Non-orthogonal Blocked Two-level Factorial Designs

by

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B.Sc. (Hons.), University of Delhi, 2020

Project Submitted in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

in the
Department of Statistics and Actuarial Science
Faculty of Science

SIMON FRASER UNIVERSITY
Summer 2023

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Abstract

When orthogonal blocking of orthogonal designs is not possible, we will have to allow either non-orthogonality between treatment factors or non-orthogonality between treatments and blocks. An example of this situation is running an experiment with a 12-run design of 5 factors in three blocks. Two approaches are studied, and their performances in estimation efficiency of treatment main effects are compared. Some best designs of 12 runs in three blocks and of 20 runs in five blocks are found and tabulated.

Keywords: Efficiency; Main effect; Orthogonal array; Orthogonal blocking

Acknowledgments

I am extremely grateful to my supervisor, Dr. Boxin Tang for his invaluable advice, continuous support, and patience during my masters study. His immense knowledge and plentiful experience has encouraged me in all the time of my academic research and daily life. This work would not have been possible without his guidance and assistance.

I would like to thank thesis examiner Owen Ward and chair Tim Swartz for taking the time to consider my work. Also, I am deeply grateful to Dr. Joan Hu and appreciate her willingness for being on my committee. I would like to express my gratitude to all the committee members for their helpful comments and suggestions.

I would also like to thank all the staff and faculty members of the Statistics and Actuarial Science Department at Simon Fraser University for the support during my time as a student in master's program. Many thanks to Ian Bercovitz who gave me an opportunity to be a part of SFU's Statistical Consulting team. It was a great experience to work with him.

At last, I would like to thank my family for their love and support.

Dedication

To my parents Jagjeet Singh and Jaspal Kaur, my brother Sehajdeep Singh and my love Karamjit Singh. None of this would have been possible without their hard work.

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Chapter 1

Introduction

In many scientific investigations, the main interest lies in the study of effects of two or more factors simultaneously. Factorial designs, especially those of two-levels, are most commonly used for such investigations. These designs are used to study the effects on the response over the range of factor levels chosen. A full factorial experimental design allows all factorial effects to be estimated independently. However, it is often costly to perform a full factorial experiment because a 2^k full factorial design requires 2^k runs to be performed, so these designs are seldom used in practise for large k. For economic reasons, fractional factorial designs, which consist of a subset or a fraction of full factorial designs are preferred. Fractional factorial designs are useful at early stages of screening investigations to systematically sift through many factors and screen out a few important ones.

1.1 Non-regular designs

Fractional factorial designs can be classified into two broad categories: regular fractional factorial designs and non-regular fractional factorial designs. Regular fractional factorial designs are constructed through defining relations among factors and have simple aliasing structure in that any two effects are either orthogonal or fully aliased. An orthogonal design is a one in which the two levels in each column occur equally often, and in any two columns all their level combinations appear the same number of times. In regular designs, any two factorial effects can be estimated independently of each other if they are not fully aliased. In contrast, non-regular fractional factorial designs exhibit some complex aliasing structure, meaning that there exist effects that are neither orthogonal nor fully aliased.

Regular factorial designs can be constructed for every run size that is a power of 2 (2^{k-m} runs with k factors). Examples of non-regular factorial designs include Plackett Burman designs (1946), which are constructed from Hadamard matrices. If a Hadamard matrix exists, then its order n has to be a multiple of 4, that is $n = 4t$ for some integer t.

Run	A	B	C	D	E	F	G	H	J
1	1	-1	-1	-1	-1	-1	-1	-1	-1
2	-1	1	1	-1	1	1	-1	-1	-1
3	-1	1	1	1	-1	-1	1	-1	-1
4	1	-1	-1	1	1	1	1	-1	-1
5	-1	1	-1	-1	-1	1	1	1	-1
6	1	-1	1	-1	1	-1	1	1	-1
7	1	-1	1	1	-1	1	-1	1	-1
8	-1	1	-1	1	1	-1	-1	1	-1
9	-1	-1	1	-1	-1	1	1	-1	1
10	1	1	-1	-1	1	-1	1	-1	1
11	1	1	-1	1	-1	1	-1	-1	1
12	-1	-1	1	1	1	-1	-1	-1	1
13	1	1	1	-1	-1	-1	-1	1	1
14	-1	-1	-1	-1	1	1	-1	1	1
15	-1	-1	-1	1	-1	-1	1	1	1
16	1	1	1	1	1	1	1	1	1

Table 1.1: Regular fractional factorial 2^{9-5} design

Table 1.1 shows a regular fractional factorial 2^{9-5} design matrix of 16 runs with 9 factors, each row representing a run and each column corresponding to a factor. The first four columns A, B, C and D are given by a full factorial design for four factors. The columns of remaining factors E, F, G, H and J are then generated using the first four columns.

$$E = ABC, \quad F = ABD, \quad G = ACD, \quad H = BCD, \quad J = AB.$$

The relation $J = AB$ implies that the main effect of factor J is fully aliased with the two-factor interaction between factors A and B. The aliasing pattern divides a set of factorial effects into groups and the effects from the same group are fully aliased with each other, and those from different groups are mutually orthogonal. When two effects are fully aliased in a regular design, it is impossible to distinguish between them based on the data in the analysis. When a two-factor interaction is fully aliased with a main effect, we often assume that the two-factor interaction is negligible. But two-factor interactions are often significant in practice. This problem can be avoided if a non-regular design is used.

Run	A	B	C	D	E	F	G	H	J
1	-1	-1	-1	-1	-1	-1	-1	-1	-1
2	1	-1	1	-1	-1	-1	1	1	1
3	1	1	-1	1	-1	-1	-1	1	1
4	-1	1	1	-1	1	-1	-1	-1	1
5	1	-1	1	1	-1	1	-1	-1	-1
6	1	1	-1	1	1	-1	1	-1	-1
7	1	1	1	-1	1	1	-1	1	-1
8	-1	1	1	1	-1	1	1	-1	1
9	-1	-1	1	1	1	-1	1	1	-1
10	-1	-1	-1	1	1	1	-1	1	1
11	1	-1	-1	-1	1	1	1	-1	1
12	-1	1	-1	-1	-1	1	1	1	-1

Table 1.2: Non-regular 12-run design

Table 1.2 shows a non-regular design of 12 runs with nine factors. The nine main effects columns $A, B, C, \ldots, H, J$ are mutually orthogonal. The interaction AB is neither orthogonal nor fully aliased with the main effect C.

Columns A, B and C have correlation coefficient $-1/3$ and thus are partially aliased with each other. The interaction column AB has correlation of $\pm 1/3$ with all other main effects $C,\ D, \ldots\ J$. Although the complex aliasing structure causes difficulty in identifying the significant effects when conducting analysis, it also gives an opportunity of estimating the interaction effect AB and the main effect C simultaneously because they are not fully aliased with each other.

