maximum possible amount. $\square$

2.6 Concluding remarks

The three- and four-column J-characteristics of a design, as we have seen, play a crucial role in its generalized resolutions and projection properties. Shi and Tang (2018) showed that these J-characteristics bear a close relationship to the *type* of Hadamard matrices. We conclude the chapter with more results on the type of certain Hadamard matrices.

The concept of type was introduced by Kimura (1994) and further studied in Kharaghani and Tayfeh-Rezaie (2013). Let H be a Hadamard matrix of order N. By permutation and negation of rows and columns, any four columns of H that can be transformed into the following form

$$\begin{bmatrix} \mathbf{1}_a & \mathbf{1}_a & \mathbf{1}_a & \mathbf{1}_a \\ \mathbf{1}_b & \mathbf{1}_b & \mathbf{1}_b & -\mathbf{1}_b \\ \mathbf{1}_b & \mathbf{1}_b & -\mathbf{1}_b & \mathbf{1}_b \\ \mathbf{1}_a & \mathbf{1}_a & -\mathbf{1}_a & -\mathbf{1}_a \\ \mathbf{1}_b & -\mathbf{1}_b & \mathbf{1}_b & \mathbf{1}_b \\ \mathbf{1}_a & -\mathbf{1}_a & \mathbf{1}_a & -\mathbf{1}_a \\ \mathbf{1}_a & -\mathbf{1}_a & -\mathbf{1}_a & \mathbf{1}_a \\ \mathbf{1}_b & -\mathbf{1}_b & -\mathbf{1}_b & -\mathbf{1}_b \end{bmatrix}$$

where $a + b = N/4$ and $0 \le b \le \lfloor N/8 \rfloor$, is said to be of type b. A Hadamard matrix is of type b if it has a set of four columns of type b but has no set of four columns of type less than b. Shi and Tang (2018) established a connection between the type of H and the $\mathrm{OA}(N, 2^{N-1}, 2)$ derived from H, which can be rephrased as the following lemma.

Lemma 2.7. *A Hadamard matrix H has type b if and only if* $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(H)| = N - 8b$.

Lemma 2.7 is useful for finding the type of a Hadamard matrix; it can also be taken as a definition of type for anyone who finds the original definition cumbersome.

Proposition 2.4. *Let H_1 and H_2 be any two Hadamard matrices of orders N_1 and N_2, respectively. Then $H_1 \otimes H_2$ has type 0.*

Proof. Let $h_1^{(1)}, h_2^{(1)}$ be two columns of H_1 and $h_1^{(2)}, h_2^{(2)}$ be two columns of H_2. Then we have that $J(h_1^{(1)} \otimes h_1^{(2)}, h_1^{(1)} \otimes h_2^{(2)}, h_2^{(1)} \otimes h_1^{(2)}, h_2^{(1)} \otimes h_2^{(2)}) = J(h_1^{(1)}, h_1^{(1)}, h_2^{(1)}, h_2^{(1)}) J(h_1^{(2)}, h_2^{(2)}, h_1^{(2)}, h_2^{(2)})$ $= N_1 N_2$. Proposition 2.4 now follows from Lemma 2.7. □

The special case that H_1 is of order 2 was considered by Shi and Tang (2018). Proposition 2.4 shows that a tensor product inevitably introduces defining words of lengths 4, and thus cannot be used to construct designs with the attractive properties as described in Section 2.3.

Proposition 2.5. *Hadamard matrices from Paley's second construction are of type 1.*

Proof. Write H in (2.2) as

$$H = \begin{bmatrix} F & G \\ G & -F \end{bmatrix}, \qquad \text{where} \quad F = \begin{bmatrix} 1 & \mathbf{1}_s^T \\ \mathbf{1}_s & K + I_s \end{bmatrix} \quad \text{and} \quad G = \begin{bmatrix} -1 & \mathbf{1}_s^T \\ \mathbf{1}_s & K - I_s \end{bmatrix}.$$

For $1 \leq i < j \leq n$, let f_i and f_j (respectively, g_i and g_j) be the ith and jth column of F (respectively, G). Then the J-characteristic of the following four columns of H

$$\begin{bmatrix} f_i & f_j & g_i & g_j \\ g_i & g_j & -f_i & -f_j \end{bmatrix}$$

is $2J(f_i, f_j, g_i, g_j) = 2J(f_i g_i, f_j g_j)$. Note that the column $f_i g_i$ is all ones except for the ith entry, which is -1. One can easily see that $2J(f_i g_i, f_j g_j) = 2\{(n-2) - 2\} = 2n - 8$. On the other hand, since $2n$ is not a multiple of 8, $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(H)|$ can be at most $2n - 8$ (Cheng, 1995). Therefore, we have $\max_{|\mathbf{u}|=4} |J_{\mathbf{u}}(H)| = 2n - 8$ and result follows by Lemma 2.7. □

Proposition 2.2 implies that appending more columns to Q_{2n} will lead to severe aliasing among certain three or four columns. As a result, we cannot obtain designs with large generalized resolutions or good projection properties from them.

Propositions 2.4 and 2.5 are worth documenting even though they are somewhat negative. They convey a message that we should look elsewhere if we want to find Hadamard matrices of large types.

Chapter 3

Minimum Aberration Factorial Designs Under A Mixed Parametrization

3.1 Introduction

Two-level factorial designs are a class of experimental plans useful in scientific and technological investigations for studying the causal relationship between several input factors and a response variable. Factorial effects are utilized to attribute changes of the mean response due to various level combinations to the factors under study. The most commonly used factorial effects are those given by the orthogonal parametrization (Box and Hunter, 1961), which is termed so because those factorial effects form a set of orthogonal treatment contrasts. When it is too expensive to examine all level combinations, factorial effects cannot be all estimated and a fractional factorial design needs to be selected to entertain the estimation of the lower-order effects. One popular approach to design selection is to employ the minimum aberration criterion (Fries and Hunter, 1980; Tang and Deng, 1999). We refer to Mee (2009), Cheng (2014) and Wu and Hamada (2021) for comprehensive accounts on factorial designs under the orthogonal parametrization.

Under the orthogonal parametrization, the two levels of the factors are symmetrical and hence equally important. While this is true in most applications, there are situations, such as in microarray experiments (Yang and Speed, 2002; Glonek and Solomon, 2004; Banerjee and Mukerjee, 2008), where one of the two levels represents a baseline or default setting and is thus more important than the other level. Investigators are interested in the impact on the mean response by changing the levels of a few factors while keeping other factors set at the baseline levels. This calls for a baseline parametrization in which factorial effects are defined in relation to the baseline levels. To select a fractional factorial design under this parametrization, Mukerjee and Tang (2012) put forward a minimum aberration criterion which aims at minimizing the bias caused by higher-order interactions on the estimation of main effects.

The blanket approach to defining factorial effects via either the orthogonal parametrization or the baseline parametrization can hardly represent all practical situations. Entirely conceivable are the scenarios that we know the importance of one of the two levels for some factors but are indifferent to the two levels for other factors. In an industrial experiment on quality improvement, besides studying the potential impact of changing the current settings of several machine components in a production line, we may also want to examine some additional factors along the way. Then the current settings may be regarded as the baseline levels for the machine components, but no importance can be attached to any of the two levels for the additional factors. To deal with such practical situations, we propose a mixed parametrization of factorial effects in which some factors have baseline levels while the others do not. Our mixed parametrization includes as special cases of both the orthogonal and baseline parametrizations.

The remainder of the chapter is arranged as follows. Section 3.2 first reviews orthogonal and baseline parametrizations, and then introduces the mixed parametrization. A connection between the mixed parametrization and the existing parametrizations is established, through which we show that orthogonal arrays are optimal for estimating the main effects under the main-effects model. To protect the main effects from the contamination of nonnegligible higher-order interactions, two minimum aberration criteria are developed in Section 3.3, depending on whether or not the main effects of the factors with baseline levels need more protection than those of the other factors. Theoretical constructions are then provided to minimize the leading terms of these criteria. In Section 3.4, we present two algorithms to search for designs that are exactly optimal or nearly optimal under these criteria. All designs with 8, 12, 16 and 20 runs are found and made available online, and selected designs are provided in Section 3.5. All the proofs are relegated to Section 3.6. The chapter is concluded with a discussion in Section 3.7.

3.2 A mixed parametrization and optimality results

Consider a factorial experiment for m two-level factors $F_1, F_2, \ldots, F_m$ in which the two levels are denoted by -1 and $+1$. Let $S = \{1, 2, \ldots, m\}$ collect the indices of these factors. Then for any subset $u \subseteq S$, there corresponds a treatment combination $\boldsymbol{x}_u = (x_{u1}, \ldots, x_{um})$ where $x_{uj} = +1$ if $j \in u$ and $x_{uj} = -1$ otherwise. We use τ_u to represent the treatment mean under the treatment combination $\boldsymbol{x}_u$.

We first review the orthogonal parametrization of factorial effects. For any subset $w = \{j_1, \ldots, j_k\} \subseteq S$, let β_w be the factorial effect involving the k factors $F_{j_1}, \ldots, F_{j_k}$ under the orthogonal parametrization. Then we have

$$\tau_u = \sum_{w \subseteq S} \beta_w \prod_{j \in w} x_{uj} \quad \text{and} \quad \beta_w = \frac{1}{2^m} \sum_{u \subseteq S} \tau_u \prod_{j \in w} x_{uj}. \tag{3.1}$$

Mathematically, the treatment means τ_u's and the factorial effects β_w's are just a linear transformation of each other. However, the β_w's are statistically meaningful because they describe the change in treatment means due to the level changes of factors indexed by w. More concretely, the factorial effect β_w defines a treatment contrast by averaging over all possible level combinations of factors not contained in w. For example, the main effects are given by $\beta_j = (1/2^m) \sum_{u \subseteq S \setminus \{j\}} (\tau_{u \cup \{j\}} - \tau_u)$ for $j = 1, \ldots, m$.

The orthogonal parametrization is well suited for situations where the two levels are symmetrical. For the opposite situations where one of the two levels corresponds to a baseline or default setting, the baseline parametrization may be more appropriate. We suppose the level -1 is the baseline level. For $w \subseteq S$, let θ_w be the factorial effect involving factors indexed by w under the baseline parametrization. Let $z_{uj} = x_{uj} + 1$ for $u \subseteq S$ and $j = 1, \ldots, m$. Then we have

$$\tau_u = \sum_{w \subseteq S} \theta_w \prod_{j \in w} z_{uj} \quad \text{and} \quad \theta_w = \frac{1}{2^{|w|}} \sum_{u \subseteq w} \tau_u \prod_{j \in w} x_{uj}, \tag{3.2}$$

where $|w|$ denotes the cardinality of w. In contrast to β_w's, the θ_w's characterize the factorial effect due to factors in w by fixing all other factors at the baseline level -1. For example, the main effects under the baseline parametrization are $\theta_j = (\tau_j - \tau_\phi)/2$ for $j = 1, \dots, m$.

In the existing work on baseline designs, the two levels ± 1 are converted to 0 and 1 by $z_{uj} = (x_{uj} + 1)/2$. Our slightly different definition transforms ± 1 to 0 and 2, which is to ensure that β_w and θ_w have the same scale and are comparable. This modification gives rise to the extra $1/2^{|w|}$ in the expression of θ_w in (3.2).

We now consider a general situation in which the two levels are asymmetrical for some factors and symmetrical for the others. Without loss of generality, we assume the level -1 is the baseline level for the first m_1 factors $F_1, \dots, F_{m_1}$, and for the remaining $m_2 = m - m_1$ factors $F_{m_1+1}, \dots, F_m$, the two levels are symmetrical. For convenience, we call the first m_1 factors B-factors and the last m_2 factors O-factors. To define a mixed parametrization of factorial effects, we need to introduce some notation. Let $S_1 = \{1, \dots, m_1\}$ and $S_2 = \{m_1 + 1, \dots, m\}$, representing the index sets of B-factors and O-factors, respectively. For $w_1 \subseteq S_1$ and $w_2 \subseteq S_2$, let $\xi_{w_1 \cup w_2}$ be the factorial effect involving factors in $w_1 \cup w_2$ under the mixed parametrization. Then we have

$$\tau_u = \sum_{w_1 \subseteq S_1} \sum_{w_2 \subseteq S_2} \xi_{w_1 \cup w_2} \prod_{j \in w_1} z_{uj} \prod_{j \in w_2} x_{uj} \quad \text{and} \quad \xi_{w_1 \cup w_2} = \frac{1}{2^{|w_1| + m_2}} \sum_{u \subseteq w_1 \cup S_2} \tau_u \prod_{j \in w_1 \cup w_2} x_{uj}, \tag{3.3}$$

where $z_{uj} = x_{uj} + 1$. Clearly, (3.3) reduces to (3.1) if $S_1 = \phi$ and to (3.2) if $S_2 = \phi$. Therefore, our mixed parametrization includes as special cases the orthogonal and baseline parametrizations. The factorial effects under the mixed parametrization inherit features of the two parametrizations introduced above—the parameter $\xi_{w_1 \cup w_2}$ measures the effect of factors in $w_1 \cup w_2$ by averaging over all level combinations of O-factors in $S_2 \setminus w_2$ while fixing the B-factors in $S_1 \setminus w_1$ at the baseline level. For example, the main effects for B-factors are given by $\xi_j = (1/2^{m_2+1}) \sum_{u \subseteq S_2} (\tau_{u \cup \{j\}} - \tau_u)$ for $j = 1, \dots, m_1$, and those for O-factors are defined as $\xi_j = (1/2^{m_2}) \sum_{u \subseteq S_2 \setminus \{j\}} (\tau_{u \cup \{j\}} - \tau_u)$ for $j = m_1 + 1, \dots, m$. The following example illustrates the three parametrizations by a 2^2 factorial.

Example 3.1. *Suppose that $m = 2$ with $m_1 = m_2 = 1$ so the first factor is a B-factor and the second is an O-factor. There are 4 treatment combinations τ_ϕ, τ_1, τ_2 and τ_{12}. Under the three parametrizations discussed above, we obtain that*

$$\beta_\phi = (\tau_\phi + \tau_1 + \tau_2 + \tau_{12})/4, \quad \theta_\phi = \tau_\phi, \quad \xi_\phi = (\tau_\phi + \tau_2)/2;$$
$$\beta_1 = \xi_1 = (-\tau_\phi + \tau_1 - \tau_2 + \tau_{12})/4, \quad \theta_1 = (\tau_1 - \tau_\phi)/2;$$
$$\beta_2 = (-\tau_\phi - \tau_1 + \tau_2 + \tau_{12})/4, \quad \theta_2 = \xi_2 = (\tau_2 - \tau_\phi)/2;$$

and $\beta_{12} = \theta_{12} = \xi_{12} = (\tau_\phi - \tau_1 - \tau_2 + \tau_{12})/4$.

As can be seen from (3.1), (3.2) and (3.3), the factorial effects under the three parametrizations are all linear transformations of the treatment means, and hence must be linearly related to each other. Sun and Tang (2022) established a linear relationship between the orthogonal and baseline parametrizations. Theorem 3.1 further reveals relationships between the mixed parametrization and the other two.

Theorem 3.1. *For any $w_1 \subseteq S_1$ and $w_2 \subseteq S_2$, we have that*

(i) $\xi_{w_1 \cup w_2} = \sum_{v_1 \supseteq w_1} (-1)^{|v_1|-|w_1|} \beta_{v_1 \cup w_2}$ *and* $\beta_{w_1 \cup w_2} = \sum_{v_1 \supseteq w_1} \xi_{v_1 \cup w_2}$*; and*

(ii) $\xi_{w_1 \cup w_2} = \sum_{v_2 \supseteq w_2} \theta_{w_1 \cup v_2}$ *and* $\theta_{w_1 \cup w_2} = \sum_{v_2 \supseteq w_2} (-1)^{|v_2|-|w_2|} \xi_{w_1 \cup v_2}$.

We note that the relationship between orthogonal and baseline parametrizations can be obtained by taking $S_1 = S$ and $S_2 = \phi$ in part (i) of Theorem 3.1. More importantly, one can easily deduce from Theorem 1 the equivalency of the three conditions: (a) $\xi_w = 0$ for all $|w| \geq k$, (b) $\beta_w = 0$ for all $|w| \geq k$, and (c) $\theta_w = 0$ for all $|w| \geq k$, for any given positive integer k. This leads to the following result.

Corollary 3.1. *The factorial effects involving k or more factors are negligible under any one parametrization implies the same under the other two parametrizations. In particular, if all interactions are negligible under one parametrization, they must be negligible under the two parametrizations, in which case we have that $\xi_j = \beta_j = \theta_j$ for $j = 1, \ldots, m$.*

Now let's focus on the estimation of main effects ξ_j's under the mixed parametrization, using a design $\mathbf{D} = (d_{ij})$ of N runs for m factors. Let $\mathbf{X}_1$ be an $N \times m$ matrix with its (i, j)th element equal to $(d_{ij}+1)$ if $j \le m_1$ and d_{ij} otherwise. Consider the following main-effects model

$$\mathbf{Y} = \mathbf{1}_N \xi_\phi + \mathbf{X}_1 \boldsymbol{\xi}_1 + \boldsymbol{\epsilon}, \tag{3.4}$$

where $\mathbf{Y} = (Y_1, \ldots, Y_N)^T$ is the vector of responses, $\mathbf{1}_N$ is a column of N ones, $\boldsymbol{\xi}_1 = (\xi_1, \ldots, \xi_m)^T$ and $\boldsymbol{\epsilon}$ is the vector of uncorrelated random errors that have a zero mean and a constant variance σ^2. The results of Corollary 3.1 imply that such a model is equivalent to a main-effects model under the orthogonal parametrization. Also note that $\xi_j = \beta_j$ for $j = 1, \ldots, m$. Then the following results follow directly from the optimality results under the orthogonal parametrization, and are parallel to Propositions 1 and 2 of Mukerjee and Tang (2012). Recall that $\mathbf{D}$ is an orthogonal array of strength t if any t columns of $\mathbf{D}$ contain all possible level combinations of -1 and $+1$ the same number of times; we denote such an array by $\mathrm{OA}(N, 2^m, t)$.

Corollary 3.2. *With reference to the model* (3.4)*, we have that*

(i) the best linear unbiased estimator $\hat{\xi}_j$ of ξ_j satisfies $\mathrm{var}(\hat{\xi}_j) \ge \sigma^2/N$ for $j = 1, \ldots, m$, where the equality holds if and only if $\mathbf{D}$ is an OA$(N, 2^m, 2)$; and

(ii) design $\mathbf{D}$ is universally optimal for estimating $\boldsymbol{\xi}_1$ if $\mathbf{D}$ is an OA$(N, 2^m, 2)$.

3.3 Two minimum aberration criteria

Corollary 3.2 shows that under the model (3.4) which ignores interactions, an orthogonal array is optimal for estimating the main effects $\boldsymbol{\xi}_1$ in a very broad sense. The best linear unbiased estimator for $(\xi_\phi, \boldsymbol{\xi}_1^T)^T$ is given by $(\hat{\xi}_\phi, \hat{\boldsymbol{\xi}}_1^T)^T = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$, where $\mathbf{X} = (\mathbf{1}_N, \mathbf{X}_1)$. However, this estimator is actually biased if interactions are not negligible. Suppose the true model is the full model

$$\mathbf{Y} = \mathbf{1}_N \xi_\phi + \mathbf{X}_1 \boldsymbol{\xi}_1 + \mathbf{X}_2 \boldsymbol{\xi}_2 + \cdots + \mathbf{X}_m \boldsymbol{\xi}_m + \boldsymbol{\epsilon},$$

where $\boldsymbol{\xi}_k$ collects all k-factor interactions ξ_w's with $|w| = k$, and $\mathbf{X}_k$ is the corresponding model matrix for $k = 1, \ldots, m$. Then the bias in the estimator $(\hat{\xi}_\phi, \hat{\boldsymbol{\xi}}_1^T)^T$ is given by

$$E\left[(\hat{\xi}_\phi, \hat{\boldsymbol{\xi}}_1^T)^T\right] - (\xi_\phi, \boldsymbol{\xi}_1^T)^T = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_2\boldsymbol{\xi}_2 + \cdots + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_m\boldsymbol{\xi}_m. \tag{3.5}$$

In this section, we concentrate on selecting an orthogonal array that minimizes the contamination of the potentially active interactions on the estimation of main effects. Two minimum aberration criteria are proposed to implement the idea, depending on whether or not the main effects of the B-factors need more protection than those of the O-factors.

3.3.1 Main effects of B-factors are more important

Under the mixed parametrization, there are two sets of main effects, one for the B-factors and the other for the O-factors. In practice, the two sets of main effects may not be of equal interest and thus ought to be treated differently. In this subsection, we consider the situation that the main effects of the B-factors are more important than those of the O-factors, and therefore need more protection from contamination by nonnegligible interactions. This is reasonable because the B-factors may well be those that have current default settings and the O-factors are some additional factors the investigator want to study. Default settings need to be protected; so do the B-factors that have default settings.

From the bias expression (3.5), one can see that for $k = 2, \ldots, m$, the k-factor interactions $\boldsymbol{\xi}_k$ contribute a bias term of $\mathbf{B}_k\boldsymbol{\xi}_k$ to the estimation of main effects for B-factors, where $\mathbf{B}_k$ collects the rows $2, \ldots, m_1 + 1$ of the matrix $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_k$. Similarly, the bias caused by $\boldsymbol{\xi}_k$ on the estimation of main effects for O-factors is $\mathbf{O}_k\boldsymbol{\xi}_k$, where $\mathbf{O}_k$ collects the last m_2 rows of the matrix $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_k$. If all components of $\boldsymbol{\xi}_k$ are equally likely to be active with the same scale, then $\pi_k^B = \mathrm{tr}(\mathbf{B}_k^T\mathbf{B}_k)$ and $\pi_k^O = \mathrm{tr}(\mathbf{O}_k^T\mathbf{O}_k)$ provide reasonable measures of the amount of bias from $\boldsymbol{\xi}_k$ on main-effects estimation for B-factors and O-factors, respectively.

Under the assumption that the main effects of B-factors are more important, it is a priority to protect these main effects from the contamination of interaction terms. On the other hand, the effect hierarchy principle says that lower-order interactions are more likely to be active than the higher-order ones. Therefore, when only two-factor interactions are present, an orthogonal array that sequentially minimizes π_2^B and π_2^O is desirable. If, in addition, there are nonnegligible three-factor interactions, we then proceed to minimize π_3^B and π_3^O. Continuing this line of arguments, we obtain the following minimum π_B-aberration criterion for design selection.

Definition 3.1. *An orthogonal array for m factors is said to have minimum π_B-aberration if it sequentially minimizes $\pi_2^B, \pi_2^O, \pi_3^B, \pi_3^O, \ldots, \pi_m^B, \pi_m^O$.*

The idea of minimum π_B-aberration criterion is similar in spirit to those of the minimum G_2-aberration under the orthogonal parametrization (Tang and Deng, 1999) and the minimum K-aberration under the baseline parametrization (Mukerjee and Tang, 2012). To find a minimum aberration design is challenging, and our problem is further complicated by the presence of two types of factors. Nevertheless, good designs can still be obtained theoretically by concentrating on the leading terms in the criterion of minimum π_B-aberration.

Given k vectors $a_1, \ldots, a_k$ where $a_j = (a_{1j}, \ldots, a_{Nj})$ for $j = 1, \ldots, k$, the J-characteristic of these vectors is defined as $J(a_1, \ldots, a_k) = \sum_{i=1}^N \prod_{j=1}^k a_{ij}$ (Tang, 2001). The next result expresses π_2^B and π_2^O in terms of the J-characteristics of columns of a design.

Lemma 3.1. *Suppose that $\mathbf{D} = (b_1, \ldots, b_{m_1}, o_1, \ldots, o_{m_2})$ is an orthogonal array of N runs for m_1 B-factors and m_2 O-factors. Then we have that*

$$\pi_2^B = \frac{3}{N^2} \sum_{i<j<k} J^2(b_i, b_j, b_k) + \frac{2}{N^2} \sum_{i<j} \sum_{k} J^2(b_i, b_j, o_k) + \frac{1}{N^2} \sum_{i} \sum_{j<k} J^2(b_i, o_j, o_k) + m_1(m_1 - 1)$$

and

$$\pi_2^O = \frac{1}{N^2} \sum_{i<j} \sum_{k} J^2(b_i, b_j, o_k) + \frac{2}{N^2} \sum_{i} \sum_{j<k} J^2(b_i, o_j, o_k) + \frac{3}{N^2} \sum_{i<j<k} J^2(o_i, o_j, o_k) + m_1 m_2.$$

The J-characteristics are 0 for any three columns of an $\mathrm{OA}(N, 2^m, 3)$, which exists whenever $m \leq N/2$ and a Hadamard matrix of order $N/2$ exists (Cheng, 2014). By Lemma 3.1, such a design minimizes the bias from two-factor interactions in estimating main effects of B-factors and O-factors. Another implication of Lemma 3.1 is that switching signs of columns of a design does not affect the values of π_2^B and π_2^O.

For $m > N/2$, we use regular designs to minimize π_2^B and π_2^O. Let the columns of $\mathbf{D}$ be selected from a saturated regular design $\mathrm{OA}(2^h, 2^{2^h-1}, 2)$ for some integer h. Such an $\mathrm{OA}(2^h, 2^{2^h-1}, 2)$ can be constructed by first writing down h independent columns that form a full factorial and then adding all possible Hadamard products thereof. We assume that the columns of a regular $\mathrm{OA}(2^h, 2^{2^h-1}, 2)$ are arranged in Yates order. For example, the 15 columns of an $\mathrm{OA}(2^4, 2^{15}, 2)$ are given by

$$(\mathbf{1}, \mathbf{2}, \mathbf{12}, \mathbf{3}, \mathbf{13}, \mathbf{23}, \mathbf{123}, \mathbf{4}, \mathbf{14}, \mathbf{24}, \mathbf{124}, \mathbf{34}, \mathbf{134}, \mathbf{234}, \mathbf{1234})$$

where $\mathbf{1}$, $\mathbf{2}$, $\mathbf{3}$ and $\mathbf{4}$ are independent columns. For experiments involving only O-factors, Chen and Hedayat (1996) showed that a design obtained by taking the last m columns of a regular $\mathrm{OA}(2^h, 2^{2^h-1}, 2)$ minimizes π_2^O among all regular designs. Inspired by their construction, we establish Theorem 3.2.

Theorem 3.2. *Suppose $\mathbf{S}$ is a regular OA$(2^h, 2^{2^h-1}, 2)$. Let $\mathbf{D}_B$ select the last m_1 columns of $\mathbf{S}$ and $\mathbf{D}_O$ select the remaining m_2 columns from the last $m = m_1 + m_2$ columns of $\mathbf{S}$ that are not already in $\mathbf{D}_B$. Then we have the following results for the design $\mathbf{D} = (\mathbf{D}_B, \mathbf{D}_O)$.*

(i) If m_1 and m satisfy that $m_1 \leq 2^h - 2^{h_1}$ and $m \geq 2^h - 2^{h_1}$ for some integer h_1, then design $\mathbf{D}$ minimizes π_2^B over all OA$(2^h, 2^m, 2)$s and sequentially minimizes π_2^B and π_2^O over all regular OA$(2^h, 2^m, 2)$s.

(ii) If m satisfies that $m = 2^h - 2^{h_1}$ for some integer h_1, then $\mathbf{D}$ sequentially minimizes π_2^B and π_2^O over all OA$(2^h, 2^m, 2)$s.

It is worth remarking that although the constructed design $\mathbf{D}$ in Theorem 3.2 is regular, its optimality properties are established in the whole class of orthogonal arrays in two of the three optimality statements. Specifically, design $\mathbf{D}$ minimizes π_2^B over all $\mathrm{OA}(2^h, 2^m, 2)$s in part (i) of Theorem 3.2, and sequentially minimizes π_2^B and π_2^O over all $\mathrm{OA}(2^h, 2^m, 2)$s in part (ii) of Theorem 3.2.

The restriction on m_1 and m values in part (i) of Theorem 3.2 is fairly mild. Because $m > N/2 = 2^{h-1}$, we see that the condition is always satisfied so long as $m_1 \leq 2^{h-1}$. Example 3.2 further illustrates Theorem 3.2 with a case for $m_1 > 2^{h-1}$.

Example 3.2. *Suppose we would like to study* $m_1 = 18$ *B-factors and* $m_2 = 7$ *O-factors with* $2^5 = 32$ *runs. Then for* $h_1 = 3$*, we have that* $m_1 \leq 32 - 2^{h_1}$ *and* $m \geq 32 - 2^{h_1}$*. Let* $\mathbf{D}_B = (\mathbf{234}, \mathbf{1234}, \mathbf{5}, \ldots, \mathbf{12345})$ *and* $\mathbf{D}_O = (\mathbf{123}, \mathbf{4}, \mathbf{14}, \mathbf{24}, \mathbf{124}, \mathbf{34}, \mathbf{134})$*. By Theorem 3.2, the design* $\mathbf{D} = (\mathbf{D}_B, \mathbf{D}_O)$ *minimizes* π_2^B *over all* $OA(32, 2^{25}, 2)s$ *and sequentially minimizes* π_2^B *and* π_2^O *over all regular* $OA(32, 2^{25}, 2)s$*.*

Remark 3.1. *As careful readers may observe, the results of Theorem 3.2 hold no matter whether baseline or orthogonal parametrization is used for each factor of the design* $\mathbf{D}$*. As long as the main effects are divided into two groups and more protection from two-factor interactions is needed for one of the two groups, the results of Theorem 3.2 are applicable. The existence of two types of factors provides a natural application scenario for these results.*

3.3.2 Main effects of all factors are equally important

If the main effects of the B-factors and the O-factors are of equal interest, then, naturally, one wishes to minimize $\pi_k = \pi_k^B + \pi_k^O$ for $k = 2, \ldots, m$, as π_k measures the contamination of k-factor interactions on the estimation of all main effects. Combined with the effect hierarchy principle, the idea can be formulated as the following minimum π-aberration criterion.

Definition 3.2. *An orthogonal array for* m *factors is said to have minimum* π*-aberration if it sequentially minimizes* $\pi_2, \pi_3, \ldots, \pi_m$*.*

Lemma 3.1 indicates that for a design $\mathbf{D} = (d_1, \ldots, d_m)$ of N runs for m factors, we have $\pi_2 = 3A_3 + m_1(m-1)$ where $A_3 = \sum_{i<j<k} J^2(d_i, d_j, d_k)/N^2$ is the leading term in the minimum G_2-aberration criterion. However, for $\pi_3, \pi_4, \ldots, \pi_m$, such a simple connection with the minimum G_2-aberration criterion no longer exists. The expressions of $\pi_3, \pi_4, \ldots, \pi_m$ become more complex as sign-switching columns of $\mathbf{D}$ may affect their values.

In the following, we focus on sequential minimization of π_2 and π_3 through the use of regular designs. Consider a regular design $\mathbf{D}$ of 2^h runs for a total of $m = 2^h - 2^{h_1}$ factors where h_1 and h are integers. Chen and Hedayat (1996) and Tang and Wu (1996) proved that A_3, and thus π_2, are minimized if and only if columns of $\mathbf{D}$ are isomorphic to the last m columns of a saturated regular design. We show that π_3 of such a design $\mathbf{D}$ is determined by the J-characteristics of the B-factors alone.

Lemma 3.2. *Suppose that* $\mathbf{D} = (b_1, \ldots, b_{m_1}, o_1, \ldots, o_{m_2})$ *is a regular* $OA(2^h, 2^m, 2)$ *that minimizes* π_2*, where* $m = 2^h - 2^{h_1}$ *for some integer* h_1*. Then we have that* $\pi_3 = c_1 \sum_{i<j<k} J(b_i, b_j, b_k) + c_0$*, where* c_0 *and* $c_1 > 0$ *are constants.*

Lemma 3.2 enables us to decide which columns should be assigned to the B-factors and how to switch their signs to minimize π_3. Note that among the last $m = 2^h - 2^{h_1}$ columns of a regular OA$(2^h, 2^{2^h-1}, 2)$, there are $h - h_1$ independent columns $(\boldsymbol{h}_1 + \mathbf{1}), \ldots, \boldsymbol{h}$. Let's arrange these $h - h_1$ columns and all their possible Hadamard products in Yates order. Then let $\mathbf{D}_B$ collect the first m_1 columns with their signs all switched, where $m_1 \leq 2^{h-h_1} - 1$. Let $\mathbf{D}_O$ include the remaining $m - m_1$ columns in the last m columns of the regular OA$(2^h, 2^{2^h-1}, 2)$. Finally, let $\mathbf{D} = (\mathbf{D}_B, \mathbf{D}_O)$. We have the following result for this design $\mathbf{D}$.