1.2 Blocking

Blocking is a commonly used technique to control systematic noises in experiments. These noises might come from day-to day variation, operator-to-operator variation, or batch-to-batch variation. Blocking can effectively eliminate systematic sources of variations and hence increases the statistical efficiency of fractional factorial designs. The essence of blocking is best summarized by a widely quoted statement in Box GE, Hunter WH, Hunter S (1978), "block what you can, randomize what you cannot".

For blocked factorial designs, it is essential to keep the block factors orthogonal to the treatment factors so that the treatment main effects are estimated without the contamination of the block effects, which are often significant. This is achieved by making sure that the two levels of each factor occur equally often within each block. For regular fractional factorial designs, blocks are constructed by using interaction columns as block factors, and then associating the distinct level combinations in these columns with different blocks. This method is referred as the method of replacement in Wu and Hamada (2000).

1.2.1 Blocking Non-regular Factorial Designs

Cheng et al. (2004) extended the method of replacement to non-regular designs. Schoen, Sartono and Goos (2013) introduced two concepts, i.e. treatment design and full design, in their approach of determining the optimal blocking arrangements. The treatment design is an orthogonal array of strength 2, denoted by $\mathrm{OA}(n, 2^k, 2)$. The full design is an orthogonal array with one extra column for the blocking factor. Let the number of blocks be denoted by q. Then, that extra column has q levels. This kind of array is denoted by $\mathrm{OA}(n, 2^k\, q^1, 2)$. All possible ways of blocking k-factor treatment designs can be obtained by enumerating all non-isomorphic full designs of the type $\mathrm{OA}(n, 2^k\, q^1, 2)$. A key feature of the approach, known as the single replacement in the literature, is that it ensures orthogonality of the blocking factor with respect to the main effects of the k treatment factors.

Run	A	B	C	D	Block
1	-1	1	-1	1	1
2	-1	-1	-1	-1	1
3	1	1	-1	-1	3
4	-1	-1	1	-1	2
5	1	-1	1	1	3
6	-1	1	1	-1	3
7	-1	1	1	1	2
8	1	1	1	1	1
9	1	1	-1	-1	2
10	-1	-1	-1	1	3
11	1	-1	-1	1	2
12	1	-1	1	-1	1

Table 1.3: Non-regular 12-run design arranged in three blocks via $\mathrm{OA}(12, 2^4\, 3^1, 2)$

As said earlier, to estimate the treatment main effects without the contamination of block effects, the block factors should be orthogonal to the treatment factors. For example, Table 1.3 shows a non-regular design of 12 runs with 4 treatment factors and strength two arranged in three blocks of size four using an $\mathrm{OA}(12, 2^4\, 3^1, 2)$. Since each factor occurs equally often within each block at each of its levels, each main effect parameter is estimated orthogonally to the block effects. Another example is a non-regular design of 20 runs with eight factors arranged in five blocks of size four from the use of an $\mathrm{OA}(20, 2^8\, 5^1, 2)$.

Run	A	B	C	D	E	F	G	H	Block
1	-1	1	-1	-1	1	1	1	1	2
2	1	1	1	1	1	1	1	1	1
3	1	1	1	1	-1	1	-1	-1	2
4	-1	1	1	-1	1	-1	-1	1	5
5	1	-1	-1	1	-1	1	1	-1	5
6	1	-1	-1	-1	-1	-1	-1	1	2
7	-1	-1	1	1	1	-1	1	-1	2
8	1	-1	-1	1	1	-1	-1	1	3
9	1	1	1	-1	-1	1	1	1	3
10	-1	1	-1	1	-1	-1	-1	1	1
11	-1	-1	1	-1	-1	-1	1	-1	1
12	1	-1	-1	-1	1	1	-1	-1	1
13	-1	-1	1	-1	1	1	-1	-1	3
14	-1	1	-1	1	1	1	-1	-1	4
15	1	1	1	-1	-1	-1	-1	-1	4
16	-1	-1	-1	-1	-1	1	1	1	4
17	-1	1	-1	1	-1	-1	1	-1	3
18	1	-1	1	1	1	-1	1	1	4
19	1	1	-1	-1	1	-1	1	-1	5
20	-1	-1	1	1	-1	1	-1	1	5

Table 1.4: Non-regular 20-run design arranged in 5 blocks via $\mathrm{OA}(20, 2^8\, 5^1, 2)$

But the orthogonality between treatment and block effects is only achieved for non-regular designs with up to a certain number of factors. In non-regular designs of 12 runs arranged in three blocks of size four, the orthogonality between treatment and block factors is present when treatment factors (k) is less than or equal to 4, i.e. an $\mathrm{OA}(12, 2^k\, 3^1, 2)$ for $k \leq 4$. This is because an $\mathrm{OA}(12, 2^k\, 3^1, 2)$ does not exist for $k \geq 5$. Similarly, in non-regular designs of 20 runs arranged into five blocks of size four, treatment and blocks effects are orthogonal when k is less than or equal to 8, i.e. an $\mathrm{OA}(20, 2^k\, 5^1, 2)$ is only available for $k \leq 8$. For the existence and non-existence of mixed-level orthogonal arrays, we refer to

Schoen, Eendebak and Nguyen (2010).

1.2.2 Non-orthogonal Blocking of Non-Regular Factorial Designs

Orthogonal blocking is not achievable for non-regular designs when the number k of factors exceeds a certain number, which is 4 for 12-run factorial designs and 8 for 20-run designs arranged in 3 and 5 blocks, respectively. For example, Tables 1.5 and 1.6 show two 12-run non-regular factorial designs with 6 factors arranged in 3 blocks.

Run	A	B	C	D	E	F	Block
1	-1	1	1	1	-1	1	1
2	1	1	-1	1	1	-1	2
3	-1	1	-1	-1	-1	1	3
4	-1	-1	1	1	1	-1	3
5	1	-1	1	-1	-1	-1	1
6	-1	1	1	-1	1	-1	1
7	1	1	-1	1	-1	-1	1
8	-1	-1	-1	1	1	1	2
9	1	1	1	-1	1	1	2
10	1	-1	-1	-1	1	1	2
11	-1	-1	-1	-1	-1	-1	3
12	1	-1	1	1	-1	1	3

Table 1.5: Non-regular 12-run design arranged in 3 blocks using one NOA$(12, 2^6\, 3^1, 2)$

Run	A	B	C	D	E	F	Block
1	1	1	1	1	-1	1	1
2	1	1	-1	-1	-1	-1	1
3	-1	-1	1	1	1	1	1
4	-1	-1	-1	-1	-1	-1	1
5	1	-1	1	-1	1	1	2
6	1	-1	-1	1	1	-1	2
7	-1	1	1	1	-1	1	2
8	-1	1	-1	-1	-1	-1	2
9	1	-1	1	-1	-1	-1	3
10	-1	1	1	-1	1	1	3
11	-1	-1	-1	1	-1	1	3
12	1	1	-1	1	1	-1	3

Table 1.6: Non-regular 12-run design arranged in 3 blocks using another NOA$(12, 2^6\, 3^1, 2)$

A few things need to be mentioned in these designs. In Table 1.5, the treatment factors are orthogonal to each other in that for any two treatment factors all the level combinations $(-1, 1)$, $(1, -1)$, $(1, 1)$, $(-1, -1)$ occur the same number of times, but the treatment factors are not orthogonal to the block effects because the two levels of each factor do not occur equally often within each block. In Table 1.6, the treatment factors are orthogonal to the block effects but treatment factors are not orthogonal to each other. Thus, either orthogonality between treatment and block effects or orthogonality between treatment factors has to be sacrificed to block a 12-run non-regular design with five or more factors in three blocks.