Theorem 3.3. *The design* $\mathbf{D}$ *sequentially minimizes* π_2 *and* π_3 *over all regular designs.*

The design $\mathbf{D}$ in Theorem 3.3 can be constructed as long as the total number m of factors satisfies $m = 2^h - 2^{h_1}$ for some integer h_1 and the number m_1 of B-factors satisfies $m_1 \leq 2^{h-h_1} - 1$. In the saturated case of $m = 2^h - 1$, such a design is obtainable for any choice of m_1 and m_2. In particular, if $m_1 = m = 2^h - 1$, then we have $\mathbf{D} = (-\mathbf{1}, -\mathbf{2}, -\mathbf{12}, -\mathbf{3}, -\mathbf{13}, \ldots, -\mathbf{123}\cdots\boldsymbol{h})$ which must have a row of -1's. Mukerjee and Tang (2012) showed that a saturated orthogonal array has minimum aberration under the baseline parametrization if it contains a run of all baseline levels. Therefore our result is consistent with theirs in this special case.

We illustrate Theorem 3.3 with an example.

Example 3.3. *Suppose 64 experiments are allowed to examine the main effects of* $m_1 = 6$ *B-factors and* $m_2 = 50$ *O-factors. Let* $\mathbf{D}_B = (-\mathbf{4}, -\mathbf{5}, -\mathbf{45}, -\mathbf{6}, -\mathbf{46}, -\mathbf{56})$ *and* $\mathbf{D}_O = (\mathbf{456}, \mathbf{14}, \ldots, \mathbf{123456})$ *which consists of all columns that do not occur in* $\mathbf{D}_B$ *but do occur* *in the last 56 columns of the regular $OA(64, 2^{63}, 2)$. According to Theorem 3.3, the design $\mathbf{D} = (\mathbf{D}_B, \mathbf{D}_O)$ sequentially minimizes π_2 and π_3 over all regular $OA(64, 2^{56}, 2)$s.*

Theorems 3.2 and 3.3 provide two theoretical constructions for minimum π_B- and π-aberration designs. These methods have some restrictions on the run size as well as the numbers of B-factors and O-factors. In the next section, we develop efficient algorithms to search for minimum π_B- and π-aberration designs for general cases.

3.4 Searching designs by algorithms

3.4.1 A complete search algorithm

Two orthogonal arrays are combinatorially isomorphic if one can be obtained from the other by permuting rows, permuting columns, switching signs of columns, or a combination of these operations (Hedayat et al., 1999). All orthogonal arrays can be generated by applying these operations to a complete set of non-isomorphic orthogonal arrays. Complete sets of non-isomorphic orthogonal arrays are available for small run sizes (Sun et al., 2008; Schoen et al., 2010), which allows us to find minimum π_B- and π-aberration designs over all orthogonal arrays.

When using an $\mathrm{OA}(N, 2^m, 2)$ as a design for m_1 B-factors and m_2 O-factors, there is no need to inspect all isomorphic operations, as many of them lead to designs with the same π_B- or π-aberration. Clearly, permuting rows, permuting the first m_1 columns and permuting the last m_2 columns won't affect the π_B- or π-aberration. In addition, we have the following results on sign-switching columns.

Lemma 3.3. *Switching the signs of O-factors in an $OA(N, 2^m, 2)$ does not change π_k^B, π_k^O and thus π_k values for $k = 2, \ldots, m$.*

Based on the above, we propose the following complete search algorithm for minimum aberration designs. The algorithm used by Mukerjee and Tang (2012) for the baseline parametrization can be seen as a special case where all factors are B-factors.

Step I: Obtain a complete list of non-isomorphic $\mathrm{OA}(N, 2^m, 2)$s.

Step II: For each array in the list, select m_1 columns for B-factors. The remaining m_2 columns are used for O-factors.

Step III: For every choice of B-factors and O-factors in Step II, switch signs of the m_1 columns of the B-factors in all possible ways. Calculate the π_k^B, π_k^O and π_k values for this design.

Note that for the minimum π-aberration criterion, only those OA$(N, 2^m, 2)$s with minimum π_2 values need to be considered in Step I. We apply this complete search algorithm to obtain minimum π_B- and π-aberration designs of $N = 8$, 12 and 16 runs for all choices of m_1 and m_2, the numbers of B-factors and O-factors. For $N = 20$ runs, the complete search is done for $m \leq 13$. All the obtained designs are available online at `https://github.com/gz-chen/Mixed-Param`.

Suppose there are $q(N, m)$ non-isomorphic OA$(N, 2^m, 2)$s to be considered in Step I. Then the total number of designs to be compared in a complete search is $q(N, m)\binom{m}{m_1}2^{m_1}$, which, as N, m and m_1 increases, soon becomes too large for computer to handle, not to mention that the computation of J-characteristics also grows rapidly and that complete sets of non-isomorphic orthogonal arrays are no longer available for large designs. Therefore, it is necessary to come up with an efficient algorithm for the cases where the complete search is impossible.

3.4.2 An algorithm based on minimum G_2-aberration designs

The aim of this subsection is to conduct an algorithmic search for large designs that perform well under the minimum π_B- or π-aberration criterion. To achieve this, several measures are taken to reduce the computation. The first is to focus on orthogonal arrays with minimum G_2-aberrations instead of all non-isomorphic ones in Step I of the complete search algorithm.

An OA$(N, 2^m, 2)$, say $\mathbf{D} = (d_1, \ldots, d_m)$, is said to have minimum G_2-aberration if it sequentially minimizes $A_3, A_4, \ldots, A_m$, where $A_k = \sum_{j_1<\cdots<j_k} J^2(d_{j_1}, \ldots, d_{j_k})/N^2$ for $k = 3, \ldots, m$. As mentioned in Section 3.3.2, a minimum G_2-aberration design minimizes π_2 in the minimum π-aberration criterion. The next result shows that such a design is also

promising in sequentially minimizing higher-order terms π_k for $k = 3, \ldots, m$ and entries in the minimum π_B-aberration criterion.

Theorem 3.4. *Suppose the B-factors of a design are generated by randomly selecting and sign-switching m_1 columns of an $OA(N, 2^m, 2)$ and the O-factors are given by the remaining columns. Let $\bar{\pi}_k$ be the average of π_k's over all possible designs generated in this way. Then, for $k = 2, \ldots, m$, we have*

$$\bar{\pi}_k = c_{k+1}^{(k)} A_{k+1} + c_k^{(k)} A_k + \cdots + c_3^{(k)} A_3 + c_0^{(k)},$$

where $c_0^{(k)}, c_3^{(k)}, \ldots, c_{k+1}^{(k)}$ are positive constants, $A_3, \ldots, A_m$ are determined by the $OA(N, 2^m, 2)$ and we define $A_{m+1} = 0$. Similar results also hold for π_k^B and π_k^O.

Theorem 3.4 provides a rationale for the use of minimum G_2-aberration designs in Step I of the complete search algorithm. Related to Theorem 3.4 is a result of Xiao and Xu (2018) who justified the use of generalized minimized aberration designs in generating space-filling designs.

Next, we improve the efficiency of Steps II and III of the complete search algorithm through a local search algorithm (Aarts and Lenstra, 2003). The idea is to iteratively replace a current design with the best one in a small neighbourhood of the current design, until no further improvement can be made. A full description of our algorithm for minimum π-aberration designs is given below.

Step I: Obtain a minimum G_2-aberration design from a list of OA$(N, 2^m, 2)$s. Randomly permute and sign-switch its columns. Denote this design by $\mathbf{D} = (b_1, \ldots, b_{m_1}, o_1 \ldots, o_{m_2})$ and calculate $\boldsymbol{\pi} = (\pi_2, \ldots, \pi_m)$ for $\mathbf{D}$.

Step II: Exchange a column b_j ($j = 1, \ldots, m_1$) and a column $\pm o_k$ ($k = 1, \ldots, m_2$). Among all $2m_1m_2$ designs generated this way, continue to the next step if none of them improves $\boldsymbol{\pi}$; otherwise select one with the least π-aberration, denote it by $\mathbf{D}$ and update $\boldsymbol{\pi}$. Then repeat this step.

Step III: Exchange a column pair (b_{j_1}, b_{j_2}) $(1 \leq j_1 < j_2 \leq m_1)$ and a column pair $(\pm o_{k_1}, \pm o_{k_2})$ $(1 \leq k_1 < k_2 \leq m_2)$. Among all $4\binom{m_1}{2}\binom{m_2}{2}$ designs generated this way, continue to the next step if none of them improves $\boldsymbol{\pi}$; otherwise select one with the least π-aberration, denote it by $\mathbf{D}$ and update $\boldsymbol{\pi}$. Then go back to Step II.

Step IV: Replace a column b_j by $-b_j$ $(j = 1, \ldots, m_1)$. Among all m_1 designs generated this way, continue to the next step if none of them improves $\boldsymbol{\pi}$; otherwise select one with the least π-aberration, denote it by $\mathbf{D}$ and update $\boldsymbol{\pi}$. Then repeat this step.

Step V: Replace a column pair (b_{j_1}, b_{j_2}) by $(-b_{j_1}, -b_{j_2})$ $(1 \leq j_1 < j_2 \leq m_1)$. Among all $\binom{m_1}{2}$ designs generated this way, continue to the next step if none of them improves $\boldsymbol{\pi}$; otherwise select one with the least π-aberration, denote it by $\mathbf{D}$ and update $\boldsymbol{\pi}$. Then go back to Step IV.

Step VI: Output the design $\mathbf{D}$ and the associated vector $\boldsymbol{\pi} = (\pi_2, \ldots, \pi_m)$.

The algorithm above generalizes that for the baseline parametrization presented in Li et al. (2014). One can replace the vector $\boldsymbol{\pi} = (\pi_2, \ldots, \pi_m)$ in the algorithm by $\boldsymbol{\pi} = (\pi_2^B, \pi_2^O, \ldots, \pi_m^B, \pi_m^O)$ if a minimum π_B-aberration design is the goal. If there is more than one minimum G_2-aberration design in Step I, then we can apply the algorithm to all those designs and then find the best output design.

To evaluate the performance of our algorithm, we apply it to 20-run designs for 13 factors. There are 730 non-isomorphic $\mathrm{OA}(20, 2^{13}, 2)$s in total, where 5 of them minimize A_3 (and equivalently, π_2) and 3 of them have the minimum G_2-aberration. Therefore in a complete search, we search 730 orthogonal arrays for minimum π_B-aberration designs and 5 orthogonal arrays for minimum π-aberration designs, whereas in the incomplete search we focus on the 3 minimum G_2-aberration designs. For each case of the number of B-factors $m_1 = 1, \ldots, 13$, we run the incomplete search algorithm 200 times for minimum π_B- and π-aberration designs separately and compare the results with those obtained from the complete search.

Under the minimum π_B-aberration criterion, we are surprised to find that all the designs obtained by the incomplete search algorithm sequentially minimize the leading terms π_2^B

and π_2^O among all orthogonal arrays. So we move on to the next term and compare the 200 π_3^B values in the incomplete search with all the π_3^B values of orthogonal arrays that have sequentially minimized π_2^B and π_2^O. For each $m_1 = 1, \ldots, 13$, the distributions of these two sets of π_3^B values can be described by two boxplots, as shown in the left panel of Figure 3.1. It can be seen that the π_3^B values from the incomplete search are all centered near the minimum π_3^B values from the complete search. A closer examination can be done by calculating the proportion of designs in the complete search that are no better than the worst design by the incomplete search algorithm. As displayed in the second and fifth rows of Table 3.1, some of these proportions are 100%, implying the 200 incomplete searches always find the design with minimum π_3^B value, and other proportions are close to 100%, showing that the even the worst design found by the incomplete search algorithm has good performance in terms of π_3^B value. Similar observations on π_3 values can also be made from the searching results for minimum π-aberration designs, as presented in the right panel of Figure 3.1 and the third and sixth rows of Table 3.1.

These empirical results demonstrate that our incomplete search algorithm can be used to obtain designs that perform well under the minimum π_B- or π-aberration criterion. We

Figure 3.1: The π_3^B and π_3 values obtained by 200 incomplete searches and the complete search. For each $m_1 = 1, \ldots, 13$, the left and right boxplots show the values from the complete and incomplete searches, respectively.

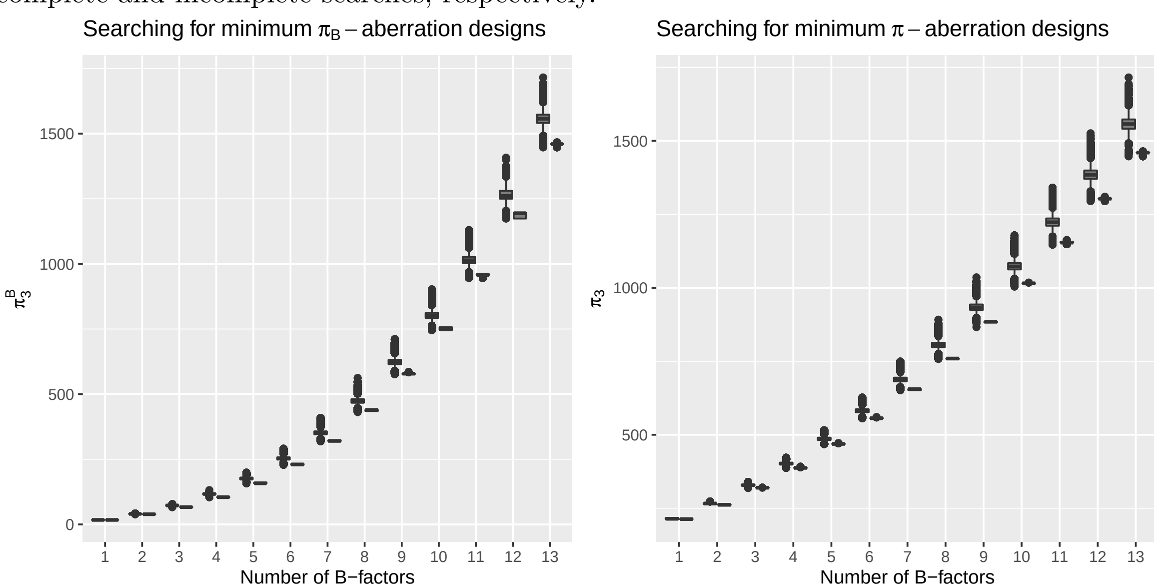


Table 3.1: Proportions of $\text{OA}(20, 2^{13}, 2)$s that are no better than the worst design found by the incomplete search algorithm.

m_1	1	2	3	4	5	6	7
π_3^B	100%	99.697%	100%	100%	99.989%	99.934%	99.967%
π_3	98.462%	98.462%	99.528%	99.633%	99.863%	99.930%	99.981%
m_1	8	9	10	11	12	13	
π_3^B	99.953%	99.919%	99.828%	99.738%	99.775%	99.824%	
π_3	99.996%	99.994%	99.984%	99.859%	99.862%	99.864%	

Table 3.2: Two saturated designs of 8 and 12 runs.

1	2	3	4	5	6	7
−	−	−	−	−	−	−
+	−	+	−	+	−	+
−	+	+	−	−	+	+
+	+	−	−	+	+	−
−	−	−	+	+	+	+
+	−	+	+	−	+	−
−	+	+	+	+	−	−
+	+	−	+	−	−	+

1	2	3	4	5	6	7	8	9	10	11
−	−	−	−	−	−	−	−	−	−	−
+	−	+	−	−	−	+	+	+	−	+
+	+	−	+	−	−	−	+	+	+	−
−	+	+	−	+	−	−	−	+	+	+
+	−	+	+	−	+	−	−	−	+	+
+	+	−	+	+	−	+	−	−	−	+
+	+	+	−	+	+	−	+	−	−	−
−	+	+	+	−	+	+	−	+	−	−
−	−	+	+	+	−	+	+	−	+	−
−	−	−	+	+	+	−	+	+	−	+
+	−	−	−	+	+	+	−	+	+	−
−	+	−	−	−	+	+	+	−	+	+

apply this algorithm to 20-run designs with more than 13 factors under the both criteria. All findings are available at `https://github.com/gz-chen/Mixed-Param`.

3.5 Some selected designs

We present minimum π_B- and π-aberration designs of 8 and 12 runs in Tables 3.3, 3.4 and 3.5. All these designs are generated by selecting and sign-switching columns of the two saturated designs displayed in Table 3.2.

3.6 Proofs

Proof of Theorem 3.1. The proof is similar to that of Theorem 1 in Sun and Tang (2022). Let $\boldsymbol{\tau}$, $\boldsymbol{\theta}$, $\boldsymbol{\beta}$ and $\boldsymbol{\xi}$ collect all τ_u's, θ_w's, β_w's and ξ_w's in Yates order. Define $\mathbf{L}_m = \otimes_{k=1}^{m}\mathbf{L}$

Table 3.3: Minimum π_B and π-aberration designs of 8 runs.

m	m_1	m_2	Columns of $\mathbf{D}_B$	Columns of $\mathbf{D}_O$	$(\pi_2^B, \pi_2^O, \pi_3^B, \pi_3^O)$	Criterion
3	1	2	-1	$(2, 4)$	$(0, 2, 0, 0)$	π_B, π
3	2	1	$(-1, -2)$	4	$(2, 2, 0, 1)$	π_B, π
4	1	3	-1	$(2, 4, 7)$	$(0, 3, 1, 3)$	π_B, π
4	2	2	$(-1, -2)$	$(4, 7)$	$(2, 4, 2, 4)$	π_B, π
4	3	1	$(-1, -2, -4)$	7	$(6, 3, 6, 4)$	π_B, π
5	1	4	-2	$(1, 3, 4, 5)$	$(1, 9, 2, 6)$	π_B
5	1	4	-1	$(2, 3, 4, 5)$	$(2, 8, 2, 4)$	π
5	2	3	$(-2, -3)$	$(1, 4, 5)$	$(4, 10, 4, 11)$	π_B
5	2	3	$(-1, -2)$	$(3, 4, 5)$	$(5, 9, 5, 8)$	π
5	3	2	$(-2, -3, -4)$	$(1, 5)$	$(9, 9, 13, 12)$	π_B
5	3	2	$(1, -2, -3)$	$(4, 5)$	$(10, 8, 5, 12)$	π
5	4	1	$(2, -3, -4, -5)$	1	$(16, 6, 28, 10)$	π_B
5	4	1	$(1, -2, -3, -4)$	5	$(17, 5, 21, 9)$	π
6	1	5	-1	$(2, 3, 4, 5, 6)$	$(2, 15, 4, 16)$	π_B, π
6	2	4	$(-1, -2)$	$(3, 4, 5, 6)$	$(6, 16, 10, 22)$	π_B
6	2	4	$(-1, -6)$	$(2, 3, 4, 5)$	$(6, 16, 12, 20)$	π
6	3	3	$(1, -2, -3)$	$(4, 5, 6)$	$(12, 15, 15, 27)$	π_B, π
6	4	2	$(1, -2, -3, -4)$	$(5, 6)$	$(20, 12, 36, 26)$	π_B, π
6	5	1	$(1, -2, -3, -4, -5)$	6	$(30, 7, 62, 18)$	π_B, π
7	1	6	-1	$(2, 3, 4, 5, 6, 7)$	$(3, 24, 7, 36)$	π_B, π
7	2	5	$(-1, -2)$	$(3, 4, 5, 6, 7)$	$(8, 25, 18, 45)$	π_B, π
7	3	4	$(1, -2, -3)$	$(4, 5, 6, 7)$	$(15, 24, 30, 52)$	π_B, π
7	4	3	$(1, -2, -3, -4)$	$(5, 6, 7)$	$(24, 21, 58, 54)$	π_B, π
7	5	2	$(1, -2, -3, -4, -5)$	$(6, 7)$	$(35, 16, 93, 48)$	π_B, π
7	6	1	$(1, 2, 3, -4, -5, -6)$	7	$(48, 9, 138, 31)$	π_B, π

Table 3.4: Minimum π_B and π-aberration designs of 12 runs for $m = 3, \ldots, 8$ factors.

m	m_1	m_2	Columns of $\mathbf{D}_B$	Columns of $\mathbf{D}_O$	$(\pi_2^B, \pi_2^O, \pi_3^B, \pi_3^O)$	Criterion
3	1	2	-1	$(2, 3)$	$(0.11, 2.22, 0.11, 0)$	π_B, π
3	2	1	$(-1, -2)$	3	$(2.22, 2.11, 0.22, 1)$	π_B, π
4	1	3	-1	$(2, 3, 4)$	$(0.33, 4, 0.44, 0)$	π_B, π
4	2	2	$(-1, -2)$	$(3, 4)$	$(2.67, 4.67, 0.67, 2.22)$	π_B, π
4	3	1	$(-1, -2, 3)$	4	$(7, 3.33, 2.33, 3.44)$	π_B, π
5	1	4	-1	$(2, 3, 4, 6)$	$(0.67, 6.67, 1.11, 0.44)$	π_B, π
5	2	3	$(-1, -2)$	$(3, 4, 6)$	$(3.33, 8, 1.56, 3.67)$	π_B
5	2	3	$(-1, -2)$	$(3, 4, 6)$	$(3.33, 8, 1.56, 3.67)$	π
5	3	2	$(-1, -2, 3)$	$(4, 6)$	$(8, 7.33, 3.67, 7.56)$	π_B, π
5	4	1	$(-1, -2, 3, -4)$	6	$(14.67, 4.67, 9.78, 7.78)$	π_B, π
6	1	5	-1	$(2, 3, 4, 5, 6)$	$(1.11, 10.56, 2.22, 7.56)$	π_B, π
6	2	4	$(-1, -2)$	$(3, 4, 5, 6)$	$(4.22, 12.44, 4.89, 12.89)$	π_B, π
6	3	3	$(-1, -2, 3)$	$(4, 5, 6)$	$(9.33, 12.33, 10.11, 18.56)$	π_B
6	3	3	$(1, -2, -3)$	$(4, 5, 10)$	$(9.33, 12.33, 11, 16.33)$	π
6	4	2	$(-1, -2, 3, -4)$	$(5, 6)$	$(16.44, 10.22, 20, 20.44)$	π_B, π
6	5	1	$(-1, -2, 3, -4, 6)$	5	$(25.56, 6.11, 36.67, 14.44)$	π_B, π
7	1	6	-2	$(1, 3, 4, 5, 6, 7)$	$(1.67, 16, 3.89, 17.33)$	π_B, π
7	2	5	$(-1, 3)$	$(2, 4, 5, 6, 7)$	$(5.33, 18.33, 9.11, 29)$	π_B
7	2	5	$(-1, -2)$	$(3, 4, 5, 6, 7)$	$(5.33, 18.33, 9.56, 25)$	π
7	3	4	$(1, -2, -3)$	$(4, 5, 6, 7)$	$(11, 18.67, 18.44, 33.33)$	π_B
7	3	4	$(-1, -3, 5)$	$(2, 4, 6, 7)$	$(11, 18.67, 19.33, 31.56)$	π
7	4	3	$(-1, 3, -4, 6)$	$(2, 5, 7)$	$(18.67, 17, 32.89, 43.33)$	π_B
7	4	3	$(1, 3, 4, 5)$	$(2, 6, 7)$	$(18.67, 17, 33.78, 37.11)$	π
7	5	2	$(-1, -2, 3, -4, 6)$	$(5, 7)$	$(28.33, 13.33, 55.22, 34.67)$	π_B, π
7	6	1	$(-1, -2, 3, -4, -5, 6)$	7	$(40, 7.67, 99.78, 23.44)$	π_B
7	6	1	$(-1, 3, 4, -5, -6, -7)$	2	$(40, 7.67, 100.67, 21.22)$	π
8	1	7	1	$(2, 3, 4, 5, 6, 7, 8)$	$(2.33, 23.33, 6.22, 38.22)$	π_B, π
8	2	6	$(-1, 3)$	$(2, 4, 5, 6, 7, 8)$	$(6.67, 26, 14.44, 53.33)$	π_B
8	2	6	$(1, -2)$	$(3, 4, 5, 6, 7, 8)$	$(6.67, 26, 15.33, 48)$	π
8	3	5	$(1, -2, 4)$	$(3, 5, 6, 7, 8)$	$(13, 26.67, 28.11, 60.78)$	π_B
8	3	5	$(1, -2, -7)$	$(3, 4, 5, 6, 8)$	$(13, 26.67, 29, 56.78)$	π
8	4	4	$(1, -2, -3, 8)$	$(4, 5, 6, 7)$	$(21.33, 25.33, 48.89, 64.44)$	π_B, π
8	5	3	$(-1, -2, 3, -4, 6)$	$(5, 7, 8)$	$(31.67, 22, 78.44, 64.67)$	π_B
8	5	3	$(-1, -2, 3, -4, 6)$	$(5, 7, 8)$	$(31.67, 22, 78.44, 64.67)$	π
8	6	2	$(1, -2, -3, -4, -7, 8)$	$(5, 6)$	$(44, 16.67, 127.33, 56.44)$	π_B, π
8	7	1	$(1, -2, 3, 4, 5, -6, -7)$	8	$(58.33, 9.33, 194.11, 35.22)$	π_B, π

Table 3.5: Minimum π_B and π-aberration designs of 12 runs for $m = 9, 10, 11$ factors.

m	m_1	m_2	Columns of $\mathbf{D}_B$	Columns of $\mathbf{D}_O$	$(\pi_2^B, \pi_2^O, \pi_3^B, \pi_3^O)$	Criterion
9	1	8	-1	$(2,3,4,5,6,7,8,9)$	$(3.11, 32.89, 9.33, 68.44)$	π_B
9	1	8	-1	$(2,3,4,5,6,7,8,9)$	$(3.11, 32.89, 9.33, 68.44)$	π
9	2	7	$(1,-2)$	$(3,4,5,6,7,8,9)$	$(8.22, 35.78, 22.89, 84.11)$	π_B
9	2	7	$(-1,-2)$	$(3,4,5,6,7,8,9)$	$(8.22, 35.78, 23.33, 82.78)$	π
9	3	6	$(1,-2,4)$	$(3,5,6,7,8,9)$	$(15.33, 36.67, 40.33, 101.33)$	π_B
9	3	6	$(-1,-2,-4)$	$(3,5,6,7,8,9)$	$(15.33, 36.67, 43.89, 96)$	π
9	4	5	$(-1,2,-3,5)$	$(4,6,7,8,9)$	$(24.44, 35.56, 68.44, 107.78)$	π_B, π
9	5	4	$(-1,-2,3,-4,6)$	$(5,7,8,9)$	$(35.56, 32.44, 106.89, 108.89)$	π_B, π
9	6	3	$(-1,-2,-3,4,7,-8)$	$(5,6,9)$	$(48.67, 27.33, 167.78, 107.44)$	π_B
9	6	3	$(-1,-2,3,-4,5,6)$	$(7,8,9)$	$(48.67, 27.33, 169.11, 102.11)$	π
9	7	2	$(-1,-2,3,-4,5,6,7)$	$(8,9)$	$(63.78, 20.22, 242.33, 85.78)$	π_B, π
9	8	1	$(1,2,-3,-4,-5,6,-7,-8)$	9	$(80.89, 11.11, 336, 52)$	π_B, π
10	1	9	-1	$(2,3,4,5,6,7,8,9,10)$	$(4, 45, 13.33, 112)$	π_B, π
10	2	8	$(-1,-2)$	$(3,4,5,6,7,8,9,10)$	$(10, 48, 32.89, 132.44)$	π_B
10	2	8	$(-1,-2)$	$(3,4,5,6,7,8,9,10)$	$(10, 48, 32.89, 132.44)$	π
10	3	7	$(-1,2,-3)$	$(4,5,6,7,8,9,10)$	$(18, 49, 59, 152.33)$	π_B
10	3	7	$(1,-2,-3)$	$(4,5,6,7,8,9,10)$	$(18, 49, 59.89, 151.44)$	π
10	4	6	$(-1,2,-3,5)$	$(4,6,7,8,9,10)$	$(28, 48, 92, 169.33)$	π_B
10	4	6	$(-1,-2,3,-4)$	$(5,6,7,8,9,10)$	$(28, 48, 95.56, 165.78)$	π
10	5	5	$(-1,-2,3,-4,6)$	$(5,7,8,9,10)$	$(40, 45, 141.11, 172.22)$	π_B
10	5	5	$(-1,-2,3,-4,6)$	$(5,7,8,9,10)$	$(40, 45, 141.11, 172.22)$	π
10	6	4	$(-1,-2,3,-4,-5,6)$	$(7,8,9,10)$	$(54, 40, 215.11, 170.22)$	π_B
10	6	4	$(-1,-2,3,-4,-5,6)$	$(7,8,9,10)$	$(54, 40, 215.11, 170.22)$	π
10	7	3	$(1,-2,-3,-4,5,-6,-7)$	$(8,9,10)$	$(70, 33, 302.78, 156.56)$	π_B
10	7	3	$(1,-2,3,4,5,-6,-7)$	$(8,9,10)$	$(70, 33, 305.44, 153.89)$	π
10	8	2	$(1,2,-3,-4,-5,6,-7,-8)$	$(9,10)$	$(88, 24, 410.67, 122.67)$	π_B, π
10	9	1	$(-1,2,-3,4,5,6,-7,-8,-9)$	10	$(108, 13, 540, 73.33)$	π_B, π
11	1	10	-1	$(2,3,4,5,6,7,8,9,10,11)$	$(5, 60, 18.33, 173.33)$	π_B, π
11	2	9	$(-1,-2)$	$(3,4,5,6,7,8,9,10,11)$	$(12, 63, 44.67, 201)$	π_B, π
11	3	8	$(1,-2,-3)$	$(4,5,6,7,8,9,10,11)$	$(21, 64, 80, 226.67)$	π_B, π
11	4	7	$(-1,-2,3,-4)$	$(5,6,7,8,9,10,11)$	$(32, 63, 125.33, 247.33)$	π_B, π
11	5	6	$(-1,-2,3,-4,6)$	$(5,7,8,9,10,11)$	$(45, 60, 181.67, 260)$	π_B, π
11	6	5	$(-1,-2,3,-4,-5,6)$	$(7,8,9,10,11)$	$(60, 55, 270, 261.67)$	π_B, π
11	7	4	$(1,-2,-3,-4,5,-6,-7)$	$(8,9,10,11)$	$(77, 48, 375.33, 249.33)$	π_B
11	7	4	$(1,-2,-3,-4,5,-6,-7)$	$(8,9,10,11)$	$(77, 48, 375.33, 249.33)$	π
11	8	3	$(1,2,-3,-4,-5,6,-7,-8)$	$(9,10,11)$	$(96, 39, 498.67, 220)$	π_B, π
11	9	2	$(-1,2,-3,4,5,6,-7,-8,-9)$	$(10,11)$	$(117, 28, 649, 170.67)$	π_B, π
11	10	1	$(-1,-2,3,-4,5,6,7,-8,-9,-10)$	11	$(140, 15, 823.33, 98.33)$	π_B, π

and $\mathbf{H}_m = \otimes_{k=1}^m \mathbf{H}$ where

$$\mathbf{L} = \begin{bmatrix} 1 & 0 \\ 1 & 2 \end{bmatrix} \qquad \text{and} \qquad \mathbf{H} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

and $\otimes_{k=1}^m$ denotes m-fold Kronecker product. Then in matrix notation (3.1), (3.2) and (3.3) can be written as

$$\boldsymbol{\tau} = \mathbf{H}_m \boldsymbol{\beta}, \quad \boldsymbol{\tau} = \mathbf{L}_m \boldsymbol{\theta} \quad \text{and} \quad \boldsymbol{\tau} = \mathbf{H}_{m_2} \otimes \mathbf{L}_{m_1} \boldsymbol{\xi}. \tag{3.6}$$

Then the results in Theorem 3.1 can be verified directly. For example, $\boldsymbol{\xi} = \otimes_{k=1}^{m_2}(\mathbf{H}^{-1}\mathbf{L}) \otimes \mathbf{I}_{2^{m_1}} \boldsymbol{\theta}$ where $\mathbf{I}_{2^{m_1}}$ is the identity matrix of order 2^{m_1}. □

Proof of Lemma 3.1. Note that the matrix $\mathbf{B}_2$, which contains the rows $2, \ldots, m_1 + 1$ of the matrix $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_2$, can be written as $\mathbf{B}_2 = (\mathbf{B}_{2,B\times B}, \mathbf{B}_{2,B\times O}, \mathbf{B}_{2,O\times O})$, where the three submatrices correspond to the interactions of two B-factors, one B-factor and one O-factor, and two O-factors, respectively. Hence $\pi_2^B = \text{tr}(\mathbf{B}_2^T\mathbf{B}_2) = \text{tr}(\mathbf{B}_{2,B\times B}^T\mathbf{B}_{2,B\times B}) + \text{tr}(\mathbf{B}_{2,B\times O}^T\mathbf{B}_{2,B\times O}) + \text{tr}(\mathbf{B}_{2,O\times O}^T\mathbf{B}_{2,O\times O})$. Since $\mathbf{D}$ is an orthogonal array, it can be easily checked that

$$\mathbf{X}^T\mathbf{X} = N \begin{bmatrix} 1 & \mathbf{1}_{m_1}^T & \mathbf{0} \\ \mathbf{1}_{m_1} & \mathbf{I}_{m_1} + \mathbf{J}_{m_1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_{m_2} \end{bmatrix} \quad \text{and} \quad (\mathbf{X}^T\mathbf{X})^{-1} = \frac{1}{N} \begin{bmatrix} m_1 + 1 & -\mathbf{1}_{m_1}^T & \mathbf{0} \\ -\mathbf{1}_{m_1} & \mathbf{I}_{m_1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_{m_2} \end{bmatrix},$$

where $\mathbf{J}_{m_1}$ is an $m_1 \times m_1$ matrix of all ones. Through some tedious algebra, one can show that $\text{tr}(\mathbf{B}_{2,B\times B}^T\mathbf{B}_{2,B\times B}) = 3\sum_{i<j<k} J^2(b_i, b_j, b_k)/N^2 + m_1(m_1 - 1)$, $\text{tr}(\mathbf{B}_{2,B\times O}^T\mathbf{B}_{2,B\times O}) = 2\sum_{i<j}\sum_k J^2(b_i, b_j, o_k)/N^2$ and $\text{tr}(\mathbf{B}_{2,O\times O}^T\mathbf{B}_{2,O\times O}) = \sum_i\sum_{j<k} J^2(b_i, o_j, o_k)/N^2$. This gives the expression of π_2^B in the Lemma. One can also define $\mathbf{O}_{2,B\times B}$, $\mathbf{O}_{2,B\times O}$ and $\mathbf{O}_{2,O\times O}$ similarly and show that $\text{tr}(\mathbf{O}_{2,B\times B}^T\mathbf{O}_{2,B\times B}) = \sum_{i<j}\sum_k J^2(b_i, b_j, o_k)/N^2$, $\text{tr}(\mathbf{O}_{2,B\times O}^T\mathbf{O}_{2,B\times O}) = 2\sum_i\sum_{j<k} J^2(b_i, o_j, o_k)/N^2 + m_1 m_2$ and $\text{tr}(\mathbf{O}_{2,O\times O}^T\mathbf{O}_{2,O\times O}) = 3\sum_{i<j<k} J^2(o_i, o_j, o_k)/N^2$, leading to the expression of π_2^O in the Lemma. □

Proof of Theorem 3.2. First, we do not assume that $\mathbf{D} = (b_1, \ldots, b_{m_1}, o_1, \ldots, o_{m_2})$ is regular. Since $\mathbf{D}$ is an orthogonal array, there exists a set of $m_3 = N - 1 - m$ orthogonal real columns $\mathbf{E} = (e_1, \ldots, e_{m_3})$ such that $e_j^T e_j = N^2$ and e_j's are orthogonal to columns of $\mathbf{D}$ and the column $\mathbf{1}_N$ for $j = 1, \ldots, m_3$. Hence, for any $1 \le i \ne j \le m_1$, we have that $\sum_{k=1}^{m_1} J^2(b_i, b_j, b_k) + \sum_{k=1}^{m_2} J^2(b_i, b_j, o_k) + \sum_{k=1}^{m_3} J^2(b_i, b_j, e_k) = N^2$. Summing this equation over all (i, j)'s, one can show that

$$\sum_{i<j} \sum_{k} J^2(b_i, b_j, o_k) = -3 \sum_{i<j<k} J^2(b_i, b_j, b_k) - \sum_{i<j} \sum_{k} J^2(b_i, b_j, e_k) + C_1 \tag{3.7}$$

for some constant C_1. Using similar arguments, we can express $\sum_i \sum_{j<k} J^2(b_i, o_j, o_k)$ and $\sum_{i<j<k} J^2(o_i, o_j, o_l)$ in terms of J-characteristics of columns not involving o_j's. In particular, we have

$$\sum_{i} \sum_{j<k} J^2(b_i, o_j, o_k) = 3 \sum_{i<j<k} J^2(b_i, b_j, b_k) + 2 \sum_{i<j} \sum_{k} J^2(b_i, b_j, e_k) + \sum_{i} \sum_{j<k} J^2(b_i, e_j, e_k) + C_2 \tag{3.8}$$

for some constant C_2 and

$$\begin{aligned} \sum_{i<j<k} J^2(o_i, o_j, o_k) = &- \sum_{i<j<k} J^2(b_i, b_j, b_k) - \sum_{i<j} \sum_{k} J^2(b_i, b_j, e_k) \\ &- \sum_{i} \sum_{j<k} J^2(b_i, e_j, e_k) - J^2(e_i, e_j, e_k) + C_3 \end{aligned} \tag{3.9}$$

for some constant C_3. Combining (3.7), (3.8) and (3.9), we have $\pi_2^B = \sum_i \sum_{j<k} J^2(b_i, e_j, e_k)/N^2$ $+ C_B$ and $\pi_2^O = -\sum_i \sum_{j<k} J^2(b_i, e_j, e_k)/N^2 - 3\sum_{i<j<k} J^2(e_i, e_j, e_k)/N^2 + C_O$ for some constants C_B and C_O. Therefore, we have proved that sequentially minimizing π_2^B and π_2^O amounts to sequentially minimizing $\sum_i \sum_{j<k} J^2(b_i, e_j, e_k)$ and $-\sum_{i<j<k} J^2(e_i, e_j, e_k)$.

Now suppose that columns of $\mathbf{D}$ are selected from a saturated regular design as specified in Theorem 3.2. Then $\mathbf{E}$ can be taken as the complement of $\mathbf{D}$ in the saturated regular design. Then we have that $J^2(b_i, e_j, e_k) = N^2$ if b_i, e_j and e_k forms a defining word and $J^2(b_i, e_j, e_k) = 0$ otherwise. It can be verified that when the conditions in part (i) of the theorem are met, b_i must contain an independent column not contained in e_j and e_k, leading to $J^2(b_i, e_j, e_k) = 0$. In addition, the results of Chen and Hedayat (1996) imply that $\sum_{i<j<k} J^2(e_i, e_j, e_k)$ is maximized by design $\mathbf{D}$ among all regular OA$(2^h, 2^m, 2)$'s, and in particular, among all OA$(2^h, 2^m, 2)$'s if $m = 2^h - 2^{h_1}$ for some integer h_1. The results of Theorem 3.2 then follow. $\square$

Proof of Lemma 3.2. We use similar notations to those in the proof of Lemma 3.1. For example, $\mathbf{B}_{3,B\times B\times B}$ is the submatrix of $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_3$ corresponding to contamination of interaction involving three B-factors on the main effects of B-factors. Then we have

$$\begin{aligned}
\mathrm{tr}(\mathbf{B}_{3,B\times B\times B}^T \mathbf{B}_{3,B\times B\times B}) =& \frac{3}{N^2} \sum_{i<j<k} \{J(b_i, b_j, b_k) + N\}^2 \\
&+ \frac{1}{N^2} \sum_{i<j<k} \sum_{l} \{J(b_i, b_j, b_k, b_l) + J(b_i, b_j, b_l) + J(b_i, b_k, b_l) + J(b_j, b_k, b_l)\}^2, \\
\mathrm{tr}(\mathbf{B}_{3,B\times B\times O}^T \mathbf{B}_{3,B\times B\times O}) =& \frac{2}{N^2} \sum_{i<j} \sum_{k} J^2(b_i, b_j, o_k) \\
&+ \frac{1}{N^2} \sum_{i<j} \sum_{k} \sum_{l} \{J(b_i, b_j, b_k, o_l) + J(b_i, b_k, o_l) + J(b_j, b_k, o_l)\}^2, \\
\mathrm{tr}(\mathbf{B}_{3,B\times O\times O}^T \mathbf{B}_{3,B\times O\times O}) =& \frac{1}{N^2} \sum_{i} \sum_{j<k} J^2(b_i, o_j, o_k) + \frac{1}{N^2} \sum_{i\neq j} \sum_{k<l} \{J(b_i, b_j, o_k, o_l) + J(b_i, o_k, o_l)\}^2, \\
\mathrm{tr}(\mathbf{B}_{3,O\times O\times O}^T \mathbf{B}_{3,O\times O\times O}) =& \frac{1}{N^2} \sum_{i} \sum_{j<k<l} J^2(b_i, o_j, o_k, o_l), \\
\mathrm{tr}(\mathbf{O}_{3,B\times B\times B}^T \mathbf{O}_{3,B\times B\times B}) =& \frac{1}{N^2} \sum_{i<j<k} \sum_{l} \{J(b_i, b_j, b_k, o_l) + J(b_i, b_j, o_l) + J(b_i, b_k, o_l) + J(b_j, b_k, o_l)\}^2, \\
\mathrm{tr}(\mathbf{O}_{3,B\times B\times O}^T \mathbf{O}_{3,B\times B\times O}) =& \frac{2}{N^2} \sum_{i<j} \sum_{k<l} \{J(b_i, b_j, o_k, o_l) + J(b_i, o_k, o_l) + J(b_j, o_k, o_l)\}^2 + \frac{1}{2} m_1 m_2 (m_1 - 1), \\
\mathrm{tr}(\mathbf{O}_{3,B\times O\times O}^T \mathbf{O}_{3,B\times O\times O}) =& \frac{3}{N^2} \sum_{i} \sum_{j<k<l} \{J(b_i, o_j, o_k, o_l) + J(o_j, o_k, o_l)\}^2, \\
\mathrm{tr}(\mathbf{O}_{3,O\times O\times O}^T \mathbf{O}_{3,O\times O\times O}) =& \frac{4}{N^2} \sum_{i<j<k<l} J^2(o_i, o_j, o_k, o_l).
\end{aligned}$$

Then π_3 is obtained by taking the sum of all the terms above. Since any two J-characteristics in the same curly bracket cannot be nonzero at the same time, their product will be zero if we expand the square term. By some tedious algebra, we have

$$\pi_3 = 4A_4 + (3m_1 - 6)A_3 + 2\pi_2^O + \frac{6}{N} \sum_{i<j<k} J(b_i, b_j, b_k) + \frac{1}{2} m_1 (m_1 - 1)(m_1 + m_2 - 2). \quad (3.10)$$

In the proof of Theorem 3.2, we have already obtained that $\pi_2^O = -\sum_i \sum_{j<k} J^2(b_i, e_j, e_k)/N^2 - 3\sum_{i<j<k} J^2(e_i, e_j, e_k)/N^2 + C_O$ for some constant C_O, where $e_1, \ldots, e_{N-1-m}$ are columns of the complement of $\mathbf{D}$. Clearly, if $e_1, \ldots, e_{N-1-m}$ takes the first $2^{h_1} - 1$ columns of a saturated regular design, then the first three terms of π_3 in (3.10) are constant. Then the result of the lemma follows. □

Proof of Theorem 3.3. Since $\mathbf{D}$ is regular, the value of $J(b_i, b_j, b_k)$ is either 0 or $\pm N$ for any $1 \leq i < j < k \leq m_1$. Thus we have

$$\pi_3 = c_1 N \sum_{i<j<k} J(b_i, b_j, b_k)/N + c_0 \geq -c_1 N \sum_{i<j<k} J^2(b_i, b_j, b_k)/N^2 + c_0 = -c_1 N A_3(\mathbf{D}_B) + c_0, \tag{3.11}$$

where $A_3(\mathbf{D}_B)$ is the A_3 value of $\mathbf{D}_B$. By results of Chen and Hedayat (1996), we have $A_3(\mathbf{D}_B)$ is maximized among all regular designs by the choice of $\mathbf{D}_B$ in the construction. In addition, since $J(b_i, b_j, b_k)/N = -J^2(b_i, b_j, b_k)/N^2$, we conclude the lower bound in (3.11) is achieved. Therefore, $\mathbf{D} = (\mathbf{D}_B, \mathbf{D}_O)$ sequentially minimizes π_2 and π_3 over all regular designs. □

Proof of Lemma 3.3. The proof can be done by a direct verification. For example, the contamination of k-factor interaction $od_{j_1} \cdots d_{j_{k-1}}$ on the estimation of main effect of d_{j_k}, where o is an O-factor and $d_{j_1}, \ldots, d_{j_k}$ are either B-factors or O-factors, will contribute a term $(\sum_{i=1}^N o_i z_{i,j_1} z_{i,j_2} \cdots z_{i,j_{k-1}} d_{i,j_k})^2/N^2$, where $z_{i,j_l} = d_{i,j_l}$ if d_{j_l} is an O-factor and $z_{i,j_l} = d_{i,j_l} + 1$ if d_{j_l} is a B-factor for $l = 1, \ldots, k-1$, in π_k^B or π_k^O depending on whether d_{j_k} is a B-factor or an O-factor. One can see that replacing o_i by $-o_i$ does not affect the value of this term. Therefore, the conclude switching the signs of O-factors in an $\mathrm{OA}(N, 2^m, 2)$ does not affect its aberration. □

Proof of Theorem 3.4. For the design $\mathbf{D}$ generated in the theorem, we study the contamination of k-factor interaction $b_{j_1} \cdots b_{j_{k_1}} o_{l_1} \cdots o_{l_{k_2}}$ $(k_1 + k_2 = k)$ on the estimation of the main effect of certain factor d_0. Such a contamination will contribute a term $Q =$

$\{\sum_{i=1}^{N}(b_{i,j_1}+1)\cdots(b_{i,j_{k_1}}+1)o_{i,l_1}\cdots o_{i,l_{k_2}}d_{i,0}\}^2/N^2$ in π_k. Thus we have

$$Q = \frac{1}{N^2}\left\{J(b_{j_1},\ldots,b_{j_{k_1}},o_{l_1},\ldots,o_{l_{k_2}},d_0)+\cdots+J(o_{l_1},\ldots,o_{l_{k_2}},d_0)\right\}^2.$$

If we expand the square and average E over all possible sign switches of B-factors, the cross-product terms will disappear and we will obtain

$$\tilde{Q} = \frac{1}{N^2}\left\{J^2(b_{j_1},\ldots,b_{j_{k_1}},o_{l_1},\ldots,o_{l_{k_2}},d_0)+\cdots+J^2(o_{l_1},\ldots,o_{l_{k_2}},d_0)\right\}.$$

If we further average $\tilde{Q}$ over all possible choices of B-factors in the orthogonal array, then one can show that the resulting term will be a linear combination of $A_{k+1}, A_k, \ldots, A_{k_2-1}$ with positive coefficients. Then the result of the theorem follows by some tedious algebra. □

3.7 Concluding remarks

In this chapter, we propose a mixed parametrization for two-level factorial experiments where there are two types of factors called B-factors and O-factors. For O-factors the two levels are symmetrical while for B-factors they are not. We establish a connection of this mixed parametrization with both the orthogonal and baseline parametrizations. To control the contamination of higher-order interactions on the estimation of main effects, we propose two minimum aberration criteria, depending on whether or not the main effects of B- and O-factors are treated equally. Theoretical constructions and algorithms are provided to obtain orthogonal arrays that are optimal or nearly optimal under these criteria.

All the designs considered in this chapter are orthogonal arrays, because, as shown in Corollary 3.2, they are optimal under the main-effects model. On the other hand, under the baseline parametrization, Mukerjee and Tang (2012) showed that one-factor-at-a-time designs may be more desirable when the biases of the main effect estimators dominate their variances. It is interesting to investigate for the mixed parametrization how to obtain designs suitable for these situations.

Most results of this chapter concern the estimation of main effects. When some two-factor interactions are also of interest, we may wish to use designs that allow the efficient estimation of these effects as well. The construction of such designs under the mixed parametrization is worthy of future research.

Chapter 4

A Study of Orthogonal Array-Based Designs Under A Broad Class of Space-Filling Criteria

4.1 Introduction

Space-filling designs spread their points in the design region in some uniform manner. Such designs are widely accepted for computer experiments, because they not only allow information to be collected from different parts of the design region, but also enjoy desirable robustness properties against model bias. We refer to Santner et al. (2018) and Fang et al. (2006) for a more comprehensive introduction to computer experiments and benefits of space-filling designs.

Among various ideas in pursuit of space-filling designs over the past few decades, distance, orthogonality and discrepancy stand out as three most commonly used criteria. One type of distance-based criteria focuses on the distances between design points and often looks for designs with large separation distances. One such criterion is the maximin distance criterion (Johnson et al., 1990), which aims to maximize the minimum pairwise distance. See Zhou and Xu (2015), Wang et al. (2018) and Li et al. (2021) for some latest developments on this topic. A space-filling design should also have small correlations among its columns. This idea leads to the criterion of orthogonality (Owen, 1994) and spawns the class of orthogonal designs. We refer to Ye (1998), Steinberg and Lin (2006), Lin et al. (2010), Sun and Tang (2017) and references therein for the evolution of this line of space-filling designs. Besides these two criteria, the discrepancy measures the uniformity of a design by quantifying the difference between the empirical distribution function of its design points and the ideal uniform distribution function. One of the most popular discrepancies is the centered L_2-discrepancy (Hickernell, 1998). A detailed account on this branch of space-filling designs is available in Fang et al. (2018). Recently, Sun et al. (2019) proposed the uniform projection criterion by averaging the centered L_2-discrepancies of all two-dimensional projections. They showed that designs optimizing this criterion tend to scatter points uniformly in all dimensions and are space-filling under different types of criteria. However, except for a few theoretical constructions, to find a space-filling design under these numerical criteria is challenging and often requires computer searches, which often deteriorate quickly in performance for large designs.

Another appealing idea towards space-filling designs is to borrow strengths from orthogonal arrays. This class of designs guarantees attractive low-dimensional stratification properties without any assistance of computers. The earliest work was the introduction of Latin hypercubes (McKay et al., 1979) which are essentially orthogonal arrays of strength one. Owen (1992) and Tang (1993) later independently put forward designs based on orthogonal arrays of strength two.

Motivated by the concept of digital (w, k, m)-nets in quasi-Monte Carlo methods (Sobol', 1967; Niederreiter, 1987), He and Tang (2013) introduced strong orthogonal arrays. As detailed in He and Tang (2013), a (w, k, m)-net in base s is equivalent to a strong orthogonal array of strength $k - w$ with s^k runs for m factors. The introduction of strong orthogonal arrays is useful for a number of reasons. Strong orthogonal arrays are more general than (w, k, m)-nets in base s as they do not require run sizes to be powers of s. The new concept is in the familiar language of orthogonal arrays, thus creating opportunities for new research. For example, He et al. (2018) proposed strong orthogonal arrays of strength 2+ by focusing on two-dimensional space-filling properties of strength-three strong orthogonal arrays (He and Tang, 2014). The mappable nearly orthogonal arrays studied by Mukerjee et al. (2014) represent another direction to improve stratification properties of ordinary orthogonal array-based designs. The precise definitions for these structures will be given in a later section. For the latest research in this field, we refer to Xiao and Xu (2018), Shi and Tang (2019), Cheng et al. (2021), Wang et al. (2022a) and Tian and Xu (2022).

Despite many construction results for designs based on orthogonal arrays, it is not very clear how the low-dimensional stratification properties owned by such designs relate to other space-filling criteria, and how different types of stratifications contribute to the overall space-filling properties. Recently, Sun and Tang (2023) provided a partial answer by connecting strong orthogonal arrays with the uniform projection criterion. They gave a decomposition of the criterion, based on which some optimality results of certain strong orthogonal arrays can be established.

In this chapter, we study the space-filling properties of orthogonal array-based designs in terms of a broad class of space-filling criteria that include the commonly used criteria of variance of distances, orthogonality and uniform projection as special cases. Under these criteria, we show that the designs which are based on orthogonal arrays are better on average than those which are not. To identify those more space-filling designs, we partition orthogonal array-based designs into classes of designs using a notion of allowable level permutations. The average performance of each class of designs is then shown to depend on two types of stratification properties. Strong orthogonal arrays of strength 2+ are justified by achieving one of them. Based on these justification results, we investigate constructions of two families of space-filling orthogonal array-based designs, including some strong orthogonal arrays of strength 2+ and some mappable nearly orthogonal arrays. The two families of designs are shown to be complementary of each other and suitable for different situations depending on the number of factors and the specific criterion used.

The remainder of the chapter is arranged as follows. Section 4.2 introduces necessary notation and background. Section 4.3 provides justifications for orthogonal array-based designs and strong orthogonal arrays, where guidance for finding more space-filling orthogonal array-based designs is also given. Section 4.4 uses this guidance to construct and study various orthogonal array-based designs. All the proofs are included in Section 4.5. The chapter is concluded by a discussion in Section 4.6.

4.2 Notation, background and preliminaries

4.2.1 Orthogonal arrays and orthogonal array-based designs

A design of n runs and m factors with the uth factor having s_u levels is represented by an $n \times m$ matrix with entries from $\mathbb{Z}_{s_u} = \{0, \ldots, s_u - 1\}$ in the uth column. Such a design is called an orthogonal array of strength t, and denoted by $\mathrm{OA}(n, m, s_1 \times \cdots \times s_m, t)$, if any of its $n \times t$ submatrices contains all possible level combinations equally often. If $s_1 = \cdots = s_m = s$, then the orthogonal array is denoted by $\mathrm{OA}(n, m, s, t)$. An $\mathrm{OA}(n, m, s, 1)$ is also called a U-type design and denoted by $\mathrm{U}(n, s^m)$ in this chapter.

Orthogonal arrays can be used to generate space-filling designs (Tang, 1993). Suppose $s = \alpha s'$, where α and s' are positive divisors of s. Given an $\mathrm{OA}(n, m, s', 2)$, say A, an orthogonal array-based design can then be obtained by the following procedure:

Step 1. Randomly permute the s' levels in each column of A.

Step 2. Next, for each column, replace the n/s' entries of level l by a random permutation of $(\alpha l, \ldots, \alpha l, \alpha l{+}1, \ldots, \alpha l{+}1, \ldots\ldots, \alpha l{+}\alpha{-}1, \ldots, \alpha l{+}\alpha{-}1)$ for $l = 0, \ldots, s'{-}1$.

The resulting design, achieving stratification over an $s' \times s'$ grid in any of its two-dimensional projections, is called an orthogonal array-based design (OABD) and denoted by $\mathrm{OABD}_\alpha(n, s^m)$. The above procedure is a more general version of constructing orthogonal array-based designs, since the original proposal of Tang (1993) was to construct orthogonal array-based Latin hypercubes, which correspond to $s = n$ in our procedure.

Example 4.1. *We illustrate the two-step procedure with the OA*$(8, 3, 2, 2)$ *denoted by* A *in* (4.1)*. Based on this orthogonal array, we first obtain* A' *by permuting the two levels in each column (Step 1); then expand the four entries of 0 by a random permutation of* $(0, 0, 1, 1)$*, and the four entries of 1 by a random permutation of* $(2, 2, 3, 3)$ *in each column* *independently (Step 2). The resulting design D is an OABD$_2(8, 4^3)$.*

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \overset{\textit{Step 1}}{\longrightarrow} \quad A' = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \quad \overset{\textit{Step 2}}{\longrightarrow} \quad D = \begin{bmatrix} 0 & 3 & 3 \\ 3 & 2 & 0 \\ 0 & 1 & 1 \\ 2 & 0 & 3 \\ 1 & 2 & 2 \\ 2 & 3 & 1 \\ 1 & 1 & 0 \\ 3 & 0 & 2 \end{bmatrix} \tag{4.1}$$

Strong orthogonal arrays, introduced by He and Tang (2013), are more space-filling than ordinary orthogonal array-based designs. We study the most economical strong orthogonal arrays, namely those of strength 2+ (He et al., 2018) and call them SOAs for convenience. An OABD$_\alpha(n, s^m)$ is an SOA and denoted by SOA$_\alpha(n, s^m)$, if any pair of columns can be collapsed into an OA$(n, 2, s \times s', 2)$ as well as an OA$(n, 2, s' \times s, 2)$, where collapsing s levels into s' levels is done by $\lfloor x/\alpha \rfloor$ for $x = 0, \ldots, s-1$ and $\lfloor \cdot \rfloor$ is the floor function. An SOA achieves $s \times s'$ and $s' \times s$ stratifications in all two-dimensions.

Another attractive class of orthogonal array-based designs is the mappable nearly orthogonal arrays (MNOAs) introduced by Mukerjee et al. (2014). An OABD$_\alpha(n, s^m)$ is an MNOA and denoted by MNOA$_\alpha(n, (s^r)^p)$ if its $m = pr$ columns can be partitioned into p disjoint groups of r columns such that any two columns from different groups form an OA$(n, 2, s, 2)$.

The following lemma, which can be proved similarly as Proposition 2 of He and Tang (2013), gives a unified characterization for U-type designs, OABDs, SOAs and MNOAs. Recall that a U(n, s^m) denotes a balanced s-level design of n runs for m factors.

Lemma 4.1. *Let $s = \alpha s'$. Then D is a $U(n, s^m)$ if and only if there exist a unique $U(n, (s')^m)$, say $A = (a_1, \ldots, a_m)$, and a unique $U(n, \alpha^m)$, say $B = (b_1, \ldots, b_m)$, such that (a_u, b_u) is an $OA(n, 2, s' \times \alpha, 2)$ for $u = 1, \ldots, m$ and that $D = \alpha A + B$. Furthermore, we have that* *(i) D is an $OABD_\alpha(n, s^m)$ if and only if A is an $OA(n, m, s', 2)$;*

(ii) D is an $SOA_\alpha(n, s^m)$ if and only if (a_u, a_v, b_v) is an $OA(n, 3, s' \times s' \times \alpha, 3)$ for all $u \neq v$;

(iii) D is an $MNOA_\alpha(n, (s^r)^p)$ if and only if A is an $OA(n, m, s', 2)$ and (a_u, b_u, a_v, b_v) is an $OA(n, 4, s' \times \alpha \times s' \times \alpha, 4)$ so long as the uth and vth columns are from different groups of the MNOA.

For any $\mathrm{U}(n, s^m)$, we use the associated matrices A and B in Lemma 4.1 without specification hereafter.

4.2.2 Optimality criteria

We first introduce the orthonormal contrasts defined by tensor products. Consider a full factorial $s_1 \times \cdots \times s_m$ design. For its uth factor taking levels from $\mathbb{Z}_{s_u}$, we define a set of s_u complex-valued functions $\kappa^{(u)}_{g_u} : \mathbb{Z}_{s_u} \to \mathbb{C}$ such that $\kappa^{(u)}_0 = 1$ and $\sum_{z_u \in \mathbb{Z}_{s_u}} \kappa^{(u)}_{g_u}(z_u)\overline{\kappa^{(u)}_{h_u}(z_u)} = s_u \delta(g_u, h_u)$ for $g_u, h_u \in \mathbb{Z}_{s_u}$, where $\overline{\kappa^{(u)}_{h_u}(z_u)}$ is the complex conjugate of $\kappa^{(u)}_{h_u}(z_u)$ and δ is the Kronecker delta function. Let $\mathcal{Z} = \mathbb{Z}_{s_1} \times \cdots \times \mathbb{Z}_{s_m}$. For $g = (g_1, \ldots, g_m) \in \mathcal{Z}$ and $z = (z_1, \ldots, z_m) \in \mathcal{Z}$, the function $\kappa_g(z) = \prod_{u=1}^m \kappa^{(u)}_{g_u}(z_u)$ is called a k-factor interaction if $wt(g) = k$, where $wt(g)$ is the number of nonzero components in g.

Let D be a design of n runs for m factors with the uth factor taking s_u levels. We denote its design points by $x_1, x_2, \ldots, x_n$. Let $X_k = (\kappa_g(x_i))_{i=1,\ldots,n; wt(g)=k}$ be the matrix of orthonormal contrast coefficients for its k-factor interactions; we refer to its (i, u)th entry by $x^{(k)}_{iu}$. Then the combinatorial uniformity of D can be described by its generalized wordlength pattern $(A_1(D), A_2(D), \ldots, A_m(D))$, where

$$A_k(D) = \frac{1}{n^2} \sum_u \left(\sum_{i=1}^n x^{(k)}_{iu} \right)^2 . \tag{4.2}$$

We have that D is an orthogonal array of strength t if and only if $A_k(D) = 0$ for $1 \leq k \leq t$. The minimum G_2-aberration (Tang and Deng, 1999; Xu and Wu, 2001) proposes to minimize $A_1(D), A_2(D), A_3(D), \ldots$ sequentially. A design D is said to be supersaturated if $m > (n-1)/(s-1)$ and a popular criterion to select such a design is to use $A_2(D)$, see, for example, Xu and Wu (2005).

To evaluate a space-filling design D for quantitative factors, it is more reasonable to consider criteria such as distance, orthogonality and discrepancy. Hereafter we always assume D is a $\mathrm{U}(n, s^m)$. Given a distance function d on $\mathbb{Z}_s = \{0, 1, \ldots, s-1\}$, we define the distance between design points $x_i = (x_{i1}, \ldots, x_{im})$ and $x_j = (x_{j1}, \ldots, x_{jm})$ to be $d_{ij} = \sum_{k=1}^{m} d(x_{ik}, x_{jk})$. The most commonly used are L_p-distances for $p = 1$ and 2 where $d(x_{ik}, x_{jk}) = |x_{ik} - x_{jk}|^p$. Note that our definition for d_{ij} does not take the pth root as in the conventional one. The maximin distance criterion (Johnson et al., 1990) seeks to maximize the minimum distance of all d_{ij}s for $1 \leq i \neq j \leq n$. For theoretical convenience, we use a surrogate criterion that aims to minimize the variance of distances d_{ij}s, that is, we minimize

$$\phi(D) = \frac{1}{n(n-1)} \sum_{i \neq j} \left(d_{ij} - \bar{d}\right)^2,$$

where $\bar{d}$ is the average of all d_{ij}s for $i \neq j$. Zhou and Xu (2015) showed that $\bar{d}$ is a constant for U-type designs. Therefore, as argued in Xiao and Xu (2018) and Wang et al. (2022c), it is reasonable to expect a design with small $\phi(D)$ to be also good under the maximin distance criterion. Let ϕ_1 and ϕ_2 be the versions of ϕ when L_1- and L_2-distances are used, respectively. Wang et al. (2022c) showed that a design with small $\phi_1(D)$ or $\phi_2(D)$ tends to perform well under the orthogonality criterion and the uniform projection criterion to be reviewed next.

The orthogonality criterion (Owen, 1994) was proposed to minimize the average squared correlations among factors. Specifically, if we let ρ_{uv} be the sample correlation between the uth and vth columns of D, then the orthogonality criterion is defined to be

$$\rho(D) = \frac{1}{m(m-1)} \sum_{u \neq v} \rho_{uv}^2.$$

Clearly, we have $0 \leq \rho(D) \leq 1$ and a design with small $\rho(D)$ is desirable.

Another class of criteria, known as discrepancies, measures uniformity by the difference between the empirical distribution function of the design points and the uniform distribution function. Among them a popular criterion is the centered L_2-discrepancy (Hickernell, 1998) given by

$$\mathrm{CD}(D) = \left(\frac{13}{12}\right)^m - \frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(1+\frac{1}{2}\left|\frac{2x_{ik}+1-s}{2s}\right| - \frac{1}{2}\left|\frac{2x_{ik}+1-s}{2s}\right|^2\right)$$
$$+ \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(1+\frac{1}{2}\left|\frac{2x_{ik}+1-s}{2s}\right| + \frac{1}{2}\left|\frac{2x_{jk}+1-s}{2s}\right| - \left|\frac{x_{ik}-x_{jk}}{2s}\right|\right).$$

Recently, Sun et al. (2019) proposed a uniform projection criterion ψ by considering two-dimensional projections of D under the centered L_2-discrepancy. Let D_{uv} be the $n \times 2$ design consisting of the uth and vth columns of D. Then

$$\psi(D) = \frac{1}{m(m-1)}\sum_{u \neq v}\mathrm{CD}(D_{uv}). \tag{4.3}$$

Sun et al. (2019) showed that ψ has a close connection with the L_1-distance and that designs minimizing $\psi(D)$ also have good projection properties in all $t > 2$ dimensions, though the definition only takes into account two-dimensions.

In this chapter, we consider a broad class of space-filling criteria χ that includes ϕ, ρ and ψ as special cases. This class of criteria is based on two-dimensional projections of D and can be written as

$$\chi(D) = \frac{1}{m(m-1)}\sum_{u \neq v} q(D_{uv}),$$

where q takes the form of

$$q(D_{uv}) = \gamma_0 + \frac{\gamma_1}{n}\sum_{i=1}^{n} g(x_{iu})g(x_{iv}) + \frac{\gamma_2}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} f(x_{iu}, x_{ju})f(x_{iv}, x_{jv})$$

where γ_0 and γ_1 are arbitrary real constants, and f and g are arbitrary real functions; and we only require that $\gamma_2 > 0$. The following lemma shows that ϕ, ρ and ψ are special cases of χ.