The blocked designs in Tables 1.5 and 1.6 suggest two approaches to the construction of nearly orthogonal blocked factorial designs.

- Minimum non-orthogonality between treatment factors while maintaining orthogonality between treatment and block effects, and
- Minimum non-orthogonality between treatment factors and block effects while maintaining orthogonality between treatment factors.

Throughout the discussion of this project, two assumptions regarding treatment and block effects are made:

- There is no interaction between treatment factors and blocks.
- Interactions among treatment factors are all negligible.

Chapter 2

Approach I: Non-orthogonality between Treatment Factors

When orthogonality is not achieved in blocked non-regular factorial designs, the effort is made to construct a non-orthogonal blocked factorial design with minimum non-orthogonality. One of the two approaches to constructing nearly orthogonal blocked factorial designs is discussed in this chapter and the degree of non-orthogonality is measured with the J-characteristics of factorial designs to find the best non-orthogonal blocked factorial designs.

2.1 J-Characteristics

Before discussing our approach, it is important to understand the measure of non-orthogonality to compare the factorial designs. Deng and Tang (1999) introduced the criteria for assessing non-regular fractional factorial designs. These criteria are defined using a set of J values called J-characteristics. Tang (2001) showed that a factorial design is uniquely determined by its J-characteristics, just as a regular design is uniquely determined by its defining relation. The set of J-characteristics naturally generalizes the concept of defining relation associated with regular designs.

Let $x_1, x_2, \ldots, x_k$ be k vectors of length n and $x_j = (x_{1j}, x_{2j}, \ldots, x_{nj})^T$ for $j = 1, 2, \ldots, k$.

Then, the J-characteristic for these k vectors is defined as

$$J(x_1, x_2, \ldots, x_k) = \sum_{i=1}^{n} x_{i1}\, x_{i2} \cdots x_{ik}.$$

For $k = 2$, $J(x_1, x_2) = x_1^T x_2$, which is the inner product of two vectors x_1 and x_2. J-characteristics generalize the inner product and are defined for any number of vectors and we present them in form of cross-product matrix to measure the degree of non-orthogonality between treatment factors, where each treatment factor (column) is a vector.

2.2 Construction of Best Non-orthogonal Blocked Designs

Orthogonal blocking of non-regular factorial designs is possible for designs with small numbers k of treatment factors. We make use of such designs to construct the best non-orthogonal blocked factorial designs when orthogonal blocking is not possible. Let m' be the highest number of treatment factors with which orthogonal blocking in q blocks is possible for non-regular factorial designs with n runs and strength 2, that is an $\mathrm{OA}(n, 2^k\, q^1, 2)$ is available for $k \leq m'$ but an $\mathrm{OA}(n, 2^k\, q^1, 2)$ does not exist for any $k \geq m' + 1$.

1. Start with an orthogonal blocked non-regular factorial design of n runs with $k = m'$ factors arranged into q blocks, i.e. an $\mathrm{OA}(n, 2^k\, q^1, 2)$ where $k = m'$.
2. Add another treatment factor (column) to the $\mathrm{OA}(n, 2^k q^1, 2)$ where $k = m'$ such that
   (a) $(k + 1)^{th}$ treatment factor is orthogonal to the block effects,
   (b) there exists the least number of non-orthogonal pairs of treatment factors i.e. J characteristic of x_i and x_j for $i < j$ is zero for the maximum number of pairs of treatment factors,
   (c) and J characteristics are minimized for non-orthogonal pairs of treatment factors.
3. Continue adding another treatment factor to the best design just obtained.

The blocked designs obtained in the above give a class of nearly orthogonal arrays. For convenience, they are called nearly orthogonal arrays of type I, and are denoted by $\mathrm{NOA}_I(n, 2^k\, q^1, 2)$ for $k \geq m' + 1$.

2.3 Examples

2.3.1 To construct best $\mathbf{NOA}_I(12, 2^5\, 3^1, 2)$

Orthogonal blocking of a 12-run non-regular factorial design in three blocks is possible for treatment factors $k \leq 4$, i.e. $m' = 4$. To construct the best $\mathrm{NOA}_I(12, 2^5\, 3^1, 2)$, we start with an $\mathrm{OA}(12, 2^4\, 3^1, 2)$ and add another treatment factor E such that factor E satisfies all the conditions in point 2 of the method in Section 2.2.

Let $X_E = (-1, 1, 1, -1, -1, 1, -1, 1, -1, 1, -1, 1)$. Thus, the full design is

Run	A	B	C	D	**E**	Block
1	1	1	-1	-1	**-1**	1
2	1	1	1	1	**1**	1
3	-1	-1	-1	-1	**1**	1
4	-1	-1	1	1	**-1**	1
5	1	-1	-1	-1	**-1**	2
6	1	-1	1	1	**1**	2
7	-1	1	1	-1	**-1**	2
8	-1	1	-1	1	**1**	2
9	1	-1	-1	1	**-1**	3
10	1	1	1	-1	**1**	3
11	-1	1	-1	1	**-1**	3
12	-1	-1	1	-1	**1**	3

Table 2.1: Best $\mathrm{NOA}_I(12, 2^5\, 3^1, 2)$.

The cross-product matrix of the treatment design is

	A	B	C	D	**E**
A	12	0	0	0	**0**
B	0	12	0	0	**0**
C	0	0	12	0	**4**
D	0	0	0	12	**0**
E	**0**	**0**	**4**	**0**	12

Table 2.2: Cross-product matrix of the treatment design in Table 2.1

The cross-product matrix in Table 2.2 shows the J-characteristics of all possible subsets of two treatment factors.

The treatment factor E is orthogonal to the block effects since we can see that the two levels of each factor occur equally often within each block.

The cross-product matrix shows that the factor E is orthogonal to all other treatment factors except factor C. Thus, non-orthogonality exists in one pair of treatment factors and has minimum J-characteristic among all possible 12-run factorial designs with five factors arranged in three blocks. Since all the conditions are satisfied, this design is one of the best $\mathrm{NOA}_I(12, 2^5\, 3^1, 2)$.

2.3.2 To construct best $\mathbf{NOA}_I(20, 2^9\, 5^1, 2)$

For 20-run non-regular designs, orthogonal blocking in five blocks is achievable when the number of treatment factors $k \leq 8$, thus $m' = 8$. Table 2.3 shows one of the best $\mathrm{NOA}_I(20, 2^9\, 5^1, 2)$ which is obtained by adding a factor J (that satisfies all the three conditions) to an $\mathrm{OA}(20, 2^8\, 5^1, 2)$.

Run	A	B	C	D	E	F	G	H	**J**	Block
1	1	-1	-1	-1	1	1	-1	-1	**-1**	1
2	-1	1	-1	1	-1	-1	-1	1	**1**	1
3	-1	-1	1	-1	-1	-1	1	-1	**1**	1
4	1	1	1	1	1	1	1	1	**-1**	1
5	1	1	1	1	-1	1	-1	-1	**-1**	2
6	-1	-1	1	1	1	-1	1	-1	**1**	2
7	-1	1	-1	-1	1	1	1	1	**1**	2
8	1	-1	-1	-1	-1	-1	-1	1	**-1**	2
9	-1	-1	1	-1	1	1	-1	-1	**-1**	3
10	1	-1	-1	1	1	-1	-1	1	**1**	3
11	-1	1	-1	1	-1	-1	1	-1	**-1**	3
12	1	1	1	-1	-1	1	1	1	**1**	3
13	1	-1	1	1	1	-1	1	1	**-1**	4
14	1	1	1	-1	-1	-1	-1	-1	**-1**	4
15	-1	1	-1	1	1	1	-1	-1	**1**	4
16	-1	-1	-1	-1	-1	1	1	1	**1**	4
17	1	1	-1	-1	1	-1	1	-1	**-1**	5
18	-1	-1	1	1	-1	1	-1	1	**1**	5
19	1	-1	-1	1	-1	1	1	-1	**-1**	5
20	-1	1	1	-1	1	-1	-1	1	**1**	5

Table 2.3: Best $\mathrm{NOA}_I(20, 2^9\, 5^1, 2)$

The cross-product matrix of the treatment design in Table 2.3 is

	A	B	C	D	E	F	G	H	**J**
A	20	0	0	0	0	0	0	0	**-12**
B	0	20	0	0	0	0	0	0	**0**
C	0	0	20	0	0	0	0	0	**0**
D	0	0	0	20	0	0	0	0	**0**
E	0	0	0	0	20	0	0	0	**0**
F	0	0	0	0	0	20	0	0	**0**
G	0	0	0	0	0	0	20	0	**0**
H	0	0	0	0	0	0	0	20	**8**
J	**-12**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	20

Table 2.4: Cross-product matrix of the treatment design in Table 2.3.

It can be noticed that non-orthogonal blocked factorial designs with orthogonality between treatment and block factors for 12-runs is possible for one non-orthogonal pair of treatments, whereas for 20-run designs, the orthogonality between treatments and blocks is only possible in presence of at least two non-orthogonal pairs of treatment factors. Thus, it seems reasonable that non-orthogonality continues to increase with an increase in the number of runs and number of factors. This is indeed the case for the best non-orthogonal blocked factorial designs of 12 and 20 runs with higher numbers of factors. Such designs can be obtained by continuing adding more columns ($m' + 2, m' + 3, \ldots$) to the best obtained designs with $m' + 1$ factors.

The next section presents the best non-orthogonal blocked 12-run and 20-run factorial designs (with orthogonality between treatment factors and block effects) with higher numbers of factors.

2.4 Best non-orthogonal blocked factorial designs with higher number of factors using Approach I

Below are the best $\text{NOA}_I(12, 2^k\, 3^1, 2)s$ and $\text{NOA}_I(20, 2^k\, 5^1, 2)s$ for $k \geq m' + 2$, we have obtained using the method presented in Section 2.2.

Run	A	B	C	D	E	F	Block
1	-1	-1	-1	-1	-1	1	1
2	1	1	1	1	-1	-1	1
3	1	1	-1	-1	1	1	1
4	-1	-1	1	1	1	-1	1
5	-1	1	1	1	-1	1	2
6	1	-1	1	-1	1	1	2
7	-1	1	-1	-1	-1	-1	2
8	1	-1	-1	1	1	-1	2
9	-1	1	-1	1	1	1	3
10	1	1	1	-1	-1	-1	3
11	-1	-1	1	-1	1	-1	3
12	1	-1	-1	1	-1	1	3

	A	B	C	D	E	F
A	12	0	0	0	0	0
B	0	12	0	0	-4	0
C	0	0	12	0	0	-4
D	0	0	0	12	0	0
E	0	-4	0	0	12	0
F	0	0	-4	0	0	12

Table 2.5: Best $\mathrm{NOA}_I(12, 2^6\,3^1, 2)$ and cross-product matrix

Run	A	B	C	D	E	F	G	Block
1	1	1	1	1	1	1	1	1
2	1	1	-1	-1	1	-1	1	1
3	-1	-1	-1	-1	-1	1	-1	1
4	-1	-1	1	1	-1	-1	-1	1
5	1	-1	1	-1	-1	-1	1	2
6	-1	1	-1	-1	1	1	-1	2
7	-1	1	1	1	1	-1	-1	2
8	1	-1	-1	1	-1	1	1	2
9	1	1	1	-1	-1	1	-1	3
10	-1	-1	1	-1	1	1	1	3
11	-1	1	-1	1	-1	-1	1	3
12	1	-1	-1	1	1	-1	-1	3

	A	B	C	D	E	F	G
A	12	0	0	0	0	0	4
B	0	12	0	0	4	0	0
C	0	0	12	0	0	0	0
D	0	0	0	12	0	-4	0
E	0	4	0	0	12	0	0
F	0	0	0	4	0	12	0
G	4	0	0	0	0	0	12

Table 2.6: Best $\mathrm{NOA}_I(12, 2^7\,3^1, 2)$ and cross-product matrix

Run	A	B	C	D	E	F	G	H	Block
1	-1	-1	-1	-1	1	1	1	1	1
2	1	1	1	1	-1	1	-1	1	1
3	1	1	-1	-1	1	-1	1	-1	1
4	-1	-1	1	1	-1	-1	-1	-1	1
5	-1	1	1	1	1	-1	1	1	2
6	-1	1	-1	-1	-1	-1	-1	1	2
7	1	-1	1	-1	-1	1	1	-1	2
8	1	-1	-1	1	1	1	-1	-1	2
9	-1	-1	1	-1	1	1	-1	1	3
10	1	1	1	-1	1	-1	-1	-1	3
11	1	-1	-1	1	-1	-1	1	1	3
12	-1	1	-1	1	-1	1	1	-1	3

	A	B	C	D	E	F	G	H
A	12	0	0	0	0	0	0	-4
B	0	12	0	0	0	-4	0	0
C	0	0	12	0	0	0	-4	0
D	0	0	0	12	-4	0	0	0
E	0	0	0	-4	12	0	0	0
F	0	-4	0	0	0	12	0	0
G	0	0	-4	0	0	0	12	0
H	-4	0	0	0	0	0	0	12