Lemma 4.2. *We have that*

(i) $\chi = \phi$ *if* $f(x,y) = d(x,y)$, $\gamma_2 = mn(m-1)/(n-1)$, $\gamma_1 = 0$ *and* $\gamma_0 = mn\sum_{x=0}^{s-1}\sum_{y=0}^{s-1} d(x,y)^2/(s^2(n-1)) - \{mn\sum_{x=0}^{s-1}\sum_{y=0}^{s-1} d(x,y)/(ns^2 - s^2)\}^2$;

(ii) $\chi = \rho$ *if* $f(x, y) = \{x - (s-1)/2\}\{y - (s-1)/2\}$, $\gamma_2 = 12^2/(s^2-1)^2$ *and* $\gamma_1 = \gamma_0 = 0$;

(iii) $\chi = \psi$ *if* $f(x, y) = 1 + |\tilde{x}|/2 + |\tilde{y}|/2 - |\tilde{x} - \tilde{y}|/2$, $g(x) = 1 + |\tilde{x}|/2 - \tilde{x}^2/2$, $\gamma_2 = 1$, $\gamma_1 = -2$ *and* $\gamma_0 = (13/12)^2$, *where* $\tilde{x} = (2x + 1 - s)/(2s)$ *and* $\tilde{y} = (2y + 1 - s)/(2s)$.

We remark that χ includes more space-filling criteria besides the three discussed here. For example, ψ would still be a member of χs if we replace the centered L_2-discrepancy in (4.3) by other discrepancies such as wrap-around discrepancy (Hickernell, 1998) and mixture discrepancy (Zhou et al., 2013).

4.3 Justification results

4.3.1 OABDs are better than U-type designs on average

Suppose we would like a design with n runs for m factors each with $s = \alpha s'$ levels. Then a U(n, s^m), say D, can be easily generated by juxtaposing m random permutations of the sequence $(0, \ldots, 0, \ldots\ldots, s-1, \ldots, s-1)$ where each level is replicated $\lambda = n/s$ times. We denote by $\bar{\chi}_u$ the average of $\chi(D)$s over all such U-type designs.

Based on an OA$(n, m, s', 2)$, an OABD$_\alpha(n, s^m)$ can be constructed as in Section 4.2.1. Let $\bar{\chi}_o$ be the average of $\chi(D)$s over all OABD$_\alpha(n, s^m)$s obtained from the given OA$(n, m, s', 2)$. Theorem 4.1 shows that $\bar{\chi}_o < \bar{\chi}_u$. This indicates that a random OABD$_\alpha(n, s^m)$ tends to be better than a random U(n, s^m) under the criterion χ. For ease of expression, we introduce the notation $S_l = \{\alpha l, \alpha l + 1, \ldots, \alpha l + \alpha - 1\}$ for $l = 0, \ldots, s' - 1$, thus the set of all levels $\mathbb{Z}_s = \{0, 1, \ldots, s-1\}$ is a union of these s' disjoint groups.

Theorem 4.1. *We have that*

$$\bar{\chi}_u - \bar{\chi}_o = \frac{\gamma_2}{n-1}\left(1 - \frac{1}{s'}\right)^2 \left(Z_\chi - \frac{(\lambda - 1)X_\chi + (\alpha\lambda - \lambda)Y_\chi}{\alpha\lambda - 1}\right)^2,$$

where $X_\chi = \sum_{x=0}^{s-1} f(x, x)/s$, $Y_\chi = \sum_{l=0}^{s'-1} \sum_{\substack{x,y \in S_l \\ x \neq y}} f(x, y)/(s'\alpha(\alpha-1))$ *and* $Z_\chi = \sum_{0 \le k \neq l \le s'-1} \sum_{x \in S_k, y \in S_l} f(x, y)/(\alpha^2 s'(s'-1))$.

We illustrate the results of Theorem 4.1 by taking $\chi = \phi$, the variance of pairwise distances between the design points. Suppose L_p-distances are used, i.e., $f(x, y) = d(x, y) =$

$|x-y|^p$. It is clear that $X_\phi = 0$. Then Y_ϕ and Z_ϕ, respectively, calculate the average distance of two distinct levels within and between the s' groups of $\mathbb{Z}_s$. Obviously, we have $X_\phi < Y_\phi < Z_\phi$ as long as $s' > 1$. In addition, when the number of levels $s = \alpha s'$ is fixed, we have that the larger s' is, the larger Z_ϕ and the smaller Y_ϕ would be, leading to a larger difference between $\bar{\phi}_u$ and $\bar{\phi}_o$ according to Theorem 4.1. This difference becomes largest when $s' = s$, in which case OABD$_\alpha(n, s^m)$s become OA$(n, m, s, 2)$s. Therefore, Theorem 4.1 suggests the use of OABD$_\alpha(n, s^m)$s with larger s', which is also intuitive as such designs achieve stratification on a finer $s' \times s'$ grid. The discussion is similar if we take χ as other criteria. Note that the relationship $X_\chi < Y_\chi < Z_\chi$ may not hold in general, but it can be verified that either

$$X_\chi < Y_\chi < Z_\chi \quad \text{or} \quad X_\chi > Y_\chi > Z_\chi \tag{4.4}$$

holds for the commonly used space-filling criteria ϕ, ρ and ψ.

Special cases of Theorem 4.1 are related to results of Xiao and Xu (2018) and Wang et al. (2021), who studied space-filling criteria such as ϕ_1 and ρ and found that permuting and expanding the levels of an orthogonal array (i.e. OABDs) is better than doing the same to a non-orthogonal array.

We conclude this subsection with a corollary on the average $A_2(D)$ of U-type designs and OABDs. A result of Xu (2003) indicates that $\phi(D)$ is equivalent to $A_2(D)$ for any U-type design if we take $d(x, y) = 1 - \delta(x, y)$, where δ is Kronecker's delta. This connection, combining with Theorem 4.1, enables us to establish that the average $A_2(D)$ of OABDs cannot be greater than that of U-type designs.

Corollary 4.1. *Let $\bar{A}_{2,u}$ and $\bar{A}_{2,o}$ be the average $A_2(D)$ over all $U(n, s^m)$s and $OABD_\alpha(n, s^m)$s, respectively. Then we have*

$$\bar{A}_{2,u} - \bar{A}_{2,o} = \frac{m(m-1)s^2}{2(n-1)} \left(1 - \frac{1}{s'}\right)^2 \left(\frac{\lambda - 1}{\alpha\lambda - 1}\right)^2.$$

4.3.2 Good classes of designs within OABDs

To find those OABDs with even better space-filling properties, we introduce the concept of *allowable permutations.*

Definition 4.1. *A permutation σ of $\mathbb{Z}_s = \{0, 1, \ldots, s-1\}$ is said to be α-allowable if for two levels $x, y \in \mathbb{Z}_s$, we have $\lfloor x/\alpha \rfloor = \lfloor y/\alpha \rfloor$ if and only if $\lfloor \sigma(x)/\alpha \rfloor = \lfloor \sigma(y)/\alpha \rfloor$.*

An α-allowable permutation preserves the group structure given by $\mathbb{Z}_s = \cup_{l=0}^{s'-1} S_l$, that is, two levels belong to the same group if and only if the permuted levels do. For example, for $s = 4$ there are eight 2-allowable permutations in total: $(0, 1, 2, 3)$, $(1, 0, 2, 3)$, $(0, 1, 3, 2)$, $(1, 0, 3, 2)$, $(2, 3, 0, 1)$, $(2, 3, 1, 0)$, $(3, 2, 0, 1)$ and $(3, 2, 1, 0)$, where each vector represents a permutation σ by $(\sigma(0), \sigma(1), \sigma(2), \sigma(3))$.

Proposition 4.1. *Let D' be the design obtained by permuting levels in each column of D independently with α-allowable permutations. Then D' is an $OABD_\alpha(n, s^m)$ if and only if D is an $OABD_\alpha(n, s^m)$. Furthermore, D' is an $SOA_\alpha(n, s^m)$ if and only if D is an $SOA_\alpha(n, s^m)$; D' is an $MNOA_\alpha(n, (s^r)^p)$ if and only if D is an $MNOA_\alpha(n, (s^r)^p)$.*

Proposition 4.1 is quite intuitive and can be verified directly. Essentially, α-allowable permutations induce a partition of all $\text{OABD}_\alpha(n, s^m)$s into classes of designs, where two designs belong to the same class if and only if they can be obtained from each other via α-allowable permutations. The next result provides a guidance on how to find good classes of OABDs.

Theorem 4.2. *Suppose D is an $OABD_\alpha(n, s^m)$. Let $\bar{\chi}(D)$ be the average of $\chi(D')$s over all designs D' obtained by conducting α-allowable level permutations to columns of D. Then*

$$\bar{\chi}(D) = \frac{2\gamma_2(Y_\chi - X_\chi)^2}{m(m-1)s^2} A_2(D) + \frac{2\alpha\gamma_2(Y_\chi - X_\chi)(Z_\chi - Y_\chi)}{m(m-1)s^2} \mu(D) + C, \tag{4.5}$$

where $\mu(D) = \sum_{u \neq v}\{A_2(a_u, b_v) + A_3(a_u, a_v, b_v)\}$ and $C = \gamma_0 + \gamma_1(\sum_{x=0}^{s-1} g(x)/s)^2 + \gamma_2(\sum_{x=0}^{s-1} \sum_{y=0}^{s-1} f(x, y)/s^2)^2$ is a constant.

The results of Theorem 4.2 can be interpreted as follows. Recall that for $1 \leq u \neq v \leq m$, according to the projection justification of minimum G_2-aberration (Tang, 2001; Ai and Zhang, 2004), the quantity $A_2(a_u, b_v) + A_3(a_u, a_v, b_v)$ is proportional to the variance of frequencies of the $s' \times s' \times \alpha$ level combinations in (a_u, a_v, b_v), or equivalently, the $s' \times s$ level combinations in (a_u, D_v), where D_v is the vth column of D. Similarly, $A_2(D_{uv})$

is proportional to the variance of frequencies of $s \times s$ level combinations in D_{uv}. Also note the coefficients for $A_2(D)$ and $\mu(D)$ are positive due to (4.4) and $\gamma_2 > 0$. Therefore, Theorem 4.2 reveals that up to a constant, the average χ-performance of the class of OADBs obtained from D by α-allowable permutations is determined by two components, the overall stratification of D over an $s \times s$ grid, represented by the term with $A_2(D) = \sum_{u<v} A_2(D_{uv})$, and the overall stratification of D over the $s \times s'$ and $s' \times s$ grids, represented by the term with $\mu(D) = \sum_{u \neq v}\{A_2(a_u, b_v) + A_3(a_u, a_v, b_v)\}$. Clearly, the second term vanishes if and only if D is an SOA$_\alpha(n, s^m)$.

Corollary 4.2. *Suppose D is an SOA$_\alpha(n, s^m)$. Then*

$$\bar{\chi}(D) = \frac{2\gamma_2(Y_\chi - X_\chi)^2}{m(m-1)s^2} A_2(D) + C. \tag{4.6}$$

Zhou and Xu (2014) considered all level permutations of a U-type design and found the average performance in terms of distance and discrepancy is determined by the generalized wordlength pattern. For comparison, we present the results for the same problem under the criterion χ.

Lemma 4.3. *Suppose D is a U(n, s^m). Let $\bar{\bar{\chi}}(D)$ be the average of $\chi(D')$s over all designs D' obtained by conducting all level permutations to columns of D. Then*

$$\bar{\bar{\chi}}(D) = \frac{2\gamma_2(W_\chi - X_\chi)^2}{m(m-1)s^2} A_2(D) + C, \tag{4.7}$$

where $W_\chi = \sum_{0 \le x \neq y \le s-1} f(x, y)/(s(s-1))$.

Note that $W_\chi = (\alpha-1)Y_\chi/(s-1) + (s-\alpha)Z_\chi/(s-1)$, which is a weighted average of Y_χ and Z_χ. Together with (4.4), we deduce that the coefficient of $A_2(D)$ in (4.6) must be less than its counterpart in (4.7). Suppose D_1 and D_2 are two U(n, s^m)s such that $A_2(D_1) = A_2(D_2)$, where D_1 is an SOA$_\alpha(n, s^m)$ but D_2 is not. Then we have $\bar{\chi}(D_1) < \bar{\bar{\chi}}(D_2)$ by Corollary 4.2 and Lemma 4.3, suggesting that compared to arbitrarily permuting the non-SOA, where a total of $(s!)^m$ designs are generated, a much smaller class of more space-filling designs, which contains $\{(s')!(\alpha!)^{s'}\}^m$ candidates, is obtained by allowably permuting the SOA. Even if D_2

is an $\mathrm{OABD}_\alpha(n, s^m)$, we still have $\bar{\chi}(D_1) < \bar{\chi}(D_2)$ by Theorem 4.2. In this sense, the class of $\mathrm{SOA}_\alpha(n, s^m)$s is superior in terms of the class of criteria χ compared with ordinary U-type designs and OABDs. We choose two sets of s, α and s' to illustrate the above results.

Example 4.2. *We consider $\chi = \phi_1$. The results for $\chi = \psi$ are similar since the ratio $(W_\chi - X_\chi)/(Y_\chi - X_\chi)$ as well as $(Z_\chi - Y_\chi)/(Y_\chi - X_\chi)$ is the same for $\chi = \phi_1$ and $\chi = \psi$.*

(i) Suppose $s = 4$ and $s' = \alpha = 2$. Then for some constant $C_{1,1}$, we have $\bar{\bar{\phi}}_1(D) = 25n/(72(n-1))A_2(D) + C_{1,1}$ if D is a $U(n, 4^m)$; $\bar{\phi}_1(D) = n/(8(n-1))A_2(D) + n/(4(n-1))\mu(D) + C_{1,1}$ if D is an $OABD_2(n, 4^m)$; and $\bar{\phi}_1(D) = n/(8(n-1))A_2(D) + C_{1,1}$ if D is an $SOA_2(n, 4^m)$. It can be seen the coefficient in (4.6) *is only* 9/25 *of the coefficient in* (4.7) *in this case.*

(ii) Suppose $s = 9$ and $s' = \alpha = 3$. Then for some constant $C_{2,1}$, we have $\bar{\bar{\phi}}_1(D) = 200n/(729(n-1))A_2(D) + C_{2,1}$ if D is a $U(n, 9^m)$; $\bar{\phi}_1(D) = 32n/(729(n-1))A_2(D) + 64n/(243(n-1))\mu(D) + C_{2,1}$ if D is an $OABD_3(n, 9^m)$; and $\bar{\phi}_1(D) = 32n/(729(n-1))A_2(D) + C_{2,1}$ if D is an $SOA_3(n, 9^m)$. It can be seen the coefficient in (4.6) *is only* 4/25 *of the coefficient in* (4.7) *in this case.*

Example 4.3. *We consider $\chi = \phi_2$. The results for $\chi = \rho$ are similar since the ratio $(W_\chi - X_\chi)/(Y_\chi - X_\chi)$ as well as $(Z_\chi - Y_\chi)/(Y_\chi - X_\chi)$ is the same for $\chi = \phi_2$ and $\chi = \rho$.*

(i) Suppose $s = 4$ and $s' = \alpha = 2$. Then for some constant $C_{1,2}$, we have $\bar{\bar{\phi}}_2(D) = 100n/(72(n-1))A_2(D) + C_{1,2}$ if D is a $U(n, 4^m)$; $\bar{\phi}_2(D) = n/(8(n-1))A_2(D) + 7n/(8(n-1))\mu(D) + C_{1,2}$ if D is an $OABD_2(n, 4^m)$; and $\bar{\phi}_2(D) = n/(8(n-1))A_2(D) + C_{1,2}$ if D is an $SOA_2(n, 4^m)$. It can be seen the coefficient in (4.6) *is only* 9/100 *of the coefficient in* (4.7) *in this case.*

(ii) Suppose $s = 9$ and $s' = \alpha = 3$. Then for some constant $C_{2,2}$, we have $\bar{\bar{\phi}}_2(D) = 50n/(9(n-1))A_2(D) + C_{2,2}$ if D is a $U(n, 9^m)$; $\bar{\phi}_2(D) = 8n/(81(n-1))A_2(D) + 208n/(81(n-1))\mu(D) + C_{2,2}$ if D is an $OABD_3(n, 9^m)$; and $\bar{\phi}_2(D) = 8n/(81(n-1))A_2(D) + C_{2,2}$ if D is an $SOA_3(n, 9^m)$. It can be seen the coefficient in (4.6) *is only* 4/225 *of the coefficient in* (4.7) *in this case.*

Besides the SOAs, we point out the MNOAs are also competitive by Theorem 4.2. Suppose D is an $\mathrm{MNOA}_\alpha(n,(s^r)^p)$. Then $A_2(D_{uv})=0$ whenever $\lfloor(u-1)/r\rfloor \neq \lfloor(v-1)/r\rfloor$ and as a result, the overall $A_2(D)$ would tend to be small. This may effectively bring $\bar{\chi}(D)$ down by minimizing its first term, in spite of the positive second term. More examples will be given in Section 4.4.2.

We conclude this section by presenting a useful and also insightful result which has been implicitly used in the proof of Theorem 4.2.

Proposition 4.2. *Suppose D is a $U(n,s^m)$. Then we have*

$$A_2(D)=A_2(A)+\mu(D)+\nu(D), \tag{4.8}$$

where $\nu(D)=A_2(B)+\sum_{u\neq v}\{A_3(a_u,b_u,b_v)+A_4(a_u,b_u,a_v,b_v)/2\}$.

Proposition 4.2 enables us to calculate $A_2(D)$ from columns of A and B directly. The terms in (4.8) all have interpretations. Specifically, $A_2(A)$ measures the difference of D from an $\mathrm{OABD}_\alpha(n,s^m)$; $A_2(A)+\mu(D)$ measures the difference of D from an $\mathrm{SOA}_\alpha(n,s^m)$; and $A_2(D)=A_2(A)+\mu(D)+\nu(D)$ measures the difference of D from an $\mathrm{OA}(n,m,s,2)$.

Remark 4.1. *Based on Proposition 4.2, we can rewrite* (4.5) *in Theorem 4.2 as*

$$\bar{\chi}(D)=\frac{2\gamma_2(Y_\chi-X_\chi)^2+2\alpha\gamma_2(Y_\chi-X_\chi)(Z_\chi-Y_\chi)}{m(m-1)s^2}\mu(D)+\frac{2\gamma_2(Y_\chi-X_\chi)^2}{m(m-1)s^2}\nu(D)+C,$$

where the first and second terms can be seen as measures of the difference and "residual difference" of D from $SOA_\alpha(n,s^m)$ and $OA(n,m,s,2)$ under χ, respectively. This decomposition has a similar flavor to Theorem 2 of Sun and Tang (2023).

4.4 Construction results

In this section, we provide construction methods for two families of OABDs, both of which have good performance under $\bar{\chi}(D)$.

4.4.1 SOAs with small $A_2(D)$

As discussed in Section 4.3.2, an $\mathrm{SOA}_\alpha(n, s^m)$, say D, tends to be more space-filling in terms of $\chi(D)$ when compared to a non-SOA with the same $A_2(D)$. By Corollary 4.2, D would be most preferable if $A_2(D)$ is small. The construction of such a design is the focus of this subsection. Define the index λ' of D to be $\lambda' = n/(ss') = n\alpha/s^2$. We have the following result for $\lambda' = 1$.

Theorem 4.3. *An $SOA_\alpha(n, s^m)$ with $\lambda' = 1$ has minimum $A_2(D)$ among all $U(n, s^m)$s, and thus minimizes $\bar{\chi}(D)$ among all $OABD_\alpha(n, s^m)$s.*

Sun and Tang (2023) also showed that $\mathrm{SOA}_\alpha(n, s^m)$s with $\lambda' = 1$ are optimal or nearly optimal in terms of $\psi(D)$. Theorem 4.3 indicates that such SOAs are optimal under $\bar{\chi}(D)$ and thus confirms their results from another perspective.

Now let's focus on the scenario $\lambda' > 1$ and $\alpha = s'$. As in He et al. (2018), we construct an $\mathrm{SOA}_{s'}(n, s^m)$ by selecting columns of A and B from a saturated regular design S of s' levels obtained by the Rao-Hamming construction. Here s' is a prime power and $n = (s')^k$ for a positive integer k. The $(n-1)/(s'-1)$ columns of S form a projective geometry. Given two distinct columns $a, b \in S$, we denote their $(s-1)$ interaction columns $a+b, \ldots, a+(s'-1)b$ by $ab, \ldots, ab^{s'-1}$ for ease of expression. Let $E = (e_1, \ldots, e_{m'})$ be the complement of A in S, where $m' = (n-1)/(s'-1) - m$. A lower bound for $A_2(D)$ can be derived under this setting.

Theorem 4.4. *Suppose D is an $SOA_{s'}(n, s^m)$ with columns of A and B selected from a regular design. Then $A_2(D) \geq \mathcal{B}(m, n, s')$ where*

$$\mathcal{B}(m, n, s') = \xi(s'-1)(2s'm - m' - m'\xi)/2$$

with $\xi = \lfloor s'm/m' \rfloor$. The lower bound is achieved if and only if the frequencies of $e_1, \ldots, e_{m'}$ in $(b_1, a_1b_1, \ldots, a_1b_1^{s'-1}, \ldots\ldots, b_m, a_mb_m, \ldots, a_mb_m^{s'-1})$ differ by at most 1.

He et al. (2018) constructed some $\mathrm{SOA}_2(16, 4^{10})$s, $\mathrm{SOA}_2(32, 4^{22})$s and an $\mathrm{SOA}_3(81, 9^{25})$. We conduct a computer search for SOAs with small $A_2(D)$s by selecting columns of A from

Table 4.1: Some four-level SOAs obtained by computer search and the recursive construction.

$n \times m$	$A_2(D)$	LB	$4n \times (4m+1)$	$A_2(\tilde{D})$	LB	$16n \times (16m+5)$	$A_2(\tilde{\tilde{D}})$	LB
16×6	$3^{\dagger}$	3	64×25	$12^{\dagger}$	12	256×101	$48^{\dagger}$	48
16×7	$6^{\dagger}$	6	64×29	$24^{\dagger}$	24	256×117	$96^{\dagger}$	96
16×8	12	11	64×33	48	42	256×133	192	166
16×9	$18^{\dagger}$	18	64×37	72	70	256×149	288	278
16×10	$30^{\dagger}$	30	64×41	120	114	256×165	480	450
32×11	3	2	128×45	12	8	512×181	48	32
32×12	$5^{\dagger}$	5	128×49	$20^{\dagger}$	20	512×197	$80^{\dagger}$	80
32×13	$8^{\dagger}$	8	128×53	$32^{\dagger}$	32	512×213	$128^{\dagger}$	128
32×14	$11^{\dagger}$	11	128×57	$44^{\dagger}$	44	512×229	$176^{\dagger}$	176
32×15	$14^{\dagger}$	14	128×61	$56^{\dagger}$	56	512×245	$224^{\dagger}$	224
32×16	$19^{\dagger}$	19	128×65	76	74	512×261	304	294
32×17	$26^{\dagger}$	26	128×69	104	102	512×277	416	406
32×18	$33^{\dagger}$	33	128×73	132	130	512×293	528	518
32×19	43	42	128×77	172	162	512×309	688	642
32×20	$54^{\dagger}$	54	128×81	216	210	512×325	864	834
32×21	72	68	128×85	288	260	512×341	1152	1028
32×22	98	86	128×89	392	332	512×357	1568	1316

those that constructed these designs and then selecting columns of B from E such that D is an SOA. The designs found are presented in the left blocks of Tables 4.1 and 4.2, where for each case the corresponding lower bound in Theorem 4.4 is given under the column LB. An A_2 value that attains the lower bound is highlighted by a dagger. As can be seen, the lower bound is attained for $m = 6, 7, 9, 10$ when $n = 16$, for $m = 12, 13, 14, 15, 16, 17, 18, 20$ when $n = 32$, and for $m = 11, 12, 13, 14, 18, 19, 21$ when $n = 81$.

Based on these designs, we propose two recursive constructions to obtain larger designs that attain or approach the lower bound. When $s' = 2$, we follow the convention to denote the two levels by $\{-1, 1\}$. Thus A, B and D are related through $D = A + B/2 + 3/2$ instead of $D = 2A + B$. Given an $\mathrm{SOA}_2(n, 4^m)$, say D, a larger design of $4n$ runs for $4m+1$ factors, say $\tilde{D}$, can be obtained by taking

$$\tilde{A} = (A, \mathbf{x}A, \mathbf{y}A, \mathbf{xy}A, \mathbf{xy}), \qquad \tilde{B} = (B, \mathbf{xy}B, \mathbf{x}B, \mathbf{y}B, \mathbf{x}), \tag{4.9}$$

Table 4.2: Some nine-level SOAs obtained by computer search and the recursive construction.

$n \times m$	$A_2(D)$	LB	$9n \times (9m+1)$	$A_2(\tilde{D})$	LB	$81n \times (81m+10)$	$A_2(\tilde{\tilde{D}})$	LB
81×11	$8^\dagger$	8	729×100	$72^\dagger$	72	6561×901	$648^\dagger$	648
81×12	$16^\dagger$	16	729×109	$144^\dagger$	144	6561×982	$1296^\dagger$	1296
81×13	$24^\dagger$	24	729×118	$216^\dagger$	216	6561×1063	$1944^\dagger$	1944
81×14	$32^\dagger$	32	729×127	$288^\dagger$	288	6561×1144	$2592^\dagger$	2592
81×15	42	40	729×136	378	360	6561×1225	3402	3240
81×16	54	48	729×145	486	432	6561×1306	4374	3888
81×17	68	66	729×154	612	588	6561×1387	5508	5286
81×18	$84^\dagger$	84	729×163	756	750	6561×1468	6804	6744
81×19	$102^\dagger$	102	729×172	918	912	6561×1549	8262	8202
81×20	126	120	729×181	1134	1074	6561×1630	10206	9660
81×21	$150^\dagger$	150	729×190	1350	1332	6561×1711	12150	11970
81×22	190	180	729×199	1710	1602	6561×1792	15390	14400
81×23	234	212	729×208	2106	1872	6561×1873	18954	16830
81×24	284	256	729×217	2556	2268	6561×1954	23004	20376
81×25	330	300	729×226	2970	2664	6561×2035	26730	23940

and $\tilde{D} = \tilde{A} + \tilde{B}/2 + 3/2$, where $\mathbf{x}$ and $\mathbf{y}$ are new independent columns. It can be verified that $\tilde{D}$ is an $\mathrm{SOA}_2(4n, 4^{4m+1})$, and calculated by Proposition 4.2 that $A_2(\tilde{D}) = 4A_2(D)$. We note that there are other choices for $\tilde{A}$ and $\tilde{B}$; for example, we may replace $\tilde{B}$ in (4.9) by $\tilde{B} = (B, \mathbf{y}B, \mathbf{xy}B, \mathbf{x}B, \mathbf{y})$ to obtain an $\mathrm{SOA}_2(4n, 4^{4m+1})$, which also has $A_2(\tilde{D}) = 4A_2(D)$.

Suppose D is an $\mathrm{SOA}_{s'}(n, s^m)$. Define the A_2-efficiency of D as $\varphi(D) = \mathcal{B}(m, n, s')/A_2(D)$. Then we have $\varphi(\tilde{D}) = h(m, n)\varphi(D)$, where

$$h(m, n) = \frac{\mathcal{B}(4m+1, 4n, 2)}{4\mathcal{B}(m, n, 2)} \tag{4.10}$$

is a measure of the efficiency of the recursive construction in (4.9). It can be checked that $h(m, n) \geq 95\%$ for all $2^4 \leq n \leq 2^{16}$ and any m such that an $\mathrm{SOA}_2(n, 4^m)$ can be constructed by Cheng et al. (2021). In particular, we have that $h(m, n) = 100\%$ if $(n-1)/3 < m \leq (n-1)/2$. Therefore, $\tilde{D}$ has small $A_2(\tilde{D})$ as long as D has small $A_2(D)$. Applying the construction successively to the designs in the left block of Table 4.1, we obtain the SOAs displayed in the middle and right blocks of the table.

Next consider $s' = 3$ and $s = 9$. Suppose A and B are selected from a three-level regular design such that $D = 3A + B$ is an $\mathrm{SOA}_3(n, 9^m)$. Let

$$\tilde{A} = (A, \mathbf{x}A, \mathbf{y}A, \mathbf{x}^2A, \mathbf{xy}A, \mathbf{x}^2\mathbf{y}A, \mathbf{y}^2A, \mathbf{xy}^2A, \mathbf{x}^2\mathbf{y}^2A, \mathbf{x}), \tag{4.11}$$

$$\tilde{B} = (B, \mathbf{y}B, \mathbf{x}^2B, \mathbf{y}^2B, \mathbf{xy}^2B, \mathbf{xy}B, \mathbf{x}B, \mathbf{x}^2\mathbf{y}^2B, \mathbf{x}^2\mathbf{y}B, \mathbf{y}), \tag{4.12}$$

where $\mathbf{x}$ and $\mathbf{y}$ are new independent columns. Then it can be verified directly that $\tilde{D} = 3\tilde{A} + \tilde{B}$ is an $\mathrm{SOA}_3(9n, 9^{9m+1})$ with $A_2(\tilde{D}) = 9A_2(D)$. Similar to in the four-level case, the choices of $\tilde{A}$ and $\tilde{B}$ are not unique. We have that $\varphi(\tilde{D}) = h'(m, n)\varphi(D)$, where

$$h'(m, n) = \frac{\mathcal{B}(9m + 1, 9n, 3)}{9\mathcal{B}(m, n, 3)} \tag{4.13}$$

measures the efficiency of the recursive construction. It can be checked that $h'(m, n) \geq 98\%$ for all $3^4 \leq n \leq 3^{10}$ and any m such that an $\mathrm{SOA}_3(n, 9^m)$ can be constructed by He et al. (2018). Particularly, we have $h'(m, n) = 100\%$ if $(n - 1)/8 < m \leq (n - 1)/5$. Applying this construction to the designs of 81 runs in Table 4.2, we obtain the SOAs of 729 and 6561 runs in the table. The two construction methods are summarized in Theorem 4.5.

Theorem 4.5. *Let $k \geq 3$ be a positive integer.*

(i) Given an $SOA_2(2^k, 4^m)$, say D_1, an $SOA_2(2^{k+2}, 4^{4m+1})$, say $\tilde{D}_1$, can be constructed such that $A_2(\tilde{D}_1) = 4A_2(D_1)$. The efficiency of this construction, as given in (4.10), has that $h(m, n) = 100\%$ for $(n - 1)/3 < m \leq (n - 1)/2$ and $h(m, n) \geq 95\%$ for all $2^4 \leq n \leq 2^{16}$ and any m such that an $SOA_2(n, 4^m)$ can be constructed by Cheng et al. (2021).

(ii) Given an $SOA_3(3^k, 9^m)$, say D_2, an $SOA_3(3^{k+2}, 9^{9m+1})$, say $\tilde{D}_2$, can be constructed such that $A_2(\tilde{D}_2) = 9A_2(D_2)$. The efficiency of this construction, as given in (4.13), has that $h'(m, n) = 100\%$ for $(n - 1)/8 < m \leq (n - 1)/5$ and $h'(m, n) \geq 98\%$ for all $3^4 \leq n \leq 3^{10}$ and any m such that an $SOA_3(n, 9^m)$ can be constructed by He et al. (2018).

We conclude this subsection with an example.

Example 4.4. *Table 4.2 has an* $SOA_3(6561, 9^{2035})$ *with* $A_2(\tilde{\tilde{D}}) = 26,730$ *and* $\varphi(\tilde{\tilde{D}}) = 89.6\%$*, obtained from the recursive construction. This SOA does not fare very well in terms of the* A_2 *value when compared with a random* $U(6561, 9^{2035})$*, which has a mean* A_2 *value of* $20,191$*. On the other hand, by dropping columns from each group of an* $MNOA_3(6561, (9^4)^{820})$ *as evenly as possible, we can obtain an* $OABD_3(6561, 9^{2035})$ *with an* A_2 *value of* $12,880$*. This motivates us to study MNOAs and related designs in the next subsection.*

4.4.2 A class of MNOAs and its variants

We now turn our attention to another family of OABDs with small $A_2(D)$. Such designs, which are inspired by a class of MNOAs, also have small $\bar{\chi}(D)$ as they minimize the first term of (4.5) in Theorem 4.2. The following lower bound on $A_2(D)$ of U-type designs, given by Xu and Wu (2005), is useful for design evaluations.