Table 2.7: Best $\mathrm{NOA}_I(12, 2^8\,3^1, 2)$ and cross-product matrix

Run	A	B	C	D	E	F	G	H	J	Block
1	-1	-1	-1	-1	-1	1	1	1	1	1
2	1	1	-1	-1	-1	-1	1	-1	-1	1
3	1	1	1	1	1	1	-1	1	1	1
4	-1	-1	1	1	1	-1	-1	-1	-1	1
5	1	-1	-1	-1	1	-1	-1	1	1	2
6	-1	1	-1	1	1	1	1	-1	1	2
7	1	-1	1	1	-1	-1	1	1	-1	2
8	-1	1	1	-1	-1	1	-1	-1	-1	2
9	1	-1	-1	1	-1	1	-1	-1	1	3
10	-1	-1	1	-1	1	1	1	1	-1	3
11	1	1	1	-1	1	-1	1	-1	1	3
12	-1	1	-1	1	-1	-1	-1	1	-1	3

	A	B	C	D	E	F	G	H	J
A	12	0	0	0	0	-4	0	0	4
B	0	12	0	0	0	-4	0	-4	0
C	0	0	12	0	4	0	0	0	-4
D	0	0	0	12	0	0	-4	0	0
E	0	0	4	0	12	0	0	0	4
F	-4	0	0	0	0	12	0	0	4
G	0	0	0	-4	0	0	12	0	0
H	0	-4	0	0	0	0	0	12	0
J	4	0	-4	0	4	4	0	0	12

Table 2.8: Best $\mathrm{NOA}_I(12, 2^9\,3^1, 2)$ and cross-product matrix

Run	A	B	C	D	E	F	G	H	J	K	Block
1	1	-1	-1	-1	1	1	-1	-1	1	-1	1
2	-1	1	-1	1	-1	-1	-1	1	-1	1	1
3	1	-1	1	-1	-1	-1	1	-1	-1	-1	1
4	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	-1	1	-1	-1	-1	-1	2
6	-1	-1	1	1	1	-1	1	-1	1	-1	2
7	-1	1	-1	-1	1	1	1	1	-1	1	2
8	1	-1	-1	-1	-1	-1	-1	1	1	1	2
9	-1	-1	1	-1	1	1	-1	-1	1	1	3
10	1	-1	-1	1	1	-1	-1	1	-1	-1	3
11	-1	1	-1	1	-1	-1	1	-1	1	1	3
12	1	1	1	-1	-1	1	1	1	1	-1	3
13	1	-1	1	1	1	-1	1	1	-1	1	4
14	1	1	1	-1	-1	-1	-1	-1	-1	-1	4
15	-1	1	-1	1	1	1	-1	-1	1	-1	4
16	-1	-1	-1	-1	-1	1	1	1	1	1	4
17	1	1	-1	-1	1	-1	1	-1	-1	-1	5
18	-1	-1	1	1	-1	1	-1	1	1	1	5
19	1	-1	-1	1	-1	1	1	-1	1	-1	5
20	-1	1	1	-1	1	-1	-1	1	-1	1	5

	A	B	C	D	E	F	G	H	J	K
A	20	0	0	0	0	0	0	0	0	-8
B	0	20	0	0	0	0	0	0	-8	0
C	0	0	20	0	0	0	0	0	0	0
D	0	0	0	20	0	0	0	0	0	0
E	0	0	0	0	20	0	0	0	0	0
F	0	0	0	0	0	20	0	0	12	0
G	0	0	0	0	0	0	20	0	0	0
H	0	0	0	0	0	0	0	20	0	12
J	0	-8	0	0	0	12	0	0	20	0
K	-8	0	0	0	0	0	0	12	0	20

Table 2.9: Best NOA$_I(20, 2^{10}\, 5^1, 2)$ and cross-product matrix

Run	A	B	C	D	E	F	G	H	J	K	L	Block
1	1	-1	-1	-1	1	1	-1	-1	1	1	-1	1
2	-1	1	-1	1	-1	-1	-1	1	-1	-1	1	1
3	-1	-1	1	-1	-1	-1	1	-1	-1	-1	-1	1
4	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	-1	1	-1	-1	-1	-1	1	2
6	-1	-1	1	1	1	-1	1	-1	1	1	1	2
7	-1	1	-1	-1	1	1	1	1	-1	1	-1	2
8	1	-1	-1	-1	-1	-1	-1	1	1	-1	-1	2
9	-1	-1	1	-1	1	1	-1	-1	1	1	-1	3
10	1	-1	-1	1	1	-1	-1	1	-1	1	1	3
11	-1	1	-1	1	-1	-1	1	-1	-1	-1	1	3
12	1	1	1	-1	-1	1	1	1	1	-1	-1	3
13	1	-1	1	1	1	-1	1	1	-1	-1	-1	4
14	1	1	1	-1	-1	-1	-1	-1	-1	1	1	4
15	-1	1	-1	1	1	1	-1	-1	1	-1	-1	4
16	-1	-1	-1	-1	-1	1	1	1	1	1	1	4
17	1	1	-1	-1	1	-1	1	-1	-1	1	-1	5
18	-1	-1	1	1	-1	1	-1	1	1	-1	1	5
19	1	-1	-1	1	-1	1	1	-1	1	-1	1	5
20	-1	1	1	-1	1	-1	-1	1	-1	1	-1	5

	A	B	C	D	E	F	G	H	J	K	L
A	20	0	0	0	0	0	0	0	0	0	0
B	0	20	0	0	0	0	0	0	-8	0	0
C	0	0	20	0	0	0	0	0	0	0	0
D	0	0	0	20	0	0	0	0	0	-8	12
E	0	0	0	0	20	0	0	0	0	12	-8
F	0	0	0	0	0	20	0	0	12	0	0
G	0	0	0	0	0	0	20	0	0	0	0
H	0	0	0	0	0	0	0	20	0	0	0
J	0	-8	0	0	0	12	0	0	20	0	0
K	0	0	0	-8	12	0	0	0	0	20	0
L	0	0	0	12	-8	0	0	0	0	0	20

Table 2.10: Best NOA$_I(20, 2^{11}\, 5^1, 2)$ and cross-product matrix

Run	A	B	C	D	E	F	G	H	J	K	L	M	Block
1	1	-1	-1	-1	1	1	-1	-1	1	1	-1	1	1
2	-1	1	-1	1	-1	-1	-1	1	-1	-1	1	-1	1
3	-1	-1	1	-1	-1	-1	1	-1	-1	-1	-1	-1	1
4	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	-1	1	-1	-1	-1	-1	1	1	2
6	-1	-1	1	1	1	-1	1	-1	1	1	1	-1	2
7	-1	1	-1	-1	1	1	1	1	-1	1	-1	-1	2
8	1	-1	-1	-1	-1	-1	-1	1	1	-1	-1	1	2
9	-1	-1	1	-1	1	1	-1	-1	1	1	-1	1	3
10	1	-1	-1	1	1	-1	-1	1	-1	1	1	-1	3
11	-1	1	-1	1	-1	-1	1	-1	-1	-1	1	1	3
12	1	1	1	-1	-1	1	1	1	1	-1	-1	-1	3
13	1	-1	1	1	1	-1	1	1	-1	-1	-1	1	4
14	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1	4
15	-1	1	-1	1	1	1	-1	-1	1	-1	-1	-1	4
16	-1	-1	-1	-1	-1	1	1	1	1	1	1	-1	4
17	1	1	-1	-1	1	-1	1	-1	-1	1	-1	1	5
18	-1	-1	1	1	-1	1	-1	1	1	-1	1	-1	5
19	1	-1	-1	1	-1	1	1	-1	1	-1	1	1	5
20	-1	1	1	-1	1	-1	-1	1	-1	1	-1	-1	5

	A	B	C	D	E	F	G	H	J	K	L	M
A	20	0	0	0	0	0	0	0	0	0	0	12
B	0	20	0	0	0	0	0	0	-8	0	0	0
C	0	0	20	0	0	0	0	0	0	0	0	0
D	0	0	0	20	0	0	0	0	0	-8	12	0
E	0	0	0	0	20	0	0	0	0	12	-8	0
F	0	0	0	0	0	20	0	0	12	0	0	0
G	0	0	0	0	0	0	20	0	0	0	0	0
H	0	0	0	0	0	0	0	20	0	0	0	-8
J	0	-8	0	0	0	12	0	0	20	0	0	0
K	0	0	0	-8	12	0	0	0	0	20	0	0
L	0	0	0	12	-8	0	0	0	0	0	20	0
M	12	0	0	0	0	0	0	-8	0	0	0	20

Table 2.11: Best NOA$_I(20, 2^{12}\, 5^1, 2)$ and cross-product matrix

Run	A	B	C	D	E	F	G	H	J	K	L	M	N	Block
1	1	-1	-1	-1	1	1	-1	-1	-1	1	-1	-1	1	1
2	-1	1	-1	1	-1	-1	-1	1	1	-1	1	-1	-1	1
3	-1	-1	1	-1	-1	-1	1	-1	-1	1	1	1	-1	1
4	1	1	1	1	1	1	1	1	1	-1	-1	1	1	1
5	1	1	1	1	-1	1	-1	-1	-1	-1	-1	1	-1	2
6	-1	-1	1	1	1	-1	1	-1	1	-1	1	-1	1	2
7	-1	1	-1	-1	1	1	1	1	-1	1	1	-1	-1	2
8	1	-1	-1	-1	-1	-1	-1	1	1	1	-1	1	1	2
9	-1	-1	1	-1	1	1	-1	-1	-1	1	-1	1	1	3
10	1	-1	-1	1	1	-1	-1	1	-1	-1	1	1	-1	3
11	-1	1	-1	1	-1	-1	1	-1	1	-1	-1	-1	-1	3
12	1	1	1	-1	-1	1	1	1	1	1	1	-1	1	3
13	1	-1	1	1	1	-1	1	1	-1	1	-1	-1	-1	4
14	1	1	1	-1	-1	-1	-1	-1	1	-1	-1	1	-1	4
15	-1	1	-1	1	1	1	-1	-1	1	1	1	1	1	4
16	-1	-1	-1	-1	-1	1	1	1	-1	-1	1	-1	1	4
17	1	1	-1	-1	1	-1	1	-1	1	1	-1	-1	-1	5
18	-1	-1	1	1	-1	1	-1	1	-1	-1	1	1	1	5
19	1	-1	-1	1	-1	1	1	-1	-1	-1	-1	-1	1	5
20	-1	1	1	-1	1	-1	-1	1	1	1	1	1	-1	5

	A	B	C	D	E	F	G	H	J	K	L	M	N
A	20	0	0	0	0	0	0	0	0	0	-12	0	0
B	0	20	0	0	0	0	0	0	12	0	0	0	-8
C	0	0	20	0	0	0	0	0	0	0	0	8	0
D	0	0	0	20	0	0	0	0	0	-12	0	0	0
E	0	0	0	0	20	0	0	0	0	8	0	0	0
F	0	0	0	0	0	20	0	0	-8	0	0	0	12
G	0	0	0	0	0	0	20	0	0	0	0	-12	0
H	0	0	0	0	0	0	0	20	0	0	8	0	0
J	0	12	0	0	0	-8	0	0	20	0	0	0	0
K	0	0	0	-12	8	0	0	0	0	20	0	0	0
L	-12	0	0	0	0	0	0	8	0	0	20	0	0
M	0	0	8	0	0	0	-12	0	0	0	0	20	0
N	0	-8	0	0	0	12	0	0	0	0	0	0	20

Table 2.12: Best NOA$_I(20, 2^{13}\, 5^1, 2)$ and cross-product matrix

Chapter 3

Approach II: Non-orthogonality between Treatment Factors and Blocks

Chapter 2 discussed one approach to constructing the best non-orthogonal blocked factorial designs by allowing non-orthogonality between treatment factors but having orthogonality between treatment factors and block effects. This chapter introduces another approach to obtaining the best non-orthogonal blocked factorial designs which allows for non-orthogonality between treatment factors and block effects while maintaining orthogonality between treatment factors. All possible 12-run and 20-run blocked factorial designs are compared and the best designs are obtained and tabulated.

3.1 Construction of the Best Non-orthogonal Blocked Factorial Design

Our second approach allows for non-orthogonality between treatment factors and block effects while maintaining the orthogonality between treatment factors. The best designs are the ones that have minimum non-orthogonality between treatment factors and block effects among all possible designs of n runs with k factors arranged in q blocks.

To obtain the best non-orthogonal blocked factorial design of n runs with k factors (where $k > m'$) arranged in q blocks,

1. Start with a non-regular fractional factorial design of n runs with k factors from using an OA$(n, 2^k, 2)$ where $k > m'$.

2. Add a q-level column such that

   (a) each entry in the added column occurs the same number of times and

   (b) the added column is orthogonal to the maximum possible number of treatment factors.

3. Measure the extent of non-orthogonality (discussed in Section 3.2) and the designs that have minimum non-orthogonality between treatment factors and block effects among all possible designs are the best non-orthogonal blocked designs.

For convenience, the blocked designs obtained this way are called nearly orthogonal arrays of type II, and are denoted by NOA$_{II}(n, 2^k\, q^1, 2)$.

3.2 Measure of Non-orthogonality between Treatment and Block Effects

Two vectors are orthogonal if each entry occurs equally often in each vector and all the level combinations occur the same number of times. If the q-level added column (blocking factor) and treatment factors have each entry occurring an equal number of times, then non-orthogonality can be measured by the variability in the frequencies of all level combinations in each treatment factor and block effect.

A two-level treatment factor u and a q-level blocking factor will have $z = 2q$ different level combinations and let the frequencies of occurrence of these level combinations be denoted by f_{u1}, $f_{u2}, \ldots, f_{uz}$. The variability in the frequencies of level combinations in a treatment factor u and block factor is measured as

$$s_u^2 = \frac{1}{z-1}\sum_{j=1}^{z}(f_{uj} - \bar{f}_u)^2,$$

where $\bar{f}_u$ is the mean of the frequencies of $z = 2q$ level combinations.