Lemma 4.4. *Suppose* D *is a* $U(n, s^m)$*. Then*

$$A_2(D) \geq m(s-1)(ms-m-n+1)/(2(n-1)) + (n-1)s^2\eta(1-\eta)/(2n),$$

where $\eta = m(n-s)/((n-1)s) - \lfloor m(n-s)/((n-1)s) \rfloor$*. The lower bound is attained if and only if the numbers of coincidences between rows of* D *differ by at most 1.*

We first investigate a class of MNOAs from Mukerjee et al. (2014). The construction is briefly described as follows. Suppose s' is a prime power. For $k \geq 2$, let Q be an $\mathrm{OA}((s')^2, s'+1, s', 2)$ and P be an $\mathrm{OA}(n, m_1, s, 2)$, where $s = (s')^2$, $n = s^k$ and $m_1 = (n-1)/(s-1)$. Obtain a $\mathrm{U}(s, s^{m_1})$, say R, by replacing the s' entries of l in turn by $\{ls', \ldots, ls'+s'-1\}$ for $l = 0, \ldots, s'-1$ in each column of Q. We then construct a design, which we denote by $D_{n,(s'+1)m_1}$, by replacing level i of P by the $(i+1)$th row of R for $i = 0, \ldots, s-1$. According to Mukerjee et al. (2014), $D_{n,(s'+1)m_1}$ is an $\mathrm{MNOA}_{s'}(n, (s^{s'+1})^{m_1})$. Examples of this class of designs include $\mathrm{MNOA}_2(16, (4^3)^5)$, $\mathrm{MNOA}_2(64, (4^3)^{21})$, $\mathrm{MNOA}_2(256, (4^3)^{85})$, $\mathrm{MNOA}_3(81, (9^4)^{10})$ and $\mathrm{MNOA}_3(729, (9^4)^{91})$.

Now let's label the columns of $D_{n,(s'+1)m_1}$ by $1, 2, \ldots, (s'+1)m_1$ and then rearrange the columns in the order of $1, s'+2, \ldots, (s'+1)m_1 - s'; 2, s'+3, \ldots, (s'+1)m_1 - s'+1; \ldots\ldots; s'+1, 2s'+2, \ldots, (s'+1)m_1$. Since any two columns from different groups of the MNOA form an OA$(n, 2, s, 2)$, it can be seen the rearranged design is a juxtaposition of $s'+1$ saturated orthogonal arrays. As in the construction of supersaturated designs (Xu and Wu, 2005), we can obtain a design for $m \leq (s'+1)m_1$ factors by taking the first m rearranged columns and denote it by $D_{n,m}$. This procedure is equivalent to dropping columns from each group of the MNOA as evenly as possible. Thus $D_{n,m}$s are still MNOAs but may have unequal group sizes. $A_2(D_{n,m})$ can be calculated as given in the following result.

Theorem 4.6. *Suppose s' is a prime or prime power and k is a positive integer. Let $s = (s')^2$ and $n = s^k$. Then $D_{n,m}$ is an OABD$_{s'}(n, s^m)$ with*

$$A_2(D_{n,m}) = \zeta(s'-1)(2s'm + 2m - m_2 - m_2\zeta)/2$$

where $m_2 = (n-1)/(s'-1)$ and $\zeta = \lfloor (s'+1)m/m_2 \rfloor$. In particular, $A_2(D_{n,m})$ attains the lower bound in Lemma 4.4 if $m = m_1 l$ or $m_1 l \pm 1$ for some integer l, where $m_1 = (n-1)/(s-1)$.

The MNOAs $D_{n,m}$s in Theorem 4.6 are attractive for small $A_2(D)$, and have nice performance under $\bar{\chi}(D)$ as we will see in Section 4.4.3. Motivated by this desirable property, we construct some OABD$_{s'}(n, s^m)$s also targeted at small $A_2(D)$ by selecting columns of A and B from S, a saturated regular design OA$(n, m_2, s', 2)$ where $m_2 = (n-1)/(s'-1)$. Then we have the following lower bound parallel to Theorem 4.4.

Theorem 4.7. *Suppose D is an OABD$_{s'}(n, s^m)$ with columns of A and B selected from a regular design. Then $A_2(D) \geq \mathcal{B}^*(m, n, s')$ where*

$$\mathcal{B}^*(m, n, s') = \zeta(s'-1)(2s'm + 2m - m_2 - m_2\zeta)/2$$

with $m_2 = (n-1)/(s'-1)$ and $\zeta = \lfloor (s'+1)m/m_2 \rfloor$. The equality holds if and only if the frequencies of the columns of S in $(a_1, b_1, a_1b_1, \ldots, a_1b_1^{s'-1}, \ldots\ldots, a_m, b_m, a_mb_m, \ldots, a_mb_m^{s'-1})$ differ by at most 1.

The $D_{n,m}$s in Theorem 4.6 attain the lower bound in Theorem 4.7, though they are constructed in a different way. Now we construct a class of OABD$_2(n, 4^m)$s for $n = 2^{2k+1}$

($k \geq 1$), a situation not covered by Theorem 4.6. Denote the final design with n runs and m factors by $D_{n,m}$. For ease of expression, we represent the ith column of $D_{n,m}$ by the pair (a_i, b_i). In the following, $\mathbf{1}$, $\mathbf{2}$, $\mathbf{3}$, $\mathbf{x}$ and $\mathbf{y}$ are independent columns. For $n = 8$, define

$$G_8^{(1)} = (\mathbf{23}, \mathbf{123}), \quad G_8^{(2)} = ((\mathbf{13}, \mathbf{1}), (\mathbf{3}, \mathbf{12})),$$
$$G_8^{(3)} = (\mathbf{12}, \mathbf{23}), \quad G_8^{(4)} = ((\mathbf{123}, \mathbf{13}), (\mathbf{2}, \mathbf{3})), \quad G_8^{(5)} = (\mathbf{1}, \mathbf{2})$$

and let $D_{8,7} = (G_8^{(1)}, G_8^{(2)}, G_8^{(3)}, G_8^{(4)}, G_8^{(5)})$. Then for $n \geq 8$, recursively define $G_{4n}^{(i)}$s based on $G_n^{(i)}$s by

$$G_{4n}^{(1)} = (G_n^{(1)}, (\mathbf{xy}, \mathbf{x}), (\mathbf{xy}, \mathbf{x})D_{n,n-1}), \quad G_{4n}^{(2)} = G_n^{(2)}, \quad G_{4n}^{(4)} = G_n^{(4)},$$
$$G_{4n}^{(3)} = (G_n^{(3)}, (\mathbf{y}, \mathbf{xy}), (\mathbf{y}, \mathbf{xy})D_{n,n-1}), \quad G_{4n}^{(5)} = (G_n^{(5)}, (\mathbf{x}, \mathbf{y}), (\mathbf{x}, \mathbf{y})D_{n,n-1}).$$

Let $D_{4n,4n-1} = (G_{4n}^{(1)}, G_{4n}^{(2)}, G_{4n}^{(3)}, G_{4n}^{(4)}, G_{4n}^{(5)})$. For any $n = 2^{2k+1}$, the design $D_{n,m}$ with $m < n-1$ is obtained by successively removing columns of $D_{n,n-1}$ from $G_n^{(5)}$ to $G_n^{(1)}$.

Theorem 4.8. *For $n = 2^{2k+1}$ ($k \geq 1$), design $D_{n,m}$ constructed above is an OABD$_2(n, 4^m)$ with*

$$A_2(D_{n,m}) = \begin{cases} 1, & \text{if } m = (n-2)/3, \\ 3m - n + 2, & \text{if } (n+1)/3 \leq m \leq (2n-4)/3, \\ n+2, & \text{if } m = (2n-1)/3, \\ 6m - 3n + 3, & \text{if } (2n+2)/3 \leq m \leq n-1. \end{cases}$$

In particular, $A_2(D_{n,m})$ attains the lower bound in Lemma 4.4 for $m = (n-2)/3$, $(2n-4)/3$, $(2n-1)/3$ and $n-1$.

Given an OABD$_{s'}(n, s^m)$, say D, we define its A_2-efficiency as $\varphi^*(D) = \mathcal{B}^*(m, n, s')/A_2(D)$. Then a simple calculation shows that $\varphi^*(D_{n,m}) = 1 - 1/(3m - n + 2)$ for $(n+1)/3 \leq m < (2n-4)/3$ and $\varphi^*(D_{n,m}) = 1$ for $(2n+2)/3 \leq m \leq n-1$. Therefore, the $D_{n,m}$s in Theorem 4.8 are quite efficient in terms of $A_2(D)$, especially for large m. Also note that when $m = (n-2)/3$, $D_{n,m}$ is actually an SOA$_2(n, 4^m)$. Thus the following result is immediate from Theorems 4.2 and 4.8.

Corollary 4.3. *Suppose $n = 2^{2k+1}$ for $k \geq 1$ and $m = (n-2)/3$. Then $D_{n,m}$ is an $SOA_2(n, 4^m)$, and thus minimizes $\bar{\chi}(D)$ among all $OABD_2(n, 4^m)$s.*

Next we construct some $\mathrm{OABD}_3(n, 9^m)$s with $n = 3^{2k+1}$ for some positive integer k. A computer search is used to address the case $n = 27$. Denote the independent columns of S, an $\mathrm{OA}(27, 13, 3, 2)$ by $\mathbf{1}$, $\mathbf{2}$ and $\mathbf{3}$. Let

$$A_{27,13} = (\mathbf{1}, \mathbf{2}, \mathbf{12}, \mathbf{12}^2, \mathbf{3}, \mathbf{13}, \mathbf{23}, \mathbf{123}, \mathbf{12}^2\mathbf{3}, \mathbf{13}^2, \mathbf{23}^2, \mathbf{123}^2, \mathbf{12}^2\mathbf{3}^2),$$

$$B_{27,13} = (\mathbf{12}, \mathbf{13}^2, \mathbf{12}^2\mathbf{3}^2, \mathbf{123}^2, \mathbf{13}, \mathbf{123}, \mathbf{1}, \mathbf{3}, \mathbf{23}, \mathbf{23}^2, \mathbf{2}, \mathbf{12}^2\mathbf{3}, \mathbf{12}^2),$$

and $D_{27,13} = 3A_{27,13} + B_{27,13}$. The designs $D_{27,m}$s for $2 \leq m < 13$ can be obtained by dropping the columns of $D_{27,13}$ from left to right. One can check directly that $D_{27,m}$s for $2 \leq m \leq 13$ are all $\mathrm{OABD}_3(27, 9^m)$s reaching the lower bound in Lemma 4.4.

For $n = 3^{2k+1}$ runs with $k \geq 2$, we can apply the technique in Section 4.4.1 again by replacing A in (4.11) by $A_{n,(n-1)/2}$, and B in (4.12) by $B_{n,(n-1)/2}$, and defining $A_{9n,(9n-1)/2} = (\tilde{A}, \mathbf{y}, \mathbf{xy}, \mathbf{x}^2\mathbf{y})$ and $B_{9n,(9n-1)/2} = (\tilde{B}, \mathbf{x}^2, \mathbf{xy}^2, \mathbf{xy})$. Then $D_{9n,(9n-1)/2} = 3A_{9n,(9n-1)/2} + B_{9n,(9n-1)/2}$ can be verified to be an $\mathrm{OABD}_3(9n, 9^{(9n-1)/2})$ that attains the lower bound in Lemma 4.4.

4.4.3 A comparison of the two families of OABDs

In this subsection, we compare two families of space-filling OABDs presented in Sections 4.4.1 and 4.4.2, where the first minimizes $\mu(D)$ and $A_2(D)$ sequentially while the second minimizes $A_2(D)$ directly.

For the first family of OABDs, the designs to be compared include $\mathrm{SOA}_2(8, 4^m)$s and $\mathrm{SOA}_3(27, 9^m)$s justified by Theorem 4.3, the $\mathrm{SOA}_2(16, 4^m)$s, $\mathrm{SOA}_2(32, 4^m)$s and $\mathrm{SOA}_3(81, 9^m)$s found by a computer search in Section 4.4.1 and the $\mathrm{SOA}_2(64, 4^m)$s obtained by a combination of a computer search and the recursive construction in Theorem 4.5. When SOAs are not available, Shi and Tang (2019) obtained some four-level designs that maximize the proportion of ordered column pairs stratified over the 4×2 grid. This is equivalent to minimizing $\mu(D)$ as implied in the proof of Theorem 4.4. For the nine-level case where such results are not available, we still use a computer search to obtain designs with small $\mu(D)$.

We then search for those with small $A_2(D)$ among these designs with minimum or small $\mu(D)$. These near SOAs are also included for comparison. The detailed constructions of all the SOAs and near SOAs mentioned above are available upon request. For the second family of OABDs, we investigate the performance of the $D_{16,m}$s, $D_{64,m}$s and $D_{81,m}$s from Theorem 4.6, the $D_{8,m}$s and $D_{32,m}$s given by Theorem 4.8, and the $D_{27,m}$s constructed at the end of Section 4.4.2.

We compare all these designs in terms of $A_2(D)$, $\mu(D)$, $\bar{\phi}_1(D)$ and $\bar{\phi}_2(D)$. Here we choose ϕ_1 and ϕ_2 as our space-filling criteria χ for the same reason as mentioned in Examples 4.2 and 4.3. In other words, the results for $\chi = \psi$ and $\chi = \rho$ are similar to those for $\chi = \phi_1$ and $\chi = \phi_2$, respectively. The comparison results are displayed in Tables 4.3, 4.4 and 4.5. The lower bounds in Lemma 4.4 are given under the columns labeled A_2^*; we mark an A_2 value by a dagger if it attains this bound. Presented in the last two columns are the values of $\bar{\phi}_{1,o}$ and $\bar{\phi}_{2,o}$ in Theorem 4.1. They represent the average performance of a random OABD, that is, a design obtained by randomly permuting and expanding the levels of an orthogonal array.

A simple calculation shows that the lower bound $\mathcal{B}(m, n, s')$ in Theorem 4.4 is less than or equal to $A_2(D_{n,m})$s when m is roughly less than $n/2$ and $n/5$ for 4-level and 9-level designs, respectively. This implies that in these cases we may find SOAs with the same or smaller $A_2(D)$s compared to $D_{n,m}$s. This is confirmed for $n = 8$ and $m \leq 3$, $n = 16$ and $m \leq 7$, $n = 32$ and $m \leq 15$, $n = 27$ and $m \leq 6$ in the tables. There are only two such designs found for $n = 64$, namely the $\mathrm{SOA}_2(64, 4^{25})$ and $\mathrm{SOA}_2(64, 4^{29})$ obtained by the recursive construction, and four such designs found for $n = 81$, namely those with $m \leq 14$. This is probably because there are too many potential SOAs for the computer to handle. Also note that in addition to the designs mentioned in Theorem 4.3 and Corollary 4.3, the $\mathrm{SOA}_2(16, 4^6)$, $\mathrm{SOA}_2(16, 4^7)$, $\mathrm{SOA}_2(32, 4^{11})$, $\mathrm{SOA}_3(81, 9^{11})$, $\mathrm{SOA}_3(81, 9^{12})$, $\mathrm{SOA}_3(81, 9^{13})$ and $\mathrm{SOA}_3(81, 9^{14})$ all reach the lower bound in Lemma 4.4 and thus are optimal under $\bar{\chi}(D)$.

When m is larger, the (near) SOAs have greater $A_2(D)$s than those of $D_{n,m}$s. Nevertheless, the (near) SOAs have smaller $\mu(D)$ and because of this, they still outperform $D_{n,m}$s under $\bar{\phi}_1(D)$ for all 8-run and 27-run cases, and for $n = 16$ and $m \leq 12$, $n = 32$ and $m \leq 21$,

Table 4.3: A comparison of SOAs and near SOAs with $D_{n,m}$s for n = 8, 16, 32.

$n \times m$	SOAs and near SOAs				$D_{n,m}$s				A_2^*	$\bar{\phi}_{1,o}$	$\bar{\phi}_{2,o}$
	$A_2(D)$	$\mu(D)$	$\bar{\phi}_1(D)$	$\bar{\phi}_2(D)$	$A_2(D)$	$\mu(D)$	$\bar{\phi}_1(D)$	$\bar{\phi}_2(D)$			
8×2	$1^\dagger$	0	1.27	14.92	$1^\dagger$	0	1.27	14.92	1	1.49	15.62
8×3	$3^\dagger$	0	1.35	19.53	$3^\dagger$	1	1.63	20.53	3	2.01	21.63
8×4	$6^\dagger$	1	1.35	23.24	$6^\dagger$	4	2.20	26.24	6	2.39	26.44
8×5	$10^\dagger$	4	1.55	27.06	$10^\dagger$	7	2.41	30.06	10	2.63	30.05
8×6	21	6	1.96	28.84	$15^\dagger$	10	2.24	31.98	15	2.72	32.46
8×7	$21^\dagger$	14	2.00	33.00	$21^\dagger$	14	2.00	33.00	21	2.67	33.67
16×6	$3^\dagger$	0	2.40	37.20	$3^\dagger$	2	2.93	39.07	3	4.24	41.90
16×7	$6^\dagger$	0	2.36	40.62	$6^\dagger$	4	3.42	44.36	6	4.70	46.97
16×8	12	0	2.49	43.56	$9^\dagger$	6	3.69	48.76	9	5.08	51.48
16×9	18	0	2.40	45.60	$12^\dagger$	8	3.73	52.27	12	5.39	55.44
16×10	30	0	2.89	47.56	$15^\dagger$	10	3.56	54.89	15	5.62	58.86
16×11	33	5	3.29	52.09	$21^\dagger$	14	4.09	58.89	21	5.79	61.73
16×12	40	9	3.73	55.33	$27^\dagger$	18	4.40	62.00	27	5.88	64.05
16×13	54	12	4.62	57.69	$33^\dagger$	22	4.49	64.22	33	5.90	65.82
16×14	105	14	9.96	63.16	$39^\dagger$	26	4.36	65.56	39	5.84	67.04
16×15	$45^\dagger$	30	4.00	66.00	$45^\dagger$	30	4.00	66.00	45	5.71	67.71
32×10	$1^\dagger$	0	4.60	64.48	$1^\dagger$	0	4.60	64.48	1	7.55	71.29
32×11	$3^\dagger$	0	4.74	68.88	$3^\dagger$	1	4.99	69.79	3	8.10	76.98
32×12	5	0	4.77	72.87	6	4	5.93	76.61	4.5	8.62	82.41
32×13	8	0	4.82	76.57	9	6	6.50	82.12	5.5	9.11	87.57
32×14	11	0	4.77	79.85	12	8	6.96	87.21	8.5	9.56	92.47
32×15	14	0	4.62	82.72	15	10	7.33	91.88	12	9.98	97.11
32×16	19	0	4.62	85.43	18	12	7.58	96.14	15	10.35	101.49
32×17	26	0	4.77	87.98	21	14	7.74	99.98	17.5	10.70	105.61
32×18	33	0	4.82	90.12	24	16	7.79	103.41	20.5	11.00	109.46
32×19	43	0	5.15	92.22	27	18	7.73	106.42	25.5	11.27	113.06
32×20	54	0	5.51	94.04	$30^\dagger$	20	7.58	109.01	30	11.51	116.39
32×21	72	0	6.67	96.35	$34^\dagger$	23	7.70	112.22	34	11.71	119.46
32×22	98	0	8.75	99.27	39	26	7.85	115.14	37.5	11.87	122.26
32×23	104	3	8.93	101.91	45	30	8.28	118.68	43.5	12.00	124.81
32×24	111	6	9.13	104.25	51	34	8.61	121.80	49.5	12.09	127.09
32×25	124	10	10.26	107.86	57	38	8.84	124.51	55	12.15	129.11
32×26	128	16	10.63	111.70	63	42	8.96	126.80	60	12.17	130.87
32×27	142	21	11.94	115.51	69	46	8.97	128.67	66	12.15	132.37
32×28	171	25	14.82	119.93	75	50	8.89	130.13	73.5	12.10	133.60
32×29	238	28	22.24	127.94	81	54	8.70	131.17	80.5	12.01	134.57
32×30	465	30	49.95	155.28	$87^\dagger$	58	8.40	131.79	87	11.89	135.28
32×31	$93^\dagger$	62	8.00	132.00	$93^\dagger$	62	8.00	132.00	93	11.73	135.73

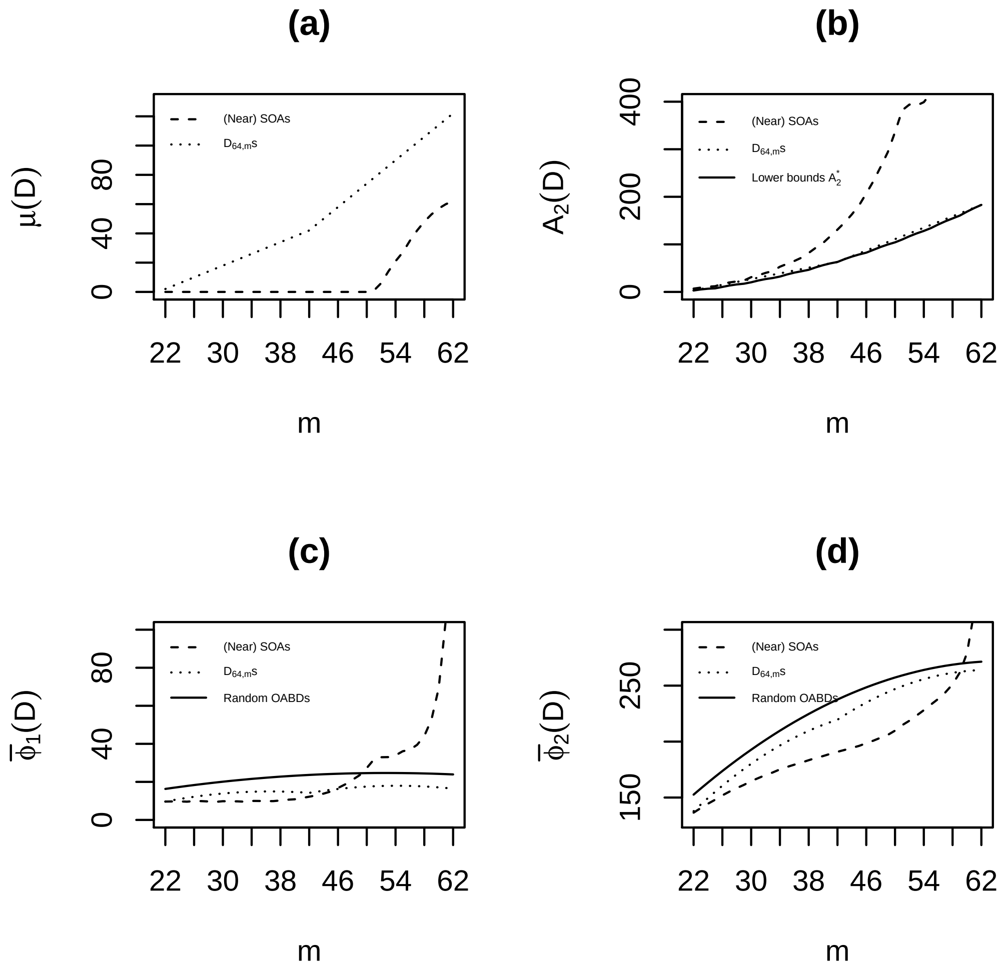
Table 4.4: A comparison of SOAs and near SOAs with $D_{n,m}$s for $n = 64$.

$n \times m$	SOAs and near SOAs				$D_{n,m}$s				A_2^*	$\bar{\phi}_{1,o}$	$\bar{\phi}_{2,o}$
	$A_2(D)$	$\mu(D)$	$\bar{\phi}_1(D)$	$\bar{\phi}_2(D)$	$A_2(D)$	$\mu(D)$	$\bar{\phi}_1(D)$	$\bar{\phi}_2(D)$			
64×22	7	0	9.65	136.49	$3^\dagger$	2	9.65	137.76	3	16.30	152.60
64×23	9	0	9.72	140.59	6	4	10.35	143.77	5.25	16.83	158.07
64×24	11	0	9.74	144.49	9	6	11.01	149.57	6.75	17.35	163.41
64×25	12	0	9.59	148.06	12	8	11.62	155.17	7.5	17.85	168.62
64×26	17	0	9.89	151.94	15	10	12.17	160.57	10.5	18.34	173.70
64×27	20	0	9.89	155.36	18	12	12.68	165.77	13.5	18.80	178.65
64×28	22	0	9.71	158.45	21	14	13.14	170.77	15.75	19.25	183.48
64×29	24	0	9.48	161.34	24	16	13.54	175.56	17.25	19.68	188.17
64×30	31	0	9.83	164.66	27	18	13.90	180.15	20.25	20.09	192.74
64×31	35	0	9.76	167.40	30	20	14.20	184.55	24	20.49	197.18
64×32	40	0	9.76	170.07	33	22	14.45	188.74	27	20.86	201.50
64×33	44	0	9.58	172.41	36	24	14.66	192.73	29.25	21.22	205.68
64×34	53	0	9.99	175.18	39	26	14.81	196.51	32.25	21.57	209.74
64×35	59	0	9.96	177.37	42	28	14.91	200.10	36.75	21.89	213.67
64×36	65	0	9.89	179.36	45	30	14.97	203.48	40.5	22.19	217.47
64×37	72	0	9.89	181.27	48	32	14.97	206.67	43.5	22.48	221.14
64×38	82	0	10.22	183.36	51	34	14.92	209.65	46.5	22.75	224.69
64×39	93	0	10.63	185.38	54	36	14.82	212.43	51.75	23.01	228.11
64×40	103	0	10.86	187.07	57	38	14.67	215.00	56.25	23.24	231.40
64×41	117	0	11.55	189.06	$60^\dagger$	40	14.47	217.38	60	23.46	234.56
64×42	131	0	12.19	190.86	$63^\dagger$	42	14.22	219.56	63	23.66	237.59
64×43	146	0	12.91	192.58	69	46	14.81	223.69	69	23.84	240.50
64×44	163	0	13.83	194.35	75	50	15.35	227.62	74.25	24.00	243.28
64×45	182	0	14.95	196.17	81	54	15.84	231.35	78.75	24.15	245.93
64×46	207	0	16.78	198.56	87	58	16.27	234.87	82.5	24.28	248.45
64×47	233	0	18.69	200.87	93	62	16.66	238.20	88.5	24.39	250.84
64×48	263	0	21.06	203.48	99	66	17.00	241.32	94.5	24.48	253.11
64×49	294	0	23.51	206.02	105	70	17.28	244.25	99.75	24.56	255.25
64×50	336	0	27.30	209.76	111	74	17.52	246.97	104.25	24.61	257.26
64×51	382	1	31.80	214.69	117	78	17.71	249.49	110.25	24.65	259.14
64×52	394	6	32.95	218.66	123	82	17.84	251.81	117	24.67	260.89
64×53	392	14	33.04	223.32	129	86	17.92	253.92	123	24.68	262.52
64×54	399	21	33.96	228.03	135	90	17.96	255.84	128.25	24.66	264.02
64×55	418	27	36.10	233.17	141	94	17.94	257.55	134.25	24.63	265.39
64×56	423	35	36.92	238.11	147	98	17.88	259.06	141.75	24.58	266.63
64×57	444	42	39.47	243.99	153	102	17.76	260.37	148.5	24.52	267.74
64×58	484	48	44.13	251.19	159	106	17.59	261.48	154.5	24.43	268.73
64×59	558	53	52.80	261.63	165	110	17.37	262.39	160.5	24.33	269.59
64×60	696	57	69.30	279.09	171	114	17.11	263.09	168.75	24.21	270.32
64×61	994	60	105.80	315.79	177	118	16.79	263.60	176.25	24.07	270.92
64×62	1953	62	225.94	435.33	$183^\dagger$	122	16.42	263.90	183	23.92	271.40
64×63	$189^\dagger$	126	16.00	264.00	$189^\dagger$	126	16.00	264.00	189	23.74	271.74

Table 4.5: A comparison of SOAs and near SOAs with $D_{n,m}$s for $n = 27$, 81.

$n \times m$	SOAs and near SOAs				$D_{n,m}$s						
	$A_2(D)$	$\mu(D)$	$\bar{\phi}_1(D)$	$\bar{\phi}_2(D)/10^2$	$A_2(D)$	$\mu(D)$	$\bar{\phi}_1(D)$	$\bar{\phi}_2(D)/10^2$	A_2^*	$\bar{\phi}_{1,o}$	$\bar{\phi}_{2,o}/10^2$
27×2	$2^\dagger$	0	8.15	4.83	$2^\dagger$	0	8.15	4.83	2	8.44	4.86
27×3	$6^\dagger$	0	11.31	7.04	$6^\dagger$	2	11.85	7.09	6	12.18	7.12
27×4	$12^\dagger$	0	13.85	9.10	$12^\dagger$	4	14.95	9.21	12	15.60	9.27
27×5	$20^\dagger$	0	15.79	11.03	$20^\dagger$	10	18.53	11.30	20	18.70	11.30
27×6	$30^\dagger$	0	17.12	12.82	$30^\dagger$	14	20.95	13.19	30	21.48	13.22
27×7	$42^\dagger$	6	19.48	14.62	$42^\dagger$	22	23.86	15.05	42	23.94	15.03
27×8	68	12	21.78	16.30	$56^\dagger$	26	25.06	16.66	56	26.08	16.73
27×9	90	18	23.19	17.83	$72^\dagger$	36	27.29	18.29	72	27.91	18.31
27×10	108	28	24.81	19.33	$90^\dagger$	46	28.91	19.79	90	29.41	19.78
27×11	134	40	26.64	20.74	$110^\dagger$	56	29.93	21.14	110	30.59	21.14
27×12	204	48	28.69	21.95	$132^\dagger$	66	30.33	22.35	132	31.46	22.38
27×13	$156^\dagger$	78	30.67	23.48	$156^\dagger$	78	30.67	23.48	156	32.00	23.51
81×11	$8^\dagger$	0	37.63	24.71	$8^\dagger$	4	38.70	24.81	8	43.64	25.18
81×12	$16^\dagger$	0	40.04	26.69	$16^\dagger$	8	42.18	26.90	16	46.97	27.25
81×13	$24^\dagger$	0	42.23	28.63	$24^\dagger$	12	45.43	28.94	24	50.19	29.29
81×14	$32^\dagger$	0	44.20	30.52	$32^\dagger$	16	48.47	30.94	32	53.31	31.29
81×15	42	0	46.03	32.37	$40^\dagger$	20	51.28	32.89	40	56.32	33.25
81×16	54	0	47.73	34.18	$48^\dagger$	24	53.87	34.80	48	59.22	35.18
81×17	68	0	49.30	35.95	$56^\dagger$	28	56.23	36.66	56	62.01	37.07
81×18	84	0	50.73	37.67	$64^\dagger$	32	58.38	38.48	64	64.70	38.92
81×19	102	0	52.03	39.35	$72^\dagger$	36	60.30	40.25	72	67.29	40.74
81×20	126	0	53.38	40.99	$80^\dagger$	40	62.00	41.98	80	69.76	42.52
81×21	150	0	54.50	42.58	$96^\dagger$	48	64.90	43.77	96	72.13	44.27
81×22	190	0	56.11	44.15	$112^\dagger$	56	67.58	45.52	112	74.40	45.98
81×23	234	0	57.68	45.67	$128^\dagger$	64	70.03	47.23	128	76.55	47.65
81×24	284	0	59.29	47.16	$144^\dagger$	72	72.27	48.89	144	78.60	49.29
81×25	330	0	60.50	48.59	$160^\dagger$	80	74.28	50.50	160	80.55	50.89
81×26	328	10	62.02	50.20	$176^\dagger$	88	76.07	52.07	176	82.38	52.45
81×27	350	18	63.86	51.73	$192^\dagger$	96	77.63	53.60	192	84.12	53.98
81×28	382	26	65.91	53.22	$208^\dagger$	104	78.98	55.08	208	85.74	55.47
81×29	430	34	68.46	54.69	$224^\dagger$	112	80.10	56.51	224	87.26	56.93
81×30	464	44	70.69	56.15	$240^\dagger$	120	81.00	57.90	240	88.67	58.35
81×31	508	52	72.61	57.52	$264^\dagger$	132	83.10	59.36	264	89.97	59.73
81×32	566	58	74.40	58.81	$288^\dagger$	144	84.98	60.77	288	91.17	61.08
81×33	650	64	77.12	60.08	$312^\dagger$	156	86.63	62.13	312	92.26	62.39
81×34	656	84	79.89	61.59	$336^\dagger$	168	88.07	63.46	336	93.25	63.66
81×35	696	100	82.88	62.99	$360^\dagger$	180	89.28	64.73	360	94.13	64.90
81×36	704	120	85.29	64.41	$384^\dagger$	192	90.27	65.96	384	94.90	66.11
81×37	782	136	89.52	65.76	$408^\dagger$	204	91.03	67.15	408	95.57	67.27
81×38	986	148	98.07	67.08	$432^\dagger$	216	91.58	68.29	432	96.12	68.40
81×39	1716	156	128.70	68.78	$456^\dagger$	228	91.90	69.39	456	96.58	69.49
81×40	$480^\dagger$	240	92.00	70.44	$480^\dagger$	240	92.00	70.44	480	96.92	70.55

Figure 4.1: Comparing 64-run (near) SOAs with $D_{64,m}$s under (a) $\mu(D)$, (b) $A_2(D)$, (c) $\bar{\phi}_1(D)$ and (d) $\bar{\phi}_2(D)$.