Thus, the total variability in the frequencies of level combinations in a factorial design with k factors is measured as

$$S^2 = \sum_{u=1}^{k} s_u^2 = \sum_{u=1}^{k} \left\{ \frac{1}{z-1} \sum_{j=1}^{z} (f_{uj} - \bar{f}_u)^2 \right\}. \tag{3.1}$$

It must be noted that an orthogonal blocked factorial design will have zero variability in the frequencies of level combinations, i.e. $S^2 = 0$. Thus, the factorial designs with minimum variability in the frequencies, i.e. minimum S^2 among all possible designs are the best non-orthogonal blocked factorial designs.

3.3 Examples

3.3.1 To construct best NOA$_{II}(12, 2^5\, 3^1, 2)$

To obtain the best non-orthogonal blocked 12-run factorial design with $k = 5$ factors arranged in $q = 3$ blocks, we need to start with an OA$(12, 2^5, 2)$.

Let the added $q = 3$ level column, i.e. the block factor, be $(0, 1, 1, 1, 0, 2, 2, 2, 0, 0, 1, 2)$. Each entry $(0, 1, 2)$ occurs four times and $z = 6$ level combinations in a treatment factor and the added block factor are $(-1, 0)$, $(-1, 1)$, $(-1, 2)$, $(1, 0)$, $(1, 1)$ and $(1, 2)$.

Run	A	B	C	D	E	**Block**
1	-1	-1	-1	-1	-1	**3**
2	-1	-1	-1	1	1	**1**
3	-1	1	1	-1	1	**1**
4	1	-1	1	1	-1	**1**
5	1	1	1	1	-1	**3**
6	1	1	-1	1	1	**2**
7	-1	1	-1	-1	-1	**2**
8	-1	1	1	1	-1	**2**
9	-1	-1	1	1	1	**3**
10	1	1	-1	-1	1	**3**
11	1	-1	-1	1	-1	**1**
12	1	-1	1	-1	1	**2**

Table 3.1: Best NOA$_{II}(12, 2^5\, 3^1, 2)$

Table 3.1 shows the best NOA$_{II}(12, 2^5\, 3^1, 2)$ with orthogonality between treatment factors and non-orthogonality between treatment factors and blocks.

The frequencies of $z = 6$ level combinations between treatments factors and block factor

Treatment factor and Block	f_1 $(-1,0)$	f_2 $(-1,1)$	f_3 $(-1,2)$	f_4 $(1,0)$	f_5 $(1,1)$	f_6 $(1,2)$
A and Block	2	2	2	2	2	2
B and Block	2	**3**	**1**	2	**1**	**3**
C and Block	2	2	2	2	2	2
D and Block	2	2	2	2	2	2
E and Block	2	2	2	2	2	2

Table 3.2: Frequencies of level combinations.

	A	B	C	D	E	Total
Block	0.0	0.8	0.0	0.0	0.0	0.8

Table 3.3: Non-orthogonality of the design in Table 3.1

are shown in Table 3.2. Since factor B and the blocking factor have an unequal number of level combinations, non-orthogonality exists which is shown in Table 3.3.

The design in Table 3.1 has non-orthogonality of 0.8 which is the least among all possible 12-run non-orthogonal blocked factorial designs with 5 factors arranged in three blocks. Thus, this design is one of the best non-orthogonal blocked 12-run factorial design, i.e. best $\mathrm{NOA}_{II}(12, 2^5\, 3^1, 2)$.

3.3.2 To construct best $\mathbf{NOA}_{II}(20, 2^9\, 5^1, 2)$

To find the best non-orthogonal blocked factorial designs, we start with a non-regular factorial design $\mathrm{OA}(20, 2^9, 2)$ and add a five-level block factor such that each entry in the block factor (added column) occurs the same number of times and the block factor is as orthogonal as possible to the treatment factors.

Table 3.5 shows the variability of the design in Table 3.4. The total variability is 4.44 which is the least among all possible factorial designs of 20 runs with 9 factors arranged in five blocks. Thus, the design in Table 3.4 is one of the best $\mathrm{NOA}_{II}(20, 2^9\, 5^1, 2)$.

Non-orthogonal blocked factorial designs with higher numbers of factors can be obtained in a similar way. The next section presents the best non-orthogonal blocked designs with higher numbers of factors for 12 and 20 runs arranged in three and five blocks, respectively.

Run	A	B	C	D	E	F	G	H	J	**Block**
1	1	-1	1	1	1	1	-1	-1	1	**5**
2	-1	1	-1	1	-1	1	1	1	1	**5**
3	-1	-1	-1	1	-1	1	-1	1	1	**5**
4	1	1	-1	1	1	-1	-1	-1	-1	**1**
5	1	1	-1	-1	1	1	-1	1	1	**1**
6	-1	-1	1	1	-1	1	1	-1	-1	**1**
7	1	-1	1	-1	1	1	1	1	-1	**3**
8	-1	-1	-1	-1	-1	-1	-1	-1	-1	**4**
9	-1	-1	1	-1	1	-1	1	1	1	**1**
10	1	1	-1	-1	-1	-1	1	-1	1	**2**
11	-1	1	1	-1	-1	-1	-1	1	-1	**3**
12	1	-1	1	1	-1	-1	-1	-1	1	**3**
13	-1	1	1	-1	1	1	-1	-1	-1	**2**
14	1	-1	-1	1	1	-1	1	1	-1	**2**
15	-1	1	-1	1	1	1	1	-1	-1	**3**
16	1	1	1	-1	-1	1	1	-1	1	**4**
17	-1	-1	-1	-1	1	-1	1	-1	1	**5**
18	1	-1	-1	-1	-1	1	-1	1	-1	**2**
19	-1	1	1	1	1	-1	-1	1	1	**4**
20	1	1	1	1	-1	-1	1	1	-1	**4**

Table 3.4: Best $\mathrm{NOA}_{II}(20, 2^9\, 5^1, 2)$

	A	B	C	D	E	F	G	H	J	Total
Block	0.4444	0.4444	0.8889	0.4444	0.4444	0.4444	0.0	0.0	1.3333	4.4444

Table 3.5: Non-orthogonality of the design in Table 3.4

3.4 Best non-orthogonal blocked designs (Higher number of factors)

Run	A	B	C	D	E	F	Block
1	-1	-1	-1	-1	-1	-1	1
2	-1	1	1	1	1	1	2
3	1	-1	-1	-1	1	1	2
4	1	-1	1	1	-1	-1	3
5	-1	1	-1	1	-1	1	1
6	1	1	1	-1	1	-1	1
7	1	-1	1	1	-1	1	1
8	-1	1	1	-1	-1	-1	2
9	1	1	-1	1	1	-1	2
10	-1	-1	-1	1	1	-1	3
11	1	1	-1	-1	-1	1	3
12	-1	-1	1	-1	1	1	3

	A	B	C	D	E	F	Total
Block	0.0	0.8	0.0	0.0	0.8	0.0	1.6

Table 3.6: Best $\text{NOA}_{II}(12, 2^6\, 3^1, 2)$ and non-orthogonality table.