$n = 64$ and $m \leq 45$, and $n = 81$ and $m \leq 37$. Under $\bar{\phi}_2(D)$ SOAs and near SOAs are better for all 8-run, 16-run, 27-run and 81-run cases, and for $n = 32$ and $m \leq 29$, and $n = 64$ and $m \leq 59$. The criterion $\bar{\phi}_2$ (and $\bar{\rho}$) favors SOA and near SOAs because it places more weight on $\mu(D)$ than $\bar{\phi}_1$ (and $\bar{\psi}$) does in (4.5).

When m is even larger, we can see that the $A_2(D)$s of SOAs and near SOAs grow so rapidly that the $D_{n,m}$s may take the lead. This observation becomes more apparent for $\bar{\phi}_1$ (and $\bar{\psi}$) as more weight is placed on $A_2(D)$ in (4.5). Indeed, a calculation for the four-level case shows that even if the lower bounds in Theorem 4.4 could be achieved by certain SOAs, the $D_{n,m}$s would have smaller $\bar{\phi}_1(D)$ (and $\bar{\psi}(D)$) when $m \geq 46$ for $n = 64$, $m \geq 93$ for

$n = 128$, $m \geq 186$ for $n = 256$, and $m \geq 372$ for $n = 512$; that is, when m is approximately greater than 0.725 times $n - 1$.

To illustrate the discussion above, we provide a visualization of the comparisons of 64-run designs in Figure 4.1. It can be clearly seen in panels (c) and (d) of Figure 4.1 that under the criteria $\bar{\phi}_1$ and $\bar{\phi}_2$, designs $D_{64,m}$s are always better than the random OABDs, while SOAs and near SOAs are the best for small m values and gradually deteriorate as m increases. The behaviors of SOAs and near SOAs are not very surprising as they first minimize the μ value as shown in panel (a) of Figure 4.1, resulting in a rapid increase of the A_2 value as m increases as shown in panel (b) of Figure 4.1.

According to these observations, we conclude that both families of designs are fruitful and have their own specialties. The SOAs and near SOAs optimize $s \times s'$ and $s' \times s$ stratifications in all two-dimensions, while $D_{n,m}$s enjoy higher proportions of column pairs stratified over the $s \times s$ grid and smaller overall $A_2(D)$. Under the class of criteria χ, the SOAs and near SOAs are appealing when the number of factors is not too large and are more welcome under L_2-distance and the orthogonality criterion than under L_1-distance and the uniform projection criterion, whereas $D_{n,m}$s are more competitive for the opposite situations.

4.5 Proofs

Proof of Lemma 4.2. To prove part (i), first note that

$$\begin{aligned}
\phi(D) &= \frac{1}{n(n-1)} \sum_{i \neq j} d_{ij}^2 - \bar{d}^2 \\
&= \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1}^{n} \left(\sum_{k=1}^{m} d(x_{ik}, x_{jk}) \right)^2 - \bar{d}^2 \\
&= \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1}^{n} \left\{ \sum_{u \neq v} d(x_{iu}, x_{ju}) d(x_{iv}, x_{jv}) + \sum_{u=1}^{m} d(x_{iu}, x_{ju})^2 \right\} - \bar{d}^2 \\
&= \sum_{u \neq v} \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1}^{n} d(x_{iu}, x_{ju}) d(x_{iv}, x_{jv}) + \frac{m}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1}^{n} d(x_{i1}, x_{j1})^2 - \bar{d}^2.
\end{aligned}$$

Then the result follows by noting that for any U-type designs, we have $\sum_{i,j} d(x_{i1}, x_{j1})^2 = n^2 \sum_{x=0}^{s-1} \sum_{y=0}^{s-1} d(x, y)^2 / s^2$ and $\bar{d} = mn \sum_{x=0}^{s-1} \sum_{y=0}^{s-1} d(x, y) / (ns^2 - s^2)$.

For part (ii), we first standardize each column of $D = (x_{iu})$ through the linear transformation $\tilde{x}_{iu} = \sqrt{12/(ns^2 - n)}(x_{iu} - (s-1)/2)$. Then we have

$$\begin{aligned}\rho(D) &= \frac{1}{m(m-1)} \sum_{u \neq v} \rho_{uv}^2 = \frac{1}{m(m-1)} \sum_{u \neq v} \left(\sum_{i=1}^{n} \tilde{x}_{iu} \tilde{x}_{iv} \right)^2 \\ &= \frac{1}{m(m-1)} \sum_{u \neq v} \sum_{i=1}^{n} \sum_{j=1}^{n} \tilde{x}_{iu} \tilde{x}_{ju} \cdot \tilde{x}_{iv} \tilde{x}_{jv}.\end{aligned}$$

The result in (ii) then follows by some tedious algebra. Part (iii) is straightfoward and is thus omitted. □

Next, we first prove Proposition 4.2 to make the logic coherent.

Proof of Proposition 4.2. For $k = 1, \ldots, m$, let $\mathbf{A}_k = (a_{iu}^{(k)})_{n \times (s'-1)}$ and $\mathbf{B}_k = (b_{iu}^{(k)})_{n \times (\alpha-1)}$ be matrices of orthonormal main-effect coefficients for the kth factor of A and B, respectively. Let $\mathbf{C}_k = (c_{iu}^{(k)})_{n \times (s'-1)(\alpha-1)}$ consist of all Hadamard products between the columns of $\mathbf{A}_k$ and $\mathbf{B}_k$. Then it is easy to verify that $(\mathbf{A}_k, \mathbf{B}_k, \mathbf{C}_k)$ is a matrix of orthonormal main-effect coefficients for the kth factor of D. Now let $\mathbf{A} = (\mathbf{A}_1, \ldots, \mathbf{A}_m)$, $\mathbf{B} = (\mathbf{B}_1, \ldots, \mathbf{B}_m)$ and $\mathbf{C} = (\mathbf{C}_1, \ldots, \mathbf{C}_m)$. Then $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ is a matrix of orthonormal main-effect coefficients for D. The expression in Proposition 4.2 follows by applying the definition (4.2) of $A_2(D)$ to this set of contrasts directly. □

To prove Theorems 4.1 and 4.2, we present two lemmas, the first of which is from Xu (2003).

Lemma 4.5. *Suppose D is a $U(n, s^m)$. Let δ_{ij} be the number of coincidences between the ith and jth runs of D. Then $\sum_{i,j} \delta_{ij} = n^2 m/s$ and $\sum_{i,j} \delta_{ij}^2 = \{2n^2 A_2(D) + n^2 m(m+s-1)\}/s^2$.*

Lemma 4.6. *Suppose D is an $OABD_\alpha(n, s^m)$. Denote by $\delta_{ij}(A)$ and $\delta_{ij}(D)$ the numbers of coincidences between the ith and jth run of A and D, respectively, and let c be any constant. Then*

$$\begin{aligned}\sum_{i=1}^{n} \sum_{j=1}^{n} \{\delta_{ij}(A) + c\delta_{ij}(D)\}^2 = \frac{2c^2 n^2}{s^2} A_2(D) &+ \frac{2c\alpha n^2}{s^2} \sum_{u \neq v} \{A_2(a_u, b_v) + A_3(a_u, a_v, b_v)\} \\ &+ \frac{mn^2}{s^2} \left\{ (m + s' - 1)(c+\alpha)^2 + s'(\alpha - 1)c^2 \right\}.\end{aligned}$$

Proof. We use the same notation as in the proof of Proposition 4.2. Note that if the kth factor of A takes the same level on the ith and jth run, then $\sum_{v=1}^{s'-1} a_{iv}^{(k)} a_{jv}^{(k)} = s' - 1$; otherwise it is equal to -1. Therefore, $\delta_{ij}(A) = (\sum_{k=1}^{m} \sum_{v=1}^{s'-1} a_{iv}^{(k)} a_{jv}^{(k)} + m)/s'$. Similarly, one can show $\delta_{ij}(D) = \{\sum_{k=1}^{m}(\sum_{v=1}^{s'-1} a_{iv}^{(k)} a_{jv}^{(k)} + \sum_{v=1}^{\alpha-1} b_{iv}^{(k)} b_{jv}^{(k)} + \sum_{v=1}^{(\alpha-1)(s'-1)} c_{iv}^{(k)} c_{jv}^{(k)}) + m\}/s$.

Let $\mathbf{J}$ be an $n \times n$ matrix of all ones. Then $\sum_{i,j}\{\delta_{ij}(A) + c\delta_{ij}(D)\}^2 = \mathrm{tr}(\{(c+\alpha)\mathbf{A}\mathbf{A}^t + c\mathbf{B}\mathbf{B}^t + c\mathbf{C}\mathbf{C}^t + (c+\alpha)m\mathbf{J}\}^2)/s^2 = (c+\alpha)^2 m^2 n^2/s^2 + (c+\alpha)^2 \mathrm{tr}(\mathbf{A}^t\mathbf{A}\mathbf{A}^t\mathbf{A})/s^2 + 2c(c+\alpha)\mathrm{tr}(\mathbf{B}^t\mathbf{A}\mathbf{A}^t\mathbf{B} + \mathbf{C}^t\mathbf{A}\mathbf{A}^t\mathbf{C})/s^2 + c^2\mathrm{tr}(\mathbf{B}^t\mathbf{B}\mathbf{B}^t\mathbf{B} + \mathbf{C}^t\mathbf{C}\mathbf{C}^t\mathbf{C} + 2\mathbf{C}^t\mathbf{B}\mathbf{B}^t\mathbf{C})/s^2 = mn^2/s^2\{(m+s'-1)(c+\alpha)^2 + s'(\alpha-1)c^2\} + 2\alpha^2 n^2/s^2 A_2(A) + 2c\alpha n^2/s^2 \sum_{u\neq v}\{A_2(a_u, b_v) + A_3(a_u, a_v, b_v)\} + 2c^2 n^2/s^2 A_2(D)$. If A is an $\mathrm{OA}(n, m, s', 2)$, then we have $\sum_{i,j}\{\delta_{ij}(A) + c\delta_{ij}(D)\}^2 = mn^2/s^2\{(m+s'-1)(c+\alpha)^2 + s'(\alpha-1)c^2\} + 2c\alpha n^2/s^2 \sum_{u\neq v}\{A_2(a_u, b_v) + A_3(a_u, a_v, b_v)\} + 2c^2 n^2/s^2 A_2(D)$. $\square$

Proof of Theorem 4.1. Let $\mathcal{D}_U$ be the set of all $\mathrm{U}(n, s^m)$s and $|\mathcal{D}_U|$ be its cardinality. Then we have

$$\bar{\chi}_u = \frac{1}{|\mathcal{D}_U|} \sum_{D\in\mathcal{D}_U} \frac{1}{m(m-1)} \sum_{u\neq v} q(D_{uv}) = \frac{1}{m(m-1)} \sum_{u\neq v} \frac{1}{|\mathcal{D}_U|} \sum_{D\in\mathcal{D}_U} q(D_{uv}).$$

Write

$$q(D_{uv}) = \gamma_0 + \frac{\gamma_1}{n}\sum_{i=1}^{n} g(x_{iu})g(x_{iv}) + \frac{\gamma_2}{n}\sum_{i=1}^{n} f(x_{iu}, x_{iu})f(x_{iv}, x_{iv}) + \frac{\gamma_2}{n^2}\sum_{i\neq j} f(x_{iu}, x_{ju})f(x_{iv}, x_{jv}).$$

Then it can be verified by distributive law that for any $u \neq v$, $\sum_{D\in\mathcal{D}_U} g(x_{iu})g(x_{iv})/|\mathcal{D}_U| = U_\chi^2$, $\sum_{D\in\mathcal{D}_U} f(x_{iu}, x_{iu})f(x_{iv}, x_{iv})/|\mathcal{D}_U| = X_\chi^2$ and $\sum_{D\in\mathcal{D}_U} f(x_{iu}, x_{ju})f(x_{iv}, x_{jv})/|\mathcal{D}_U| = M_0^2$, where $M_0 = \lambda^2 \sum_{0\leq k\neq l\leq s-1} f(k,l)/(n(n-1)) + \lambda(\lambda-1)\sum_{k=0}^{s-1} f(k,k)/(n(n-1)) = \{(\lambda-1)X_\chi + \lambda(\alpha-1)Y_\chi + (n-\alpha\lambda)Z_\chi\}/(n-1)$ and $U_\chi = \sum_{k=0}^{s-1} g(k)/s$. The definitions for X_χ, Y_χ and Z_χ are given in the theorem. Therefore, we have

$$\bar{\chi}_u = \gamma_0 + \gamma_1 U_\chi^2 + \frac{\gamma_2}{n} X_\chi^2 + \gamma_2\left(1 - \frac{1}{n}\right) M_0^2. \tag{4.14}$$

On the other hand, let $\mathcal{D}_O$ be the set of all $\mathrm{OABD}_\alpha(n, s^m)$s generated from the given A and $|\mathcal{D}_O|$ be its cardinality. Let A_{uv} be the matrix consisting of the uth and vth column of A.

Then similarly we have

$$\bar{\chi}_o = \frac{1}{m(m-1)} \sum_{u \neq v} \frac{1}{|\mathcal{D}_O|} \sum_{D \in \mathcal{D}_O} q(D_{uv}) \tag{4.15}$$

with

$$\frac{1}{|\mathcal{D}_O|} \sum_{D \in \mathcal{D}_O} q(D_{uv}) = \gamma_0 + \gamma_1 U_\chi^2 + \frac{\gamma_2}{n} X_\chi^2 + \frac{\gamma_2}{n^2} \sum_{i \neq j} M_1^{\delta_{ij}(A_{uv})} M_2^{2-\delta_{ij}(A_{uv})}, \tag{4.16}$$

where $M_1 = \{(\lambda-1)X_\chi + (\alpha\lambda - \lambda)Y_\chi\}/(\alpha\lambda - 1)$, $M_2 = Z_\chi$ and $\delta_{ij}(A_{uv})$ is the number of coincidences between the ith and jth row of A_{uv}. Note that $\delta_{ij}(A_{uv})$ can only take values of 0, 1 and 2. It can be checked that

$$M_1^{\delta_{ij}(A_{uv})} M_2^{2-\delta_{ij}(A_{uv})} = M_2^2 - (M_1 - M_2)(M_1 - 3M_2)\delta_{ij}(A_{uv})/2 + (M_1 - M_2)^2 \delta_{ij}^2(A_{uv})/2. \tag{4.17}$$

The result follows by combining equations (4.14), (4.15), (4.16), (4.17), Lemma 4.5 and some tedious algebra. □

Proof of Corollary 4.1. The result follows directly by Theorem 4.1 and Lemma 4.5. □

Proof of Theorem 4.2. Let $\mathcal{D}$ be the set of all D's obtained by applying allowable permutations to D and $|\mathcal{D}|$ be its cardinality. Then we have

$$\bar{\chi}(D) = \frac{1}{\mathcal{D}} \sum_{D' \in \mathcal{D}} \chi(D') = \frac{1}{m(m-1)} \sum_{u \neq v} \bar{q}(D_{uv}), \tag{4.18}$$

where $\bar{q}(D_{uv})$ is the average of $q(D'_{uv})$s for all D'_{uv}s obtained by applying allowable permutations to D_{uv}. Let $\mathcal{D}_{uv}$ be the set of all such D'_{uv}s and $|\mathcal{D}_{uv}|$ be its cardinality. Also denote the ith row of D'_{uv} by (x'_{iu}, x'_{iv}). Then we have

$$\begin{aligned}
\bar{q}(D_{uv}) &= \frac{1}{|\mathcal{D}_{uv}|} \sum_{D'_{uv} \in \mathcal{D}_{uv}} \left\{ \gamma_0 + \frac{\gamma_1}{n} \sum_{i=1}^n g(x'_{iu}) g(x'_{iv}) + \frac{\gamma_2}{n^2} \sum_{i=1}^n \sum_{j=1}^n f(x'_{iu}, x'_{ju}) f(x'_{iv}, x'_{jv}) \right\} \\
&= \gamma_0 + \gamma_1 U_\chi^2 + \frac{\gamma_2}{n^2} \sum_{i=1}^n \sum_{j=1}^n X_\chi^{\delta_{ij}(D_{uv})} Y_\chi^{\delta_{ij}(A_{uv}) - \delta_{ij}(D_{uv})} Z_\chi^{2-\delta_{ij}(A_{uv})},
\end{aligned} \tag{4.19}$$

where $\delta_{ij}(A_{uv})$ and $\delta_{ij}(D_{uv})$ are the number of coincidences between the ith and jth runs of A_{uv} and D_{uv} respectively. Since $(\delta_{ij}(D_{uv}), \delta_{ij}(A_{uv}))$ can only take values of $(2,2)$, $(1,2)$, $(1,1)$, $(0,2)$, $(0,1)$ and $(0,0)$, it can be verified that $X_\chi^{\delta_{ij}(D_{uv})} Y_\chi^{\delta_{ij}(A_{uv})-\delta_{ij}(D_{uv})} Z_\chi^{2-\delta_{ij}(A_{uv})} = Z_\chi^2 + \{2Z_\chi(X_\chi - Y_\chi) - (X_\chi^2 - Y_\chi^2)/2\}\delta_{ij}(D_{uv}) + (2Y_\chi Z_\chi - 3Z_\chi^2/2 - Y_\chi^2/2)\delta_{ij}(A_{uv}) + \{(Z_\chi - Y_\chi)^2/2\}\{\delta_{ij}(A_{uv}) + (Y_\chi - X_\chi)/(Z_\chi - Y_\chi)\delta_{ij}(D_{uv})\}^2$. Then the result follows by combining this with Lemmas 4.5, 4.6, equations (4.18) and (4.19), and some tedious algebra. □

Proof of Lemma 4.3. The proof can be done similarly as in that of Theorem 4.2. Let $\mathcal{D}$ and $\mathcal{D}_{uv}$ be the sets of all D's and D'_{uv}s obtained by applying all possible level permutations to columns of D and D_{uv}, respectively. Denote the ith row of D'_{uv} by (x'_{iu}, x'_{iv}). Then the equation (4.18) still holds and equation (4.19) becomes

$$\bar{q}(D_{uv}) = \gamma_0 + \gamma_1 U_\chi^2 + \frac{\gamma_2}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} X_\chi^{\delta_{ij}(D_{uv})} W_\chi^{2-\delta_{ij}(D_{uv})}.$$

Since $\delta_{ij}(D_{uv})$ can only take values of 0, 1 and 2, we have, as in (4.17), $X_\chi^{\delta_{ij}(D_{uv})} W_\chi^{2-\delta_{ij}(D_{uv})} = W_\chi^2 + (W_\chi - X_\chi)(X - 3W_\chi)\delta_{ij}(D_{uv})/2 + (W_\chi - X_\chi)^2\{\delta_{ij}(D_{uv})\}^2/2$. Then the result follows similarly as in the proof of Theorem 4.2. □

Proof of Theorem 4.3. For a $\mathrm{U}(n, s^m)$, Tang (2001) and Ai and Zhang (2004) showed that minimizing $A_2(D)$ is equivalent to minimizing the average variance of frequencies of s^2 level combinations over all the two-dimensional projections of D. Now suppose D is an $\mathrm{SOA}_\alpha(n, s^m)$ with $\lambda' = 1$. For any two-dimensional projection of D, $n = ss'$ of the s^2 level combinations occurs. Therefore $A_2(D)$ is minimized among all $\mathrm{U}(n, s^m)$s, leading to the conclusion in Theorem 4.3. □

Proof of Theorem 4.4. For ease of expression, we consider $s' = 2$. The proof for the case $s' > 2$ is similar. By Proposition 4.2, we have $A_2(D) = \sum_{u<v} A_2(D_{uv})$ where $A_2(D_{uv}) = A_2(b_u, b_v) + A_2(a_u b_u, b_v) + A_2(b_u, a_v b_v) + A_2(a_u b_u, a_v b_v)$. Hence there are only two possible cases for $A_2(D_{uv})$: (i) $A_2(D_{uv}) = 0$ if $(b_u, a_u b_u)$ and $(b_v, a_v b_v)$ are totally distinct, or (ii) $A_2(D_{uv}) = 1$ if $(b_u, a_u b_u)$ and $(b_v, a_v b_v)$ share a common column. Note that entries of $(b_1, a_1 b_1, \ldots, b_m, a_m b_m)$ must be from $e_1, \ldots, e_{n-1-m}$ since D is an SOA. Let $f_1, \ldots, f_{n-1-m}$

be the frequencies of $e_1, \ldots, e_{n-1-m}$ in $(b_1, a_1b_1, \ldots, b_m, a_mb_m)$. Therefore, $A_2(D) = \sum_{k=1}^{n-1-m} f_k(f_k-1)/2$. Minimizing $A_2(D)$ under the constraint $\sum_{k=1}^{n-1-m} f_k = 2m$ leads to the inequality in Theorem 4.4 for $s' = 2$. $\square$

Proof of Theorem 4.6. The fact that $A_2(D_{n,m})$ reaches the bound of Lemma 4.4 if $m = m_1 l$ or $m_1 l \pm 1$ for some integer l is immediate since the condition of equality is achieved (Xu and Wu, 2005). Therefore, $A_2(D_{n,(s'+1)m_1}) = m_2 s'(s-1)/2$. On the other hand, since $D_{n,(s'+1)m_1}$ is an $\mathrm{MNOA}_{s'}(n, (s^{s'+1})^{m_1})$, we have $A_2(D_{uv}) = 0$ if $\lfloor (u-1)/m_1 \rfloor \neq \lfloor (v-1)/m_1 \rfloor$. Note that $A_2(D_{uv}) \leq s-1$ if for all $u \leq v$. Therefore, $A_2(D_{n,(s'+1)m_1}) = \sum_{u<v} A_2(D_{uv}) \leq m_2 s'(s-1)/2$. Since $A_2(D_{n,(s'+1)m_1}) = m_2 s'(s-1)/2$, we conclude $A_2(D_{uv}) = s-1$ if $\lfloor (u-1)/m_1 \rfloor = \lfloor (v-1)/m_1 \rfloor$. Then the expression of $A_2(D_{n,m})$ is straightforward. $\square$

Proof of Theorem 4.7. The proof is similar to that of Theorem 4.4, with a slight difference being that, for example when $s' = 2$, we have $A_2(D) = \sum_{u<v}\{A_2(a_u, b_v) + A_2(a_v, b_u) + A_2(b_u, b_v) + A_2(a_u, a_vb_v) + A_2(a_ub_u, a_v) + A_2(a_ub_u, b_v) + A_2(b_u, a_vb_v) + A_2(a_ub_u, a_vb_v)\} = \sum_{k=1}^{n-1} f'_k(f'_k-1)/2$, where $f'_1, \ldots, f'_{n-1}$ are the frequencies of columns of S in $(a_1, b_1, a_1b_1, \ldots, a_m, b_m, a_mb_m)$. $\square$

Proof of Theorem 4.8. That $D_{n,n-1}$ reaches the lower bound in Theorem 4.7 can be proved using induction by combining two facts, both of which can be easily verified. First, $D_{8,7}$ reaches the lower bound. Second, if $D_{n,n-1}$ reaches the lower bound, then $D_{4n,4n-1}$ also does. The $A_2(D_{n,m})$s for $m \leq n-1$ can be calculated by observation. For example, when $(2n+2)/3 < m \leq n-1$, we have $A_2(D_{n,m-1}) = A_2(D_{n,m}) - 6$ and so on. A direct verification shows that $A_2(D_{n,m})$ attains the lower bound in Lemma 4.4 if $m = (n-2)/3$, $(2n-4)/3$, $(2n-1)/3$ or $n-1$. $\square$

4.6 Concluding remarks

In this chapter, we investigate orthogonal array-based designs under a broad class of space-filling criteria which includes the variance of L_p-distances, column orthogonality and uniform projection criterion. Under these criteria, we justify the use of OABDs by showing (Theorem 4.1) that they tend to be more space-filling than random U-type designs. Next, we show

(Theorem 4.2) that the average performance of the class of $\mathrm{OABD}_\alpha(n, s^m)$s obtained by allowable level permutations is determined by two components, i.e., the stratification over an $s \times s$ grid represented by $A_2(D)$ and the stratification over an $s \times s'$ as well as an $s' \times s$ grid represented by $\mu(D)$. An SOA achieves the stratification of the second kind and thus tends to be more space-filling than a non-SOA with the same $A_2(D)$. Based on these results, we study two families of OABDs, where the first seeks to minimize $A_2(D)$ among SOAs while the second focuses on minimizing $A_2(D)$ directly. The two families of designs are both attractive and have complementary performance under the class of criteria.

Several directions are worthy of future research. As pointed out in Section 4.3.2, a total of $\{(s')!(\alpha!)^{s'}\}^m$ designs can be generated from a specific $\mathrm{OABD}_\alpha(n, s^m)$ by α-allowable permutations. Notwithstanding being much fewer than the designs generated by all level permutations (Zhou and Xu, 2014) or the OABDs from permuting and expanding a specific $\mathrm{OA}(n, m, s', 2)$ (Xiao and Xu, 2018), the class of designs soon becomes exceedingly large for moderate m. For example, there are over 1 billion candidate designs by allowably permuting a 4-level design with 10 factors. Therefore, it is of great practical value to give a theoretical or algorithmic construction for how to select α-allowable permutations to obtain more space-filling designs.

This chapter focuses on two-dimensional properties so all the designs considered are based on orthogonal arrays of strength 2. The results of Zhou and Xu (2014) imply that higher-dimensional projections also affect space-filling measures such as the centered L_2-discrepancy and the minimum distance of the design. Therefore, it is of great interest to examine the performance of strong orthogonal arrays of strength 3, which achieve a stratification over the $s' \times s' \times s'$ grids in addition to the $s \times s'$ and $s' \times s$ grids, and analyze what roles these stratification properties play in the overall space-filling properties of the resulting design.

The issue as to which specific criterion shall be used in practice is an important one. The orthogonality criterion ρ may be suitable if a polynomial model is deemed appropriate. When Gaussian processes are employed (Johnson et al., 1990), the criterion ϕ_2 is linked to squared exponential functions while ϕ_1 appears more relevant to an Ornstein-Uhlenbeck process. The design community welcomes any systematic and comprehensive investigation on this matter.

Chapter 5

Using Nonregular Designs to Generate Space-Filling Designs

5.1 Introduction

In designing computer experiments, it is desirable to have design points scattered in the design region in some uniform fashion. Such designs are broadly referred to as space-filling designs (Santner et al., 2018; Fang et al., 2006). Use of space-filling designs in computer experiments is intuitively appealing as one would like to have every portion of a design region represented, and can also be theoretically justified in terms of their performances in the mean squared prediction error (Vazquez and Bect, 2011). Space-filling designs can be constructed by optimizing a uniformity criterion such as that of distance or discrepancy (Johnson et al., 1990; Fang et al., 2000). Orthogonality also plays a role in constructing space-filling designs (Ye, 1998; Bingham et al., 2009; Georgiou et al., 2014).

We consider space-filling designs based on orthogonal arrays. Designs of this type are attractive because they enjoy some guaranteed low-dimensional projection properties. This line of research started with the introduction of Latin hypercubes by McKay et al. (1979), and went further with OA-based designs (Owen, 1992; Tang, 1993). Recently, He and Tang (2013) introduced a class of new designs, namely strong orthogonal arrays. These arrays, being more space-filling than comparable orthogonal arrays, have found applications in optimizing the braking performances for freight trains (Nikiforova et al., 2021).

Most economical strong orthogonal arrays (SOAs) are those of strength 2+ that focus on two-dimensional projection properties. Construction of SOAs of strength 2+ has been largely based on regular designs (He et al., 2018; Shi and Tang, 2019). This method puts a severe restriction on the run sizes of the resulting designs as they must be prime powers. Cheng et al. (2021) considered the use of two-level nonregular designs but their results are limited to designs of run sizes that are multiples of 16.

In this chapter, we develop a general method of constructing space-filling designs using nonregular designs. Designs so constructed have very flexible run sizes compared to those constructed from regular designs. One challenging complication with using nongular designs is that it is often impossible to obtain SOAs of strength 2+. We meet this challenge by proposing two criteria for design evaluation under the new situation. Apart from some theoretical results, computer searches are conducted to find space-filling designs using two-level nonregular designs of up to 40 runs and three-level nonregular designs of 27 and 54 runs. One of the interesting findings is a strength 2+ SOA of 54 runs for 12 factors.

Section 5.2 of the chapter introduces notation and necessary background. Section 5.3 develops our method of constructing space-filling designs using two-level nonregular designs and presents corresponding theoretical and computational results. In Section 5.4, we show how the ideas of Section 5.3 can be generalized and used to construct some space-filling designs from three-level nonregular designs. The chapter is then concluded by a discussion in Section 5.5.

5.2 Notation and background

An $n \times m$ matrix with entries from $\{0, 1, \ldots, s_j - 1\}$ in the jth column is called an orthogonal array of n runs, m factors and strength t, and denoted by $\mathrm{OA}(n, m, s_1 \times \cdots \times s_m, t)$, if any of its $n \times t$ submatrix contains all possible t-tuples as its rows the same number of times. Two orthogonal arrays are said to be *isomorphic* if one can be obtained from the other by permuting the columns, the rows, the levels of each factor, or a combination of the above. If $s_1 = \cdots = s_m = s$, the orthogonal array is said to be *symmetric* and is denoted by $\mathrm{OA}(n, m, s, t)$. For convenience, when $s = 2$, the two levels are denoted by $\{-1, +1\}$ instead of $\{0, 1\}$. For an $\mathrm{OA}(n, m, s, 2)$ to exist, we must have $m \leq (n-1)/(s-1)$; and when the equality holds, the array is said to be *saturated*. If an orthogonal array can be generated by adding interaction columns to the columns of a full factorial design, then it is called a *regular design*; otherwise it is called a *nonregular design*.

Saturated two-level orthogonal arrays of strength 2 are equivalent to Hadamard matrices. An $n \times n$ matrix H with entries from $\{-1, +1\}$ is called a Hadamard matrix of order n if $HH^T = nI_n$, where I_n is the identity matrix of order n. A Hadamard matrix is said to be normalized if its first column consists of all ones. Two Hadamard matrices are said to be *isomorphic* if one can be obtained from the other by a sequence of operations involving permuting the rows or columns and negating a row or a column. Given a normalized Hadamard matrix H, an $\mathrm{OA}(n, n-1, 2, 2)$ can be obtained from H by deleting the first column.

A two-level orthogonal array can be studied using its J-characteristics (Tang, 2001). Let $a_i = (a_{1i}, \ldots, a_{ni})^T$ $(1 \leq i \leq k)$ be k columns with entries from ± 1. Then the J-characteristic of $a_1, \ldots, a_k$ is defined to be $J(a_1, \ldots, a_k) = \sum_{j=1}^{n} a_{j1} \cdots a_{jk}$. An orthogonal array $D = (d_1, \ldots, d_m)$ is of strength t if and only if $J(d_{i_1}, \ldots, d_{i_k}) = 0$ for all $1 \leq i_1 \leq \cdots \leq i_k \leq m$ and $k \leq t$. For more information on orthogonal arrays and Hadamard matrices, we refer to Hedayat et al. (1999) and Cheng (2014).

Strong orthogonal arrays (SOAs) were introduced by He and Tang (2013). An $n \times m$ matrix with entries from $\{0, 1, \ldots, s^t - 1\}$ is called an SOA of n runs, m factors, s^t levels and strength t, and denoted by $\mathrm{SOA}(n, m, s^t, t)$, if any of its $n \times g$ $(1 \leq g \leq t)$ submatrix can be collapsed into an $\mathrm{OA}(n, g, s^{u_1} \times \cdots \times s^{u_g}, g)$ for any positive integers $u_1, \ldots, u_g$ satisfying $u_1 + \cdots + u_g = t$, where collapsing s^t levels into s^{u_j} levels is done by $\lfloor a/s^{t-u_j} \rfloor$ for $a = 0, 1, \ldots s^t - 1$. Among SOAs of varying strengths, those of strength 3 are particularly interesting because, in addition to the $s \times s \times s$ stratification property in three dimensions enjoyed by orthogonal arrays of strength 3, SOAs of strength 3 possess the $s^2 \times s$ and $s \times s^2$ stratification properties in two-dimensions at almost no extra cost (He and Tang, 2014). More specifically, if an $\mathrm{OA}(n, m, s, 3)$ is available, then one can construct an $\mathrm{SOA}(n, m', s^3, 3)$ for $m' = m$ or $m' = m - 1$ depending on whether or not the $\mathrm{OA}(n, m, s, 3)$ is semi-embeddable.

Most economical are SOAs of strength 2+ (He et al., 2018), as they can accommodate many more factors than SOAs of strength 3 for given run size. An SOA$(n, m, s^2, 2)$ is said to be of strength 2+, and denoted by SOA$(n, m, s^2, 2+)$, if they have the the $s^2 \times s$ and $s \times s^2$ stratification properties in two-dimensions. The following is a useful characterization for SOAs of strength 2+ (He et al., 2018).

Lemma 5.1. *An SOA$(n, m, s^2, 2+)$, say D, exists if and only if there exist $n \times m$ arrays $A = (a_1, \ldots, a_m)$ and $B = (b_1, \ldots, b_m)$, both of s levels, such that A is an OA$(n, m, s, 2)$ and (a_i, b_i, a_j) is an OA$(n, 3, s, 3)$ for all $1 \leq i \neq j \leq m$. The three arrays A, B and D are related through*

$$D = \begin{cases} sA + B, & \text{if } s \geq 3, \\ A + B/2 + 3/2, & \text{if } s = 2. \end{cases} \tag{5.1}$$

The slightly different expression for $s = 2$ in Lemma 5.1 is because we use ± 1 to denote the two levels for arrays with $s = 2$ levels.

For latest developments on SOAs and related designs, we refer to Wang et al. (2022a) and Tian and Xu (2022).

5.3 Results from using two-level nonregular designs

5.3.1 Non-empty-cell designs and measures of 4×2 uniformity

He et al. (2018) considered the construction of SOAs of strength 2+ using two-level regular designs. If we use S to denote a saturated regular design of n runs for $n-1$ factors, then their approach is to use array A with its columns selected from S and array B with its columns selected from $S \setminus A$ to obtain design $D = A + B/2 + 3/2$. They showed that D is an SOA of strength 2+ if and only if $S \setminus A$ is second order saturated (SOS). According to Block and Mee (2003), a design is SOS if it allows estimation of a saturated model consisting of all main effects plus a set of two-factor interactions.

We follow the same spirit for the case of nonregular designs. We now let S be a saturated two-level design of n runs for $n-1$ factors, which does not have to be regular. Our goal is then to find array A with its columns selected from S and array B with its columns selected from $S \setminus A$ so that the resulting design $D = A + B/2 + 3/2$ is most space-filling in two-dimensions. We would like D to be an SOA of strength 2+ but this is often impossible. For example, when n is a multiple of 4 but not of 8, it is impossible to obtain an SOA of strength 2+ as such an array must have a run size that is a multiple of 8.

For convenience, we consider ordered two-dimensional projection designs of $D = (d_1, \ldots, d_m)$, which are given by $D_{ij} = (d_i, d_j)$ for all $i \neq j$. Then design D is an SOA of strength 2+ if every D_{ij} can be collapsed into an $\mathrm{OA}(n, 2, 4 \times 2, 2)$, thus achieving a stratification on a 4×2 grid. When it is not possible for D_{ij} to have this property, a minimum requirement for D_{ij} to be space-filling is that it has at least one point in each of the 8 cells given by the 4×2 grid. This idea leads to the type of designs we call non-empty-cell designs.

Definition 5.1. *Design D is said to be a non-empty-cell design if $D_{ij} = (d_i, d_j)$ contains all possible 4×2 level combinations after collapsing the 4 levels of d_j into 2 levels for all $i \neq j$.*

As indicated in Lemma 5.1, the property of D_{ij} on the 4×2 grid is completely determined by (a_i, b_i, a_j). Clearly, a non-empty-cell design requires that (a_i, b_i, a_j) contains all possible level combinations. From a result of Cheng (1995), we know (a_i, b_i, a_j) contains $[n - |J(a_i, b_i, a_j)|]/8$ copies of a complete 2^3 factorial plus $|J(a_i, b_i, a_j)|/4$ copies of a half-replicate of 2^3 factorial. The following result is immediate.

Proposition 5.1. *D is a non-empty-cell design if and only if $|J(a_i, b_i, a_j)| < n$ for all $i \neq j$.*

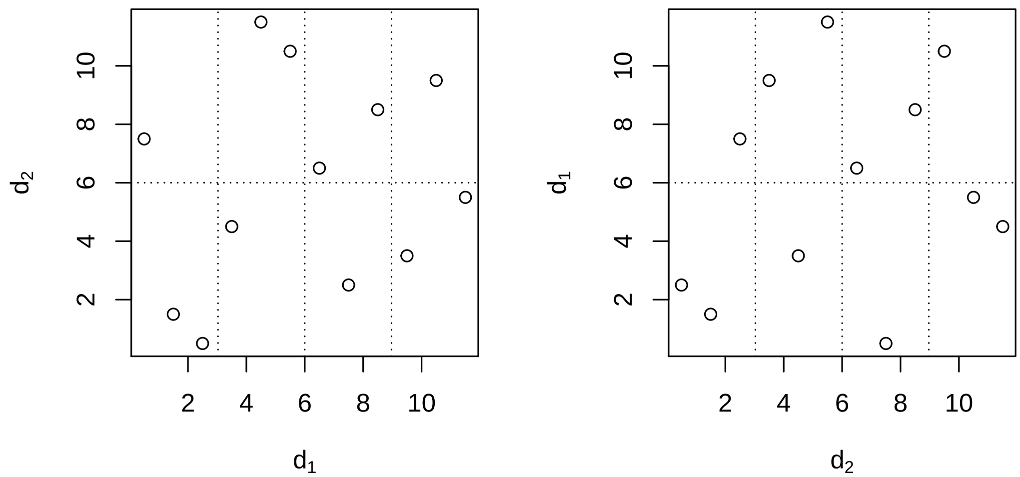
Based on Proposition 5.1 and the results of Cheng (1995) and Bulutoglu and Cheng (2003), we obtain the following sufficient conditions for non-empty-cell designs.

Corollary 5.1. *Design D is a non-empty-cell design if (i) n is not a multiple of 8, or (ii) S is a Paley design of $n \geq 12$ runs, the one obtained from the Hadamard matrix by Paley's first construction.*

We note that Paley designs of $n \leq 8$ runs are regular and cannot be used to construct non-empty-cell designs.

Example 5.1. *A non-empty-cell design D of 12 runs for 10 factors can be constructed by taking the first 10 columns of the 12-run Paley design as A and 10 copies of the 11th column*

Figure 5.1: The points of (d_1, d_2) and (d_2, d_1) over a 4×2 grid.



as B. To illustrate the non-empty-cell idea, we expand design D into a Latin hypercube as follows: for each column, replace the 3 entries of x by a random permutation of $3x + 0.5$, $3x + 1.5$ and $3x + 2.5$ for $x = 0, 1, 2, 3$. Figure 5.1 displays (d_1, d_2) and (d_2, d_1) seen from a 4×2 grid; as clearly shown, each of the eight cells of the grid contains at least one point.

In the regular case, we know that D is an SOA of strength 2+ if and only if $S \setminus A$ is an SOS design (He et al., 2018). This equivalence relationship, however, does not hold in general when S is nonregular. But we can show that a nonregular SOS design does imply the existence of a non-empty-cell design.

Corollary 5.2. *A non-empty-cell design D can be constructed if $S \setminus A$ is an SOS design.*

Proof. Since $S \setminus A$ is SOS, for any $1 \le i \le m$, there exist $e_1^{(i)}, e_2^{(i)} \in S \setminus A$ such that $|J(a_i, e_1^{(i)}, e_2^{(i)})| > 0$. Take $b_i = e_1^{(i)}$. For this choice of $B = (b_1, \ldots, b_m)$, we will show that $|J(a_i, b_i, a_j)| < n$ for all $j \neq i$. Suppose this is not the case. Then there exist $i \neq j$ such that $|J(a_i, b_i, a_j)| = n$, meaning that $a_j = \pm a_i b_i$, where $a_i b_i$ denotes the Hadamard product of a_i and b_i. Then a_j and $e_2^{(i)}$ cannot be orthogonal since $|J(a_j, e_2^{(i)})| = |J(a_i, b_i, e_2^{(i)})| = |J(a_i, e_1^{(i)}, e_2^{(i)})| > 0$, which leads to a contradiction. $\square$

Corollaries 5.1 and 5.2 give sufficient conditions for non-empty-cell designs. Identifying non-empty-cell designs is just a first step in making design D space-filling on the 4×2 grid. We now introduce two criteria to measure the 4×2 uniformity of D.

After projecting D_{ij} onto the 4×2 grid, the argument following Definition 5.1 implies that among the eight cells, four of them contain $[n - |J(a_i, b_i, a_j)|]/8$ points and the other four contain $[n + |J(a_i, b_i, a_j)|]/8$ points. A simple calculation shows that the variance of the numbers of points in eight cells is $V_{ij} = [J(a_i, b_i, a_j)]^2/64$. Therefore, different values of $|J(a_i, b_i, a_j)|$ correspond to different 4×2 patterns and a small $|J(a_i, b_i, a_j)|$ is preferred. Note that, as a by-product of Cheng's (1995) result, $|J(a_i, b_i, a_j)|$ can only take values of $n - 8k$ for $0 \leq k \leq \lfloor n/8 \rfloor$. Let f_k be the proportion of the ordered pairs (i, j)'s such that $|J(a_i, b_i, a_j)| = n - 8k$ for $0 \leq k \leq \lfloor n/8 \rfloor$. We define the 4×2 projection frequency vector of D to be

$$F(D) = (f_0, f_1, \ldots, f_{\lfloor n/8 \rfloor}).$$

The vector $F(D)$ summarizes the information on the 4×2 projection properties of the design D. In particular, if $f_0 = 0$, then D is a non-empty-cell design; if n is a multiple of 8 and $f_{n/8} = 1$, then D is an SOA of strength 2+.

To eliminate the worst 4×2 projections of design D, we sequentially minimize $f_0, f_1, \ldots, f_{\lfloor n/8 \rfloor - 1}$ and this is our first criterion. This criterion can be regarded as a natural refinement for seeking non-empty-cell designs. Though intuitively attractive, the first criterion is stringent and theoretically burdensome. Our second criterion aims at minimizing the average of V_{ij}'s over all possible (i, j)'s, that is, we seek to minimize the average variance

$$V(D) = \frac{1}{m(m-1)} \sum_{1 \leq i \neq j \leq m} V_{ij} = \frac{1}{64m(m-1)} \sum_{1 \leq i \neq j \leq m} [J(a_i, b_i, a_j)]^2. \tag{5.2}$$

In terms of $F(D)$, we have $V(D) = \sum_{k=0}^{\lfloor n/8 \rfloor} \left(\frac{n}{8} - k\right)^2 f_k$, which is a weighted average of f_k's. Thus the second criterion can be seen as a relaxed version of the first one. We should remark that designs minimizing $V(D)$ do not have to be non-empty-cell designs. In the following, we will call the two criteria Criterion 1 and Criterion 2, respectively, and focus on theoretical and computational methods to optimize them.

Finally, we note that our definitions of the two criteria are similar to those of minimum G- and G_2-aberration for fractional factorial designs proposed by Deng and Tang (1999) and Tang and Deng (1999).

5.3.2 Some theoretical results on $V(D)$

In this subsection, we present some theoretical results on $V(D)$ which, as we will see, are useful in finding optimal designs under both criteria. We start with a simple lemma.

Lemma 5.2. *Let $S \setminus A = E = \{e_1, \ldots, e_{n-m-1}\}$.*

(i) When $m = n-2, n-3$, we have $V(D) = n^2/[64(n-3)]$ for any choice of A and B.

(ii) For $e \in E$, define $P_i(e) = \sum_{j=1}^{m}[J(a_i, e, a_j)]^2$. Then for given A, array B minimizes $V(D)$ if and only if $P_i(b_i) = \min_{e\in E} P_i(e)$.

The proof of Lemma 5.2 is straightforward. Despite being mathematically simple, Lemma 5.2 provides some interesting insights. For example, an SOA of strength 2+ can be characterized as $P_i(b_i) = 0$ for every $i = 1, \ldots, m$. That $P_i(b_i) = 0$ is equivalent to that $a_i b_i$ is orthogonal to all a_j; the latter is precisely the condition for constructing SOAs of strength 2+ in Theorem 5 of Cheng et al. (2021). More importantly, Lemma 5.2 allows us to establish the next result.

Theorem 5.1. *If D is an SOA of strength 2+, then $S \setminus A$ must be an SOS design.*

Proof. Since D is an SOA of strength 2+, we have that for every a_i, there exists b_i from $S \setminus A$ such that $a_i b_i$ is orthogonal to all a_j. Since $a_i b_i$ is also orthogonal to 1_n, it must be a linear combination of $e_1, \ldots, e_{n-m-1}$, which implies that a_i is a linear combination of $b_i e_1, \ldots, b_i e_{n-m-1}$. Noting that b_i is from E, we see that every a_i is a linear combination of some $e_{j_1} e_{j_2}$ with $j_1 \neq j_2$. This means that the linear space spanned by $a_1, \ldots, a_m, e_1, \ldots, e_{n-m-1}$, which has rank $n-1$, is a linear subspace of the linear space spanned by $e_1, \ldots, e_{n-m-1}$ and all $e_{j_1} e_{j_2}$ with $j_1 \neq j_2$. Therefore the set of vectors $e_1, \ldots, e_{n-m-1}$ and all $e_{j_1} e_{j_2}$ with $j_1 \neq j_2$ has rank $n-1$, showing that $E = S \setminus A$ is SOS. □

Consider the following three statements: (a) D is an SOA of strength 2+; (b) $S \setminus A$ is SOS; and (c) D is a non-empty-cell design. In the regular case, the three statements are all equivalent. For the nonregular case, we have that (a) implies (b) by Theorem 5.1 and that (b) implies (c) by Corollary 5.2. When n is not a multiple of 8, we can easily find an example for which (c) is true but (b) is not and an example for which (b) is true but (a) is not. This completely settles the relationship between D being an SOA of strength 2+ and $S \setminus A$ being SOS in the nonregular case.

Example 5.2. *The statement (b) does not imply (a) even if n is a multiple of 8. Consider the $OA(24, 23, 2, 2)$ obtained from the Hadamard matrix labelled had.24.34 at Dr. Neil Sloane's website* `http://neilsloane.com/hadamard/` *and denote its columns by $1, \ldots, 23$. It can checked that the design $E = (11, 12, 13, 14, 15, 17, 18, 19, 20, 21, 22)$ is SOS. We take $A = S \backslash E = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 16, 23)$, and accordingly, choose $B = (13, 18, 17, 21, 22, 22, 14, 20, 14, 18, 11, 11)$ to minimize $V(D)$ by Lemma 5.2. Then we have $P_4(b_4) = 64$ and $P_i(b_i) = 0$ for $i \neq 4$. Thus D is not an SOA of strength 2+. On the other hand, the fact that E is SOS guarantees that D must be a non-empty-cell design.*

Part (i) of Lemma 5.2 says that $V(D)$ is constant when E has one or two columns. When E contains more than two columns, we derive the following lower bounds for $V(D)$ and also the conditions when they can be attained.

Theorem 5.2. *Let $J_0 = n - 8\lfloor n/8 \rfloor$. For $1 < m < \binom{n-1-m}{2}$, we have $V(D) \geq J_0^2/64$, where the equality holds if and only if $|J(a_i, b_i, a_j)| = J_0$ for $1 \leq i \neq j \leq m$. For $\binom{n-1-m}{2} \leq m \leq n-2$, we have*

$$V(D) \geq \frac{1}{64m(m-1)} \left\{ mn^2 - \binom{n-1-m}{2} n^2 + R(m,n) \right\}, \tag{5.3}$$

where $R(m,n) = J_0^2 \cdot [\binom{n-1-m}{2}(n-3) - m(n-2-m)]$ and the equality holds if and only if $|J(e_j, e_k, e_l)| = J_0$ for $1 \leq j \neq k \neq l \neq j \leq n-1-m$ and that for $1 \leq i \leq m$, there exists $e^{(i)} \in E$ such that $|J(a_i, e_j, e_k)| = J_0$ for any $e^{(i)} \neq e_j \neq e_k \neq e^{(i)}$.

Proof. The first inequality is obvious. For the second inequality, we give a proof for the case that n is a multiple of 8. Then $J_0 = 0$ and the result follows by noting that

$$V(D) = \frac{1}{64m(m-1)} \sum_{i=1}^{m} \left\{ n^2 - \max_{e \in E} \sum_{j=1}^{n-1-m} [J(a_i, e_j, e)]^2 \right\},$$

and that $\sum_{i=1}^{m} \max_{e\in E} \sum_{j=1}^{n-1-m} [J(a_i, e_j, e)]^2 \leq \sum_{i=1}^{m} \sum_{j<k}^{n-1-m} [J(a_i, e_j, e_k)]^2 = \sum_{j<k}^{n-1-m}\{n^2-$

$\sum_{l=1}^{n-1-m}[J(e_j, e_k, e_l)]^2\} \leq \binom{n-1-m}{2}n^2$, where the first equality holds if and only if for $1 \leq i \leq m$ there exists $e^{(i)} \in E$ such that $J(a_i, e_j, e_k) = 0$ for any $e^{(i)} \neq e_j \neq e_k \neq e^{(i)}$ and the last equality holds if and only if E has strength three, i.e., $J(e_j, e_k, e_l) = 0$ for $1 \leq j \neq k \neq l \neq j \leq n-1-m$. The proof for the case that n is not a multiple of 8 is similar, with the only difference being that the J-characteristic of any three columns is at least 4. $\square$

Next, we present two construction methods to attain lower bounds in Theorem 5.2. Before we proceed, we note the following useful fact.

Remark 5.1. *Suppose that design D with m columns attains the bound of Theorem 5.2. Then we can construct a design D' with m' columns where $m < m' \leq n-2$ that also attains the bound, which can be done by moving some columns from E to A as additional a_i's and taking any columns from the rest columns of E as corresponding b_i's.*

Construction 1: Suppose that $D = A + B/2 + 3/2$ of n runs for m factors attains the lower bound in Theorem 5.2. We construct design $\tilde{D} = \tilde{A} + \tilde{B}/2 + 3/2$, with $\tilde{A}$ and $\tilde{B}$ defined as

$$\tilde{A} = (a_1^+, \ldots, a_m^+, a_1^-, \ldots, a_m^-, e_1^-, \ldots, e_{n-1-m}^-), \quad \tilde{B} = (b_1^+, \ldots, b_m^+, b_1^+, \ldots, b_m^+, 1_n^-, \ldots, 1_n^-)$$

where, for any column c, we use c^+ and c^- to denote $[1\ 1]^T \otimes c$ and $[1\ -1]^T \otimes c$, respectively. Then we can verify that design $\tilde{D}$, which has $2n$ runs and $n+m-1$ factors, also attains the lower bound in Theorem 5.2 provided that (i) n is a multiple of 8 or that (ii) n is not a multiple of 8 but $m = n-3$.

Example 5.3. *Let $S = (s_1, \ldots, s_{11})$ be the 12-run Paley design. Take $A = (s_1 \ldots, s_9)$ and B as 9 copies of s_{10}. Then $D = A + B/2 + 3/2$ attains the lower bound by Lemma 5.2 and Theorem 5.2. Apply Construction 1 by letting $\tilde{A} = (s_1^+, \ldots, s_9^+, s_1^-, \ldots, s_9^-, s_{10}^-, s_{11}^-)$ and $\tilde{B} = (s_{10}^+, \ldots, s_{10}^+, s_{10}^+, \ldots, s_{10}^+, 1_{12}^-, 1_{12}^-)$. Then the 24×20 design $\tilde{D} = \tilde{A} + \tilde{B}/2 + 3/2$ also attains the bound; note that columns of $\tilde{A}$ and $\tilde{B}$ are taken from the saturated design* *consisting of* 1_{12}^-, s_i^+ *and* s_i^- *for* $i = 1, \ldots, 11$. *Applying Construction 1 successively, we obtain* 48×43, 96×90 *designs and so on, all of which attain the bound in Theorem 5.2.*

It can easily be checked that when regular S is used, the second equality conditions in Theorem 5.2 hold if and only if E has resolution V, a situation covered by Theorem 3 of Shi and Tang (2019). Inspired by this connection, we put forward the following construction.

Construction 2: Suppose that E is an $\mathrm{OA}(n, n-1-m, 2, 4)$ such that all its main effects and two-factor interactions can be embedded into a saturated orthogonal array S. Let $A = S \setminus E = (a_1, \ldots, a_m)$. For $1 \leq i \leq m$, choose $b_i = e_1^{(i)}$ if a_i can be written as $e_1^{(i)} e_2^{(i)}$ for some $e_1^{(i)}, e_2^{(i)} \in E$, otherwise choose $b_i = e_1$. Then $D = A + B/2 + 3/2$ attains the lower bound in Theorem 5.2.

Finding a required E in Construction 2 is not an easy task in general. Nonetheless, an interesting example can be given. Let $E = (e_1, \ldots, e_{15})$ be an $\mathrm{OA}(128, 15, 2, 4)$ which can be obtained, for example, from the shortened Nordstrom-Robinson code (Xu, 2005). By a result of Verheiden (1978), the 120 columns in the form of e_i $(1 \leq i \leq 15)$ and $e_j e_k$ $(1 \leq j \neq k \leq 15)$ can be embedded into an $\mathrm{OA}(128, 127, 2, 2)$. Applying Construction 2, we obtain a design D of 128 runs for $m = 112$ factors that attains the lower bound in Theorem 5.2. By Remark 5.1, designs of 128 runs for m' factors where $113 \leq m' \leq 126$ can all be constructed to attain the lower bound. The approach of Shi and Tang (2019) for regular designs effectively maximizes $f_{n/8}$ in our notation. One can check that for $112 \leq m' \leq 115$, the designs constructed here are better than those from regular designs in terms of $V(D)$.

Constructions 1 and 2 do not apply when n is a multiple of 4 but not a multiple of 8, except for $m = n - 3$ in Construction 1. We conclude this subsection with a remark that provides a result for this case.

Remark 5.2. *When* n *is a multiple of 4 such that* $n/2 - 1 = 4k + 1$ *is a prime power where* k *is an integer, Shi and Tang (2023) constructed an* $OA(n/2, n/4, 2, 2)$ *with generalized resolution* $4 - 4/n$. *Let the columns of this* $OA(n/2, n/4, 2, 2)$ *be denoted by* $s_1, \ldots, s_{n/4}$, *and take* $A = (s_1, \ldots, s_{n/4-1})$ *and* $B = (s_{n/4}, \ldots, s_{n/4})$. *Then* $D = A + B/2 + 3/2$, *a design of* n *runs for* $m = n/2 - 1$ *factors, has* $V(D) = 1/4$ *and thus attains the lower bound in Theorem*

5.2. We will see in the next subsection that for $n = 20, 28$ *and 36, designs with more factors can be found to still have* $V(D) = 1/4$.

5.3.3 Some computational results

In this subsection, we conduct computer searches to find the best designs D under each of the two criteria for n = 16, 20, 24, 28, 32, 36 and 40. For n = 16, 20 and 24, there are exactly 5, 3 and 130 non-isomorphic saturated orthogonal arrays. We take all of them as S and for each S consider all possible $\binom{n-1}{m}$ choices of A. For n = 28, 32, 36 and 40, we obtain 487, 22, 235 and 98 non-isomorphic saturated orthogonal arrays, respectively. These orthogonal arrays are derived from non-isomorphic Hadamard matrices we can find from the web. Taking each array as S, we then either consider all choices of A from S if $\binom{n-1}{m}$ does not exceed 200,000 or consider 200,000 A's selected randomly from S otherwise. After A is chosen and fixed, the columns of B are selected from $S \setminus A$ to optimize Criterion 1 or Criterion 2.

Ingram and Tang (2005) proposed using minimum G_e-aberration with sufficiently large e as a computationally efficient surrogate for minimum G-aberration. A similar approach can be applied in our computer search under Criterion 1. Our surrogate criterion is to minimize $\sum_{1 \le i \ne j \le m} |J(a_i, b_i, a_j)/n|^p$. It can be shown that if $p > \log(m^2 - m)/[\log(n) - \log(n-8)]$, then the surrogate criterion is equivalent to Criterion 1. We take $p = \lfloor \log(m^2 - m)/[\log(n) - \log(n-8)] \rfloor + 1$ in our search.

The search results are displayed in Tables 5.1 and 5.2. For given n and $m \le n-2$, we present $F(D)$ and $V(D)$ of the best design found under each of the two criteria. Only one entry of $F(D)$ and $V(D)$ combination is given if the same design can be found to optimize both criteria. We mark an $F(D)$ entry or a $V(D)$ entry with an asterisk if it is optimal, which is judged to be so either because the search is complete or by the lower bounds of $V(D)$ in Theorem 5.2. More details about the underlying designs, including the design matrices, are available online at `https://github.com/gz-chen/Nonregular-SOA`. All the designs in Tables 5.1 and 5.2 are non-empty-cell designs since they all have $f_0 = 0$

Example 5.4. *The* 16×14 *design can be constructed from the* $OA(16, 15, 2, 2)$ *from the Hadamard matrix labelled had.16.4 at Dr. Sloan's website by taking the first 14 columns as*

Table 5.1: Designs of 16, 20, 24, 28 and 32 runs by computer search under Criteria 1 and 2

<table>
<tr><th>$n \times m$</th><th>Criterion 1: $F(D)$ and $64V(D)$</th><th>Criterion 2: $F(D)$ and $64V(D)$</th></tr>
<tr><td>16×14</td><td colspan="2">(0, 0.308, 0.692)*; 19.69*</td></tr>
<tr><td>16×13</td><td colspan="2">(0, 0.308, 0.692)*; 19.69*</td></tr>
<tr><td>16×12</td><td colspan="2">(0, 0.273, 0.727)*; 17.45*</td></tr>
<tr><td>16×11</td><td colspan="2">(0, 0.182, 0.818)*; 11.64*</td></tr>
<tr><td>16×10</td><td colspan="2">(0, 0, 1)*; 0*</td></tr>
<tr><td>20×18</td><td colspan="2">(0, 0.059, 0.941)*; 23.53*</td></tr>
<tr><td>20×17</td><td colspan="2">(0, 0.059, 0.941)*; 23.53*</td></tr>
<tr><td>20×16</td><td colspan="2">(0, 0.054, 0.946)*; 22.93*</td></tr>
<tr><td>20×15</td><td colspan="2">(0, 0.043, 0.957)*; 21.49*</td></tr>
<tr><td>20×14</td><td colspan="2">(0, 0.022, 0.978)*; 18.81*</td></tr>
<tr><td>20×13</td><td colspan="2">(0, 0, 1)*; 16*</td></tr>
<tr><td>24×22</td><td colspan="2">(0, 0, 0.429, 0.571)*; 27.43*</td></tr>
<tr><td>24×21</td><td colspan="2">(0, 0, 0.429, 0.571)*; 27.43*</td></tr>
<tr><td>24×20</td><td colspan="2">(0, 0, 0.403, 0.597)*; 25.77*</td></tr>
<tr><td>24×19</td><td colspan="2">(0, 0, 0.351, 0.649)*; 22.46*</td></tr>
<tr><td>24×18</td><td colspan="2">(0, 0, 0.281, 0.719)*; 17.99*</td></tr>
<tr><td>24×17</td><td>(0, 0, 0.206, 0.794)*; 13.18</td><td>(0, 0.007, 0.162, 0.831); 12.24*</td></tr>
<tr><td>24×16</td><td colspan="2">(0, 0, 0.112, 0.888)*; 7.20*</td></tr>
<tr><td>24×15</td><td colspan="2">(0, 0, 0.076, 0.924)*; 4.88*</td></tr>
<tr><td>24×14</td><td colspan="2">(0, 0, 0.049, 0.951)*; 3.16*</td></tr>
<tr><td>24×13</td><td colspan="2">(0, 0, 0.026, 0.974)*; 1.64*</td></tr>
<tr><td>24×12</td><td colspan="2">(0, 0, 0.008, 0.992)*; 0.48*</td></tr>
<tr><td>24×11</td><td colspan="2">(0, 0, 0, 1)*; 0*</td></tr>
<tr><td>28×26</td><td colspan="2">(0, 0, 0.120, 0.880)*; 31.36*</td></tr>
<tr><td>28×25</td><td colspan="2">(0, 0, 0.120, 0.880)*; 31.36*</td></tr>
<tr><td>28×24</td><td colspan="2">(0, 0, 0.114, 0.886)*; 30.61*</td></tr>
<tr><td>28×23</td><td colspan="2">(0, 0, 0.101, 0.899)*; 28.90*</td></tr>
<tr><td>28×22</td><td colspan="2">(0, 0, 0.078, 0.922)*; 25.97*</td></tr>
<tr><td>28×21</td><td colspan="2">(0, 0, 0.452, 0.955); 23.01</td></tr>
<tr><td>28×20</td><td colspan="2">(0, 0, 0.032, 0.968); 20.04</td></tr>
<tr><td>28×19</td><td colspan="2">(0, 0, 0.018, 0.982); 18.25</td></tr>
<tr><td>28×18</td><td colspan="2">(0, 0, 0.010, 0.990); 17.25</td></tr>
<tr><td>28×17</td><td colspan="2">(0, 0, 0, 1)*; 16*</td></tr>
<tr><td>32×30</td><td colspan="2">(0, 0, 0, 0.552, 0.448)*; 35.31*</td></tr>
<tr><td>32×29</td><td colspan="2">(0, 0, 0, 0.552, 0.448)*; 35.31*</td></tr>
<tr><td>32×28</td><td>(0, 0, 0, 0.533, 0.467); 34.12</td><td>(0, 0, 0.007, 0.503, 0.491); 33.86*</td></tr>
<tr><td>32×27</td><td>(0, 0, 0, 0.509, 0.491); 32.55</td><td>(0, 0, 0.120, 0, 0.880); 30.63*</td></tr>
<tr><td>32×26</td><td>(0, 0, 0, 0.468, 0.532); 29.93</td><td>(0, 0, 0.098, 0, 0.902); 25.21*</td></tr>
<tr><td>32×25</td><td>(0, 0, 0, 0.417, 0.583); 26.67</td><td>(0, 0, 0.067, 0, 0.933); 17.07*</td></tr>
<tr><td>32×24</td><td>(0, 0, 0, 0.271, 0.728); 17.39</td><td>(0, 0, 0.043, 0, 0.957); 11.13</td></tr>
<tr><td>32×23</td><td>(0, 0, 0, 0.190, 0.810); 12.14</td><td>(0, 0, 0.024, 0, 0.976); 6.07</td></tr>
<tr><td>32×22</td><td colspan="2">(0, 0, 0, 0, 1)*; 0*</td></tr>
</table>

A and 14 copies of the last column as B. After projecting all its two-dimensions onto the 4×2 *grid, 30.8% of them have the property that four cells contain one point and the other four contain three points; 69.2% of them achieve stratification on the* 4×2 *grid, ie, all eight cells contain exactly two points.*

Table 5.2: Designs of 36 and 40 runs by computer search under Criteria 1 and 2

<table>
<tr><th>$n \times m$</th><th>Criterion 1: $F(D)$ and $64V(D)$</th><th>Criterion 2: $F(D)$ and $64V(D)$</th></tr>
<tr><td>36×34</td><td colspan="2">(0, 0, 0, 0.182, 0.818)*; 39.27*</td></tr>
<tr><td>36×33</td><td colspan="2">(0, 0, 0, 0.182, 0.818)*; 39.27*</td></tr>
<tr><td>36×32</td><td colspan="2">(0, 0, 0, 0.175, 0.825)*; 38.45*</td></tr>
<tr><td>36×31</td><td colspan="2">(0, 0, 0, 0.161, 0.839)*; 36.65*</td></tr>
<tr><td>36×30</td><td colspan="2">(0, 0, 0, 0.138, 0.862)*; 33.66*</td></tr>
<tr><td>36×29</td><td colspan="2">(0, 0, 0, 0.108, 0.892); 29.87</td></tr>
<tr><td>36×28</td><td colspan="2">(0, 0, 0, 0.086, 0.914); 27.01</td></tr>
<tr><td>36×27</td><td colspan="2">(0, 0, 0, 0.057, 0.943); 23.29</td></tr>
<tr><td>36×26</td><td colspan="2">(0, 0, 0, 0.031, 0.969); 19.94</td></tr>
<tr><td>36×25</td><td colspan="2">(0, 0, 0, 0.007, 0.993); 16.85</td></tr>
<tr><td>36×24</td><td colspan="2">(0, 0, 0, 0, 1)*; 16*</td></tr>
<tr><td>40×38</td><td colspan="2">(0, 0, 0, 0.034, 0.539, 0.427); 43.24*</td></tr>
<tr><td>40×37</td><td colspan="2">(0, 0, 0, 0.024, 0.560, 0.396); 43.24*</td></tr>
<tr><td>40×36</td><td>(0, 0, 0, 0.021, 0.582, 0.398); 42.51</td><td>(0, 0, 0.006, 0.038, 0.455, 0.503); 41.90*</td></tr>
<tr><td>40×35</td><td>(0, 0, 0, 0.018, 0.571, 0.411); 41.09</td><td>(0, 0, 0.008, 0.035, 0.403, 0.555); 39.15</td></tr>
<tr><td>40×34</td><td>(0, 0, 0, 0.013, 0.569, 0.418); 39.81</td><td>(0, 0, 0.004, 0.075, 0.217, 0.704); 35.59</td></tr>
<tr><td>40×33</td><td>(0, 0, 0, 0.010, 0.561, 0.430); 38.30</td><td>(0, 0, 0.006, 0.057, 0.203, 0.735); 30.79</td></tr>
<tr><td>40×32</td><td>(0, 0, 0, 0.006, 0.566, 0.428); 37.75</td><td>(0, 0, 0.009, 0.039, 0.183, 0.768); 27.03</td></tr>
<tr><td>40×31</td><td>(0, 0, 0, 0.002, 0.576, 0.421); 37.44</td><td>(0, 0, 0.008, 0.016, 0.234, 0.742); 23.47</td></tr>
<tr><td>40×30</td><td>(0, 0, 0, 0.001, 0.503, 0.497); 32.44</td><td>(0, 0, 0.005, 0.032, 0.153, 0.810); 20.67</td></tr>
<tr><td>40×29</td><td>(0, 0, 0, 0, 0.414, 0.586); 26.48</td><td>(0, 0, 0, 0.026, 0.167, 0.807); 17.33</td></tr>
<tr><td>40×28</td><td>(0, 0, 0, 0, 0.278, 0.722); 17.78</td><td>(0, 0, 0, 0.022, 0.149, 0.828); 15.32</td></tr>
<tr><td>40×27</td><td>(0, 0, 0, 0, 0.237, 0.762); 15.23</td><td>(0, 0, 0, 0.014, 0.138, 0.848); 12.49</td></tr>
<tr><td>40×26</td><td>(0, 0, 0, 0, 0.205, 0.795); 13.10</td><td>(0, 0, 0, 0.009, 0.135, 0.855); 11.03</td></tr>
<tr><td>40×25</td><td>(0, 0, 0, 0, 0.167, 0.833); 10.67</td><td>(0, 0, 0, 0.005, 0.120, 0.875); 8.96</td></tr>
<tr><td>40×24</td><td>(0, 0, 0, 0, 0.114, 0.886); 7.30</td><td>(0, 0, 0, 0.002, 0.089, 0.909); 6.14</td></tr>
<tr><td>40×23</td><td colspan="2">(0, 0, 0, 0, 0.091, 0.909); 5.82</td></tr>
<tr><td>40×22</td><td colspan="2">(0, 0, 0, 0, 0.054, 0.946); 3.46</td></tr>
<tr><td>40×21</td><td colspan="2">(0, 0, 0, 0, 0.048, 0.952); 3.05</td></tr>
<tr><td>40×20</td><td colspan="2">(0, 0, 0, 0, 0.024, 0.976); 1.52</td></tr>
<tr><td>40×19</td><td colspan="2">(0, 0, 0, 0, 0, 1)*; 0*</td></tr>
</table>

From Cheng et al. (2021), we know that when n is a multiple of 16, SOAs of strength 2+ can be constructed in both regular and nonregular cases for m values much larger than $n/2$. For examples, SOAs of strength 2+ can be constructed for $n = 32$ and $m = 22$ and for

$n = 48$ and $m = 34$. One surprise in Tables 5.1 and 5.2 is that no SOA of strength 2+ is found for $n = 24$ and 40 with $m \geq n/2$. This seems to suggest that SOAs of strength 2+ do not exist for $m \geq n/2$ when n is a multiple of 8 but not a multiple of 16. At the moment, we are unable to prove or disprove this statement and thus leave it as a conjecture for future research.

Another interesting finding in Tables 5.1 and 5.2 is the existence of a 20×13 design, a 28×17 design and a 36×24 design, all with $V(D) = 1/4$ which corresponds to $|J(a_i, b_i, a_j)| = 4$. When n is a multiple of 4 but not a multiple of 8, the best scenario is that $|J(a_i, b_i, a_j)| = 4$ for all $i \neq j$. A design with this property has its points most uniformly distributed in the 8 cells given by the 4×2 grid when projected onto any two-dimension. As discussed in Remark 5.2, whenever n is a multiple of 4 such that $n/2 - 1 = 4k + 1$ is a prime power where k is an integer, a design D can be constructed for $m = n/2 - 1$ factors with the property that $|J(a_i, b_i, a_j)| = 4$ for all $i \neq j$. This design D has an extra property that $|J(a_i, a_j, a_k)| = 4$ for all $i < j < k$ and therefore its points are most uniformly distributed in the 8 cells given by the $2 \times 2 \times 2$ grid when projected onto any three-dimension.

5.4 Results from using three-level nonregular designs

In this section, we consider using three-level nonregular designs to construct space-filling designs, which provides an opportunity for the resulting designs to achieve uniformity on a finer 9×3 grid than the 4×2 grid. The ideas in Section 5.3 are generalized to deal with the new situation. We present computer search results for designs of 27 and 54 runs.

5.4.1 Designs of 27 runs

Our approach is similar to Section 5.3. We construct design D by $D = 3A + B$, where A selects its columns from S, an $\mathrm{OA}(27, 13, 3, 2)$, and B selects its columns from $S \setminus A$. In all, there are 68 non-isomorphic $\mathrm{OA}(27, 13, 3, 2)$s (Schoen et al., 2010), and we use all of them as our S. By examining all projection designs $D_{ij} = (d_i, d_j)$ on the 9×3 grid, we find 9 possible patterns, which are labelled as patterns (a)–(i) in Table 5.3. The 9×3 grid gives 27 cells. For each pattern, Table 5.3 gives the numbers of cells that have 0, 1, 2 and 3 points. For example, in pattern (a) 18 cells have 0 points and 9 cells have 3 points. For another example, in pattern (i), all 27 cells contain exactly one point. The last row of the table gives the variance of the numbers of points over the 9×3 grid. The nine patterns are ordered from left to right such that both the number of empty cells and the variance are non-increasing. In this order, each pattern is more desirable than the preceding one.

Table 5.3: The nine patterns of projection designs D_{ij}'s when viewed on the 9×3 grid from considering all 68 non-isomorphic $\mathrm{OA}(27, 13, 3, 2)$s.

Pattern	(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)	(i)
0 points	18	12	9	9	8	7	6	4	0
1 points	0	6	10	9	12	13	15	19	27
2 points	0	6	7	9	6	7	6	4	0
3 points	9	3	1	0	1	0	0	0	0
Variance	2.00	1.11	0.74	0.67	0.67	0.52	0.44	0.30	0.00

Following the same idea as in the 4×2 case, we define the 9×3 projection frequency vector to be $F(D) = (f_0, \ldots, f_8)$, where $f_0, \ldots, f_8$ are the proportions of pattern (a),..., pattern (i), respectively, out of $m(m-1)$ ordered two-dimensionl projection designs D_{ij}'s, and further define $V(D)$ to be the average of the variances of D_{ij}'s for all $i \neq j$. Similarly, Criterion 1 sequentially minimizes the entries of $F(D)$ and Criterion 2 minimizes $V(D)$. We conduct a complete search over the 68 non-isomorphic orthogonal arrays under each criterion, and report our results in Table 5.4. In addition to $F(D)$ and $V(D)$, Table 5.4 also includes in the last column another measure $\rho(D)$ of design quality in terms of the number of empty cells. Let n_{ij} be the number of empty cells when design D_{ij} is viewed on the 9×3 grid. Then $\rho(D)$ is defined as

$$\rho(D) = \frac{\sum_{i \neq j} n_{ij}}{27m(m-1)},$$

which is the proportion of the total number of empty cells over the total number of cells when all projection designs D_{ij}'s are considered on the 9×3 grid.

Since $n = 27$, a non-empty-cell design must be an $\mathrm{SOA}(27, m, 9, 2+)$. According to our computer search, an $\mathrm{SOA}(27, m, 9, 2+)$ can be found for $m = 6$, which confirms a theoretical result in (He et al., 2018). Designs optimizing Criterion 2 are often not unique and we select the one to include in Table 5.4 that has the smallest $\rho(D)$ among these designs. Interested readers can find the design matrices and other details of the underlying designs in Table 5.4 at `https://github.com/gz-chen/Nonregular-SOA`.

Table 5.4: Designs of 27 runs from a complete search under Criteria 1 and 2.

m	Criterion	$F(D)$	$V(D)$	$\rho(D)$
12	1	(0, 0, 0, 0, 0.182, 0, 0.545, 0, 0.273)	0.36	17.51%
12	2	(0.182, 0, 0, 0, 0, 0, 0, 0, 0.818)	0.36	12.12%
11	1	(0, 0, 0, 0, 0.182, 0, 0.545, 0, 0.273)	0.36	17.51%
11	2	(0.182, 0, 0, 0, 0, 0, 0, 0, 0.818)	0.36	12.12%
10	1	(0, 0, 0, 0, 0.089, 0.244, 0.378, 0.156, 0.133)	0.40	19.67%
10	2	(0.156, 0, 0, 0, 0, 0, 0, 0, 0.844)	0.31	10.37%
9	1	(0, 0, 0, 0, 0, 0, 0.667, 0, 0.333)	0.30	14.81%
9	2	(0.125, 0, 0, 0, 0, 0, 0, 0, 0.875)	0.25	8.33%
8	1	(0, 0, 0, 0, 0, 0, 0.643, 0, 0.357)	0.29	14.29%
8	2	(0.107, 0, 0, 0, 0, 0, 0, 0, 0.893)	0.21	7.14%
7	1	(0, 0, 0, 0, 0, 0, 0.429, 0.190, 0.381)	0.25	12.34%
7	2	(0.071, 0, 0, 0, 0, 0, 0, 0, 0.929)	0.14	4.76%
6	1,2	(0, 0, 0, 0, 0, 0, 0, 0, 1)	0	0.00%

5.4.2 Designs of 54 runs

It is known that an OA$(54, 25, 3, 2)$ can be constructed by the Addelman-Kempthorne's method (Hedayat et al., 1999). To the best of our knowledge, OA$(54, 25, 3, 2)$s have not been enumerated. We would like to consider more OA$(54, 25, 3, 2)$s but the one by Addelman-Kempthorne construction is the only one we can find. We therefore use this OA$(54, 25, 3, 2)$ as our S, and construct design $D = 3A + B$ by selecting the columns of A from S and the columns of B from $S \setminus A$. Examining the projection designs D_{ij}'s on the 9×3 grid, we find five possible patterns, which are given as pattern (a) to (e) in Table 5.5. The five patterns are ordered so that both the variance and the number of empty cells are non-increasing. Therefore, any pattern is more desirable than the preceding one. We then define $F(D)$ and $V(D)$ and their associated Criteria 1 and 2 in the same way as in Subsection 4.1.

Table 5.5: The five patterns of projection designs D_{ij}'s when viewed on the 9×3 grid from considering the OA$(54, 25, 3, 2)$ by Addelman-Kempthorne construction.

Pattern	(a)	(b)	(c)	(d)	(e)
0 points	18	12	9	0	0
1 points	0	0	0	18	0
2 points	0	0	0	0	27
3 points	0	12	18	0	0
4 points	0	0	0	9	0
5 points	0	0	0	0	0
6 points	9	3	0	0	0
Variance	8.00	4.00	2.00	2.00	0.00

Table 5.6: Designs of 54 runs by computer search under Criteria 1 and 2.

m	Criterion	$F(D)$	$V(D)$	$\rho(D)$
24	1,2	(0.011, 0.011, 0.130, 0.130, 0.717)	0.65	5.56%
23	1	(0, 0.030, 0.170, 0.095, 0.706)	0.65	6.98%
23	2	(0.012, 0, 0.134, 0.119, 0.735)	0.60	5.27%
22	1	(0, 0, 0.117, 0.214, 0.669)	0.66	3.90%
22	2	(0.013, 0.006, 0.175, 0.019, 0.786)	0.52	7.00%
21	1	(0, 0, 0.095, 0.229, 0.676)	0.65	3.17%
21	2	(0.005, 0, 0.152, 0.057, 0.786)	0.46	5.40%
20	1	(0, 0, 0.079, 0.261, 0.661)	0.68	2.63%
20	2	(0.005, 0, 0.179, 0, 0.816)	0.40	6.32%
19	1	(0, 0, 0.050, 0.289, 0.661)	0.68	1.66%
19	2	(0, 0, 0.187, 0, 0.813)	0.37	6.24%
18	1	(0, 0, 0.039, 0.265, 0.696)	0.61	1.31%
18	2	(0, 0, 0.137, 0.039, 0.823)	0.35	4.58%
17	1	(0, 0, 0.015, 0.353, 0.632)	0.74	0.49%
17	2	(0.004, 0, 0.125, 0.022, 0.849)	0.32	4.41%
16	1	(0, 0, 0.013, 0.188, 0.800)	0.40	0.42%
16	2	(0, 0, 0.117, 0.017, 0.867)	0.27	3.89%
15	1	(0, 0, 0, 0.171, 0.829)	0.34	0.00%
15	2	(0, 0, 0.067, 0.043, 0.890)	0.22	2.22%
14	1	(0, 0, 0, 0.132, 0.868)	0.26	0.00%
14	2	(0, 0, 0.044, 0.033, 0.923)	0.15	1.47%
13	1	(0, 0, 0, 0.090, 0.910)	0.18	0.00%
13	2	(0, 0, 0.019, 0, 0.981)	0.04	0.64%
12	1,2	(0, 0, 0, 0, 1)	0	0.00%

For $m \geq 17$, our search is complete in that all possible $\binom{25}{m}$ choices for A are considered. For $12 \leq m \leq 16$, we randomly select 200,000 A's in order to save time. Once A is chosen, the columns of B are selected from $S \setminus A$ to optimize either criteria. The search results are presented in Table 5.6. Again, the designs optimizing Criterion 2 are not unique and those presented in Table 5.6 also minimize $\rho(D)$ among those designs that minimize $V(D)$. We see from Table 5.6 that non-empty-cell designs becomes available for $m \leq 15$. More details about the designs listed in Table 5.6 can be found on-line at `https://github.com/gz-chen/Nonregular-SOA`.

Most interesting among our findings in Table 5.6 is the existence of an SOA$(54, 12, 9, 2+)$. For $n = 54$, an SOA of strength 3 is available only for 5 factors and for $n = 81$, an SOA of strength 3 is available for 10 factors (He and Tang, 2014). The two SOAs of strength 3 achieve stratifications on the 9×3 grid in two-dimensions and stratifications on the $3 \times 3 \times 3$

grid in three-dimensions. By sacrificing the three-dimensional projection property, we obtain a design of 54 runs that can accommodate 12 factors. We document this design in a lemma.

Lemma 5.3. *There exists an* $SOA(54, 12, 9, 2+)$.

5.5 Concluding remarks

This chapter investigates the construction of space-filling designs using two- and three-level nonregular designs. We put forward a class of designs called non-empty-cell designs and two criteria to optimize the $s^2 \times s$ uniformity. Various theoretical and computational results are presented. Designs studied in this chapter are more general than those obtained from regular designs in that they have more flexible run sizes and often possess better space-filling properties in terms of the two criteria.

Designs constructed in this chapter have 4 or 9 levels. If more levels are preferred, we can use them to construct Latin hypercube designs by level expansion in the same way as constructing OA-based Latin hypercubes in Tang (1993). The resulting designs inherit the projection properties of the base designs.

Throughout the chapter, the columns of A and B are selected from a saturated or nearly saturated orthogonal array S. This need not be so. The general problem of interest would be to consider as A all possible orthogonal arrays of strength two and as B all possible orthogonal arrays of strength one. Although it may be computationally unwieldy, the general setting could offer some theoretical insights. For example, our current approach in Section 5.3 does not allow us to construct a design of 16 runs for 15 factors. However, a computer search without restricting to a saturated orthogonal array shows that there do exist many SOA$(16, 15, 4, 2)$s with non-empty 4×2 cells.

Computations in the chapter are currently carried out either by complete search or by a large number of random tries. It will be worthwhile to look into an algorithmic search, especially if one wishes to expand our design tables to include larger run sizes. Familiar algorithms, such as simulated annealing, coordinate exchange or particle swarms, are all potentially useful. We leave this to future exploration.

Bibliography

E. Aarts and J. K. Lenstra, editors. *Local Search in Combinatorial Optimization*. Princeton, New Jersey: Princeton University Press, 2003.

M.-Y. Ai and R.-C. Zhang. Projection justification of generalized minimum aberration for asymmetrical fractional factorial designs. *Metrika*, 60(3):279–285, 2004.

T. Banerjee and R. Mukerjee. Optimal factorial designs for cDNA microarray experiments. *Ann. Appl. Stat.*, 2(1):366–385, 2008.

D. Bingham, R. R. Sitter, and B. Tang. Orthogonal and nearly orthogonal designs for computer experiments. *Biometrika*, 96(1):51–65, 2009.

R. M. Block and R. W. Mee. Second order saturated resolution iv designs. *J. Stat. Theory Appl.*, 2:96–112, 2003.

G. Box and J. Tyssedal. Projective properties of certain orthogonal arrays. *Biometrika*, 83 (4):950–955, 1996.

G. E. P. Box and N. R. Draper. A basis for the selection of a response surface design. *J. Amer. Statist. Assoc.*, 54:622–654, 1959.

G. E. P. Box and J. S. Hunter. The 2^{k-p} fractional factorial designs. *Technometrics*, 3: 311–351, 1961.

G. E. P. Box and K. B. Wilson. On the experimental attainment of optimum conditions. *J. Roy. Statist. Soc. Ser. B*, 13:1–38; discussion: 38–45, 1951.

D. A. Bulutoglu and C.-S. Cheng. Hidden projection properties of some nonregular fractional factorial designs and their applications. *Ann. Statist.*, 31(3):1012–1026, 2003.

N. A. Butler. Results for two-level fractional factorial designs of resolution IV or more. *J. Statist. Plann. Inference*, 137(1):317–323, 2007.

G. Chen and B. Tang. A study of orthogonal array-based designs under a broad class of space-filling criteria. *Ann. Statist.*, 50(5):2925–2949, 2022a.

G. Chen and B. Tang. Using nonregular designs to generate space-filling designs. *J. Statist. Plann. Inference*, 221:201–211, 2022b.

H. Chen and A. S. Hedayat. 2^{n-l} designs with weak minimum aberration. *Ann. Statist.*, 24(6):2536–2548, 1996.

C.-S. Cheng. Orthogonal arrays with variable numbers of symbols. *Ann. Statist.*, 8(2): 447–453, 1980.

C.-S. Cheng. Some projection properties of orthogonal arrays. *Ann. Statist.*, 23(4):1223–1233, 1995.

C.-S. Cheng. Some hidden projection properties of orthogonal arrays with strength three. *Biometrika*, 85(2):491–495, 1998.

C.-S. Cheng. *Theory of Factorial Design: Single- and Multi-Stratum Experiments*. Boca Raton, Florida: CRC Press, 2014.

C.-S. Cheng, Y. He, and B. Tang. Minimal second order saturated designs and their applications to space-filling designs. *Statist. Sinica*, 31(2):867–890, 2021.

W. G. Cochran. Long-term agricultural experiments (with discussion). *J. R. Stat. Soc. Suppl.*, 6:104–148, 1939.

W. G. Cochran and G. M. Cox. *Experimental Designs, 2nd ed.* New York: Wiley, 1957.

D. R. Cox. *Planning of Experiments*. New York: Wiley, 1958.

L.-Y. Deng and B. Tang. Generalized resolution and minimum aberration criteria for Plackett-Burman and other nonregular factorial designs. *Statist. Sinica*, 9(4):1071–1082, 1999.

K.-T. Fang, D. K. J. Lin, P. Winker, and Y. Zhang. Uniform design: theory and application. *Technometrics*, 42(3):237–248, 2000.

K.-T. Fang, R. Li, and A. Sudjianto. *Design and Modeling for Computer Experiments*. Boca Raton, Florida: Chapman & Hall/CRC, 2006.

K.-T. Fang, M.-Q. Liu, H. Qin, and Y.-D. Zhou. *Theory and Application of Uniform Experimental Designs*. Beijing: Science Press; Singapore: Springer, 2018.

D. J. Finney. The fractional replication of factorial experiments. *Ann. Eugen.*, 12:291–301, 1945.

R. A. Fisher. The arrangement of field experiments. *J. Ministry Agric.*, 33:503–513, 1926.

R. A. Fisher. *Design of Experiments*. Edinburg, U.K.: Oliver and Boyd, 1935.

A. Fries and W. G. Hunter. Minimum aberration 2^{k-p} designs. *Technometrics*, 22(4): 601–608, 1980.

S. D. Georgiou, S. Stylianou, K. Drosou, and C. Koukouvinos. Construction of orthogonal and nearly orthogonal designs for computer experiments. *Biometrika*, 101(3):741–747, 2014.

G. F. V. Glonek and P. J. Solomon. Factorial and time course designs for cDNA microarray experiments. *Biostatistics*, 5(1):89–111, 2004.

H. Hasse. Zur Theorie der abstrakten elliptischen Funktionenkörper. I-III. *J. Reine Angew. Math.*, 175:55–62, 69–88, 193–208, 1936.

Y. He and B. Tang. Strong orthogonal arrays and associated Latin hypercubes for computer experiments. *Biometrika*, 100(1):254–260, 2013.

Y. He and B. Tang. A characterization of strong orthogonal arrays of strength three. *Ann. Statist.*, 42(4):115–128, 2014.

Y. He, C.-S. Cheng, and B. Tang. Strong orthogonal arrays of strength two plus. *Ann. Statist.*, 46(2):457–468, 2018.

A. S. Hedayat, N. J. A. Sloane, and J. Stufken. *Orthogonal Arrays: Theory and Applications*. Springer Series in Statistics. New York: Springer-Verlag, 1999.

F. J. Hickernell. A generalized discrepancy and quadrature error bound. *Math. Comp.*, 67 (221):299–322, 1998.

D. Ingram and B. Tang. Minimum G aberration design construction and design tables for 24 runs. *J. Qual. Technol.*, 37(2):101–114, 2005.

M. E. Johnson, L. M. Moore, and D. Ylvisaker. Minimax and maximin distance designs. *J. Statist. Plann. Inference*, 26(2):131–148, 1990.

H. Kharaghani and B. Tayfeh-Rezaie. Hadamard matrices of order 32. *J. Combin. Des.*, 21 (5):212–221, 2013.

H. Kimura. Classification of Hadamard matrices of order 28. *Discrete Math.*, 133(1-3): 171–180, 1994.

P. Li, A. Miller, and B. Tang. Algorithmic search for baseline minimum aberration designs. *J. Statist. Plann. Inference*, 149:172–182, 2014.

W. Li, M.-Q. Liu, and B. Tang. A method of constructing maximin distance designs. *Biometrika*, 108(4):845–855, 2021.

C. D. Lin, D. Bingham, R. R. Sitter, and B. Tang. A new and flexible method for constructing designs for computer experiments. *Ann. Statist.*, 38(3):1460–1477, 2010.

R. J. MacKay and R. W. Oldford. Scientific method, statistical method and the speed of light. *Statist. Sci.*, 15(3):254–278, 2000.

M. D. McKay, R. J. Beckman, and W. J. Conover. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics*, 21(2):239–245, 1979.

R. Mee. *A Comprehensive Guide to Factorial Two-Level Experimentation*. New York: Springer Science & Business Media, 2009.

R. Mukerjee and B. Tang. Optimal fractions of two-level factorials under a baseline parameterization. *Biometrika*, 99(1):71–84, 2012.

R. Mukerjee, F. Sun, and B. Tang. Nearly orthogonal arrays mappable into fully orthogonal arrays. *Biometrika*, 101(4):957–963, 2014.

H. Niederreiter. Point sets and sequences with small discrepancy. *Monatsh. Math.*, 104(4): 273–337, 1987.

N. D. Nikiforova, R. Berni, G. Arcidiacono, L. Cantone, and P. Placidoli. Latin hypercube designs based on strong orthogonal arrays and Kriging modelling to improve the payload distribution of trains. *J. Appl. Stat.*, 48(3):498–516, 2021.

A. B. Owen. Orthogonal arrays for computer experiments, integration and visualization. *Statist. Sinica*, 2(2):439–452, 1992.

A. B. Owen. Controlling correlations in latin hypercube samples. *J. Amer. Statist. Assoc.*, 89(428):1517–1522, 1994.

R. E. A. C. Paley. On orthogonal matrices. *J. Math. Phys.*, 12(1-4):311–320, 1933.

R. L. Plackett and J. P. Burman. The design of optimum multifactorial experiments. *Biometrika*, 33:305–325, 1946.

C. R. Rao. Factorial experiments derivable from combinatorial arrangements of arrays. *J. Roy. Statist. Soc. Suppl.*, 9:128–139, 1947.

J. Sacks and D. Ylvisaker. Some model robust designs in regression. *Ann. Statist.*, 12(4): 1324–1348, 1984.

J. Sacks, W. J. Welch, T. J. Mitchell, and H. P. Wynn. Design and analysis of computer experiments. *Statist. Sci.*, 4(4):409–435, 1989.

T. J. Santner, B. J. Williams, and W. I. Notz. *The Design and Analysis of Computer Experiments, Second Edition.* Springer Series in Statistics. New York: Springer, 2018.

E. D. Schoen and R. W. Mee. Two-level designs of strength 3 and up to 48 runs. *J. R. Stat. Soc. Ser. C. Appl. Stat.*, 61(1):163–174, 2012.

E. D. Schoen, P. T. Eendebak, and M. V. M. Nguyen. Complete enumeration of pure-level and mixed-level orthogonal arrays. *J. Combin. Des.*, 18(2):123–140, 2010.

E. D. Schoen, N. Vo-Thanh, and P. Goos. Two-level orthogonal screening designs with 24, 28, 32, and 36 runs. *J. Amer. Statist. Assoc.*, 112(519):1354–1369, 2017.

C. Shi and B. Tang. Designs from good Hadamard matrices. *Bernoulli*, 24(1):661–671, 2018.

C. Shi and B. Tang. Design selection for strong orthogonal arrays. *Canad. J. Statist.*, 47 (2):302–314, 2019.

C. Shi and B. Tang. On construction of nonregular two-level factorial designs with maximum generalized resolution. *Statist. Sinica*, 33:593–607, 2023.

I. M. Sobol'. Distribution of points in a cube and approximate evaluation of integrals. *Ž. Vyčisl. Mat i Mat. Fiz.*, 7:784–802, 1967.

H. M. Stark. On the Riemann hypothesis in hyperelliptic function fields. In *Analytic number theory (Proc. Sympos. Pure Math., Vol. XXIV, St. Louis Univ., St. Louis, Mo., 1972)*, pages 285–302, 1973.

D. M. Steinberg and D. K. J. Lin. A construction method for orthogonal Latin hypercube designs. *Biometrika*, 93(2):279–288, 2006.

J. Stufken and B. Tang. Complete enumeration of two-level orthogonal arrays of strength d with $d+2$ constraints. *Ann. Statist.*, 35(2):793–814, 2007.

C.-Y. Sun and B. Tang. Relationship between orthogonal and baseline parameterizations and its applications to design constructions. *Statist. Sinica*, 32(1):239–250, 2022.

C.-Y. Sun and B. Tang. Uniform projection designs and strong orthogonal arrays. *J. Amer. Statist. Assoc.*, 118(541):417–423, 2023.

D. X. Sun, W. Li, and K. Q. Ye. Algorithmic construction of catalogs of non-isomorphic two-level orthogonal designs for economic run sizes. *Statist. Appl.*, 6(1–2):141–155, 2008.

F. Sun and B. Tang. A general rotation method for orthogonal Latin hypercubes. *Biometrika*, 104(2):465–472, 2017.

F. Sun, Y. Wang, and H. Xu. Uniform projection designs. *Ann. Statist.*, 47(1):641–661, 2019.

G. Taguchi. *Introduction to Quality Engineering.* Tokyo: Asian Productivity Organization, 1986.

B. Tang. Orthogonal array-based Latin hypercubes. *J. Amer. Statist. Assoc.*, 88(424): 1392–1397, 1993.

B. Tang. Theory of J-characteristics for fractional factorial designs and projection justification of minimum G_2-aberration. *Biometrika*, 88(2):401–407, 2001.

B. Tang. Orthogonal arrays robust to nonnegligible two-factor interactions. *Biometrika*, 93 (1):137–146, 2006.

B. Tang and L.-Y. Deng. Minimum G_2-aberration for nonregular fractional factorial designs. *Ann. Statist.*, 27(6):1914–1926, 1999.

B. Tang and C. F. J. Wu. Characterization of minimum aberration 2^{n-k} designs in terms of their complementary designs. *Ann. Statist.*, 24(6):2549–2559, 1996.

Y. Tian and H. Xu. A minimum aberration-type criterion for selecting space-filling designs. *Biometrika*, 109(2):489–501, 2022.

A. R. Vazquez and H. Xu. Construction of two-level nonregular designs of strength three with large run sizes. *Technometrics*, 61(3):341–353, 2019.

A. R. Vazquez, P. Goos, and E. D. Schoen. Constructing two-level designs by concatenation of strength-3 orthogonal arrays. *Technometrics*, 61(2):219–232, 2019.

A. R. Vazquez, E. D. Schoen, and P. Goos. Two-level orthogonal screening designs with 80, 96, and 112 runs, and up to 29 factors. *J. Qual. Technol.*, 54(3):338–358, 2022.

E. Vazquez and J. Bect. Sequential search based on kriging: convergence analysis of some algorithms. *Proceedings of the 58th World Statistical Congress of the ISI*, pages 1241–1250, 2011.

E. Verheiden. Integral and rational completions of combinatorial matrices. *J. Combin. Theory Ser. A*, 25(3):267–276, 1978.

C. Wang, J. Yang, and M.-Q. Liu. Construction of strong group-orthogonal arrays. *Statist. Sinica*, 32:1225–1243, 2022a.

J. C. Wang and C.-F. J. Wu. A hidden projection property of Plackett-Burman and related designs. *Statist. Sinica*, 5(1):235–250, 1995.

L. Wang, Q. Xiao, and H. Xu. Optimal maximin L_1-distance Latin hypercube designs based on good lattice point designs. *Ann. Statist.*, 46(6B):3741–3766, 2018.

Y. Wang, F. Wang, Y. Yuan, and Q. Xiao. Connecting U-type designs before and after level permutations and expansions. *J. Stat. Theory Pract.*, 15(4):Paper No. 81, 19, 2021.

Y. Wang, S. Liu, and D. K. J. Lin. On definitive screening designs using Paley's conference matrices. *Statist. Probab. Lett.*, 181:Paper No. 109267, 6, 2022b.

Y. Wang, F. Sun, and H. Xu. On design orthogonality, maximin distance, and projection uniformity for computer experiments. *J. Amer. Statist. Assoc.*, 117(537):375–385, 2022c.

C. F. J. Wu. Post-Fisherian experimentation: from physical to virtual. *J. Amer. Statist. Assoc.*, 110(510):612–620, 2015.

C. F. J. Wu and M. S. Hamada. *Experiments: Planning, Analysis, and Optimization, 3rd ed.* Hoboken, New Jersey: Wiley, 2021.

Q. Xiao and H. Xu. Construction of maximin distance designs via level permutation and expansion. *Statist. Sinica*, 28(3):1395–1414, 2018.

H. Xu. Minimum moment aberration for nonregular designs andsupersaturated designs. *Statist. Sinica*, 13(3):691–708, 2003.

H. Xu. Some nonregular designs from the Nordstrom-Robinson code and their statistical properties. *Biometrika*, 92(2):385–397, 2005.

H. Xu and C. F. J. Wu. Generalized minimum aberration for asymmetrical fractional factorial designs. *Ann. Statist.*, 29(4):1066–1077, 2001.

H. Xu and C. F. J. Wu. Construction of optimal multi-level supersaturated designs. *Ann. Statist.*, 33(6):2811–2836, 2005.

H. Xu, F. K. H. Phoa, and W. K. Wong. Recent developments in nonregular fractional factorial designs. *Stat. Surv.*, 3:18–46, 2009.

Y. H. Yang and T. Speed. Design issues for cDNA microarray experiments. *Nature Genet.*, 3(8):579–588, 2002.

F. Yates. Incomplete randomized blocks. *Ann. Eugen.*, 7:121–140, 1936.

K. Q. Ye. Orthogonal column Latin hypercubes and their application in computer experiments. *J. Amer. Statist. Assoc.*, 93(444):1430–1439, 1998.

Y. Zhou and H. Xu. Space-filling properties of good lattice point sets. *Biometrika*, 102(4): 959–966, 2015.

Y.-D. Zhou and H. Xu. Space-filling fractional factorial designs. *J. Amer. Statist. Assoc.*, 109(507):1134–1144, 2014.

Y.-D. Zhou, K.-T. Fang, and J.-H. Ning. Mixture discrepancy for quasi-random point sets. *J. Complexity*, 29(3-4):283–301, 2013.