Run	A	B	C	D	E	F	G	Block
1	-1	-1	-1	-1	-1	-1	-1	1
2	-1	-1	1	1	1	1	1	1
3	1	1	-1	-1	-1	1	1	2
4	-1	1	-1	1	1	-1	-1	2
5	1	1	1	-1	1	-1	1	1
6	1	- 1	1	1	-1	1	-1	1
7	1	-1	-1	1	1	-1	1	2
8	1	1	1	1	-1	-1	-1	3
9	-1	1	1	-1	1	1	-1	2
10	1	-1	-1	-1	1	1	-1	3
11	-1	-1	-1	-1	-1	-1	1	3
12	-1	1	-1	1	-1	1	1	3

	A	B	C	D	E	F	G	Total
Block	0.0	0.8	0.8	0.0	0.8	0.0	0.0	2.4

Table 3.7: Best $\text{NOA}_{II}(12, 2^7\, 3^1, 2)$ and non-orthogonality table.

Run	A	B	C	D	E	F	G	H	Block
1	-1	-1	-1	-1	-1	-1	-1	-1	1
2	-1	-1	-1	1	1	1	1	1	1
3	1	1	1	-1	-1	1	1	1	1
4	-1	1	1	-1	1	-1	-1	1	3
5	1	-1	1	1	1	-1	1	-1	2
6	1	1	-1	1	-1	1	-1	-1	2
7	1	1	-1	-1	1	-1	1	-1	3
8	1	-1	1	1	-1	-1	-1	1	3
9	-1	1	1	1	1	1	-1	-1	1
10	1	-1	-1	-1	1	1	-1	1	2
11	-1	1	-1	1	-1	-1	1	1	2
12	-1	-1	1	-1	-1	1	1	-1	3

	A	B	C	D	E	F	G	H	Total
Block	0.8	0.0	0.8	0.8	0.0	0.8	0.0	0.0	3.2

Table 3.8: Best $\text{NOA}_{II}(12, 2^8\, 3^1, 2)$ and non-orthogonality table.

Run	A	B	C	D	E	F	G	H	J	Block
1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1
2	-1	-1	-1	-1	1	1	1	1	1	3
3	-1	1	1	1	-1	-1	-1	1	1	3
4	1	-1	1	1	-1	1	1	-1	-1	3
5	1	1	-1	1	1	-1	1	-1	1	1
6	1	1	1	-1	1	1	-1	1	-1	1
7	-1	1	1	-1	-1	1	1	-1	1	2
8	-1	1	-1	1	1	1	-1	-1	-1	3
9	-1	-1	1	1	1	-1	1	1	-1	1
10	1	1	-1	-1	-1	-1	1	1	-1	2
11	1	-1	1	-1	1	-1	-1	-1	1	2
12	1	-1	-1	1	-1	1	-1	1	1	2

	A	B	C	D	E	F	G	H	J	Total
Block	0.8	0.0	0.0	0.8	0.8	0.8	0.0	0.0	0.8	4

Table 3.9: Best $\text{NOA}_{II}(12, 2^9\, 3^1, 2)$ and non-orthogonality table.

Run	A	B	C	D	E	F	G	H	J	K	Block
1	-1	1	1	-1	-1	-1	-1	1	-1	1	1
2	-1	1	1	-1	1	1	-1	-1	-1	-1	1
3	-1	1	1	1	1	-1	-1	1	1	-1	1
4	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1
5	-1	-1	-1	1	-1	1	-1	1	1	1	2
6	-1	-1	-1	-1	1	-1	1	-1	1	1	3
7	1	-1	1	1	1	1	-1	-1	1	1	3
8	1	1	1	1	-1	-1	1	1	-1	1	5
9	1	-1	-1	1	1	-1	1	1	-1	-1	2
10	-1	-1	1	1	-1	1	1	-1	-1	-1	2
11	1	1	1	-1	-1	1	1	-1	1	1	2
12	1	1	-1	-1	-1	-1	1	-1	1	-1	4
13	-1	1	-1	1	-1	1	1	1	1	-1	3
14	-1	-1	1	-1	1	-1	1	1	1	1	4
15	1	1	-1	1	1	-1	-1	-1	-1	1	4
16	1	-1	1	1	-1	-1	-1	-1	1	-1	5
17	1	-1	-1	-1	-1	1	-1	1	-1	1	3
18	1	-1	1	-1	1	1	1	1	-1	-1	4
19	-1	1	-1	1	1	1	1	-1	-1	1	5
20	1	1	-1	-1	1	1	-1	1	1	-1	5

	A	B	C	D	E	F	G	H	J	K	Total
Block	1.3	0.9	0.4	0.9	0.4	0.9	1.3	0.0	0.4	0.4	7.1

Table 3.10: Best $\mathrm{NOA}_{II}(20, 2^{10}\, 5^1, 2)$ and non-orthogonality table.

Run	A	B	C	D	E	F	G	H	J	K	L	Block
1	1	-1	-1	1	1	-1	1	1	-1	-1	-1	1
2	-1	1	1	-1	1	-1	1	1	1	1	-1	1
3	1	1	-1	-1	1	1	-1	1	1	-1	-1	1
4	1	1	-1	-1	-1	-1	1	-1	1	-1	1	1
5	1	-1	1	1	-1	-1	-1	-1	1	-1	1	2
6	-1	-1	-1	1	-1	1	-1	1	1	1	1	2
7	-1	1	-1	1	-1	1	1	1	1	-1	-1	2
8	-1	-1	-1	-1	1	-1	1	-1	1	1	1	5
9	1	-1	1	1	1	1	-1	-1	1	1	-1	4
10	-1	1	1	-1	1	1	-1	-1	-1	-1	1	4
11	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	4
12	1	1	-1	1	1	-1	-1	-1	-1	1	-1	5
13	-1	1	-1	1	1	1	1	-1	-1	1	1	2
14	-1	1	1	1	1	-1	-1	1	1	-1	1	3
15	1	1	1	1	-1	-1	1	1	-1	1	1	4
16	-1	-1	1	1	-1	1	1	-1	-1	-1	-1	5
17	1	1	1	-1	-1	1	1	-1	1	1	-1	3
18	1	-1	1	-1	1	1	1	1	-1	-1	1	3
19	1	-1	-1	-1	-1	1	-1	1	-1	1	1	3
20	-1	1	1	-1	-1	-1	-1	1	-1	1	-1	5

	A	B	C	D	E	F	G	H	J	K	L	Total
Block	0.9	0.0	0.9	1.3	0.4	0.9	0.4	0.9	0.9	0.4	0.9	8

Table 3.11: Best $\mathrm{NOA}_{II}(20, 2^{11}\, 5^1, 2)$ and non-orthogonality table.

Run	A	B	C	D	E	F	G	H	J	K	L	M	Block
1	-1	1	1	1	1	-1	-1	1	1	-1	1	1	1
2	1	1	1	1	-1	-1	1	1	-1	1	1	-1	1
3	1	1	-1	1	1	-1	-1	-1	-1	1	-1	1	1
4	-1	1	1	-1	-1	-1	-1	1	-1	1	-1	1	1
5	-1	1	1	-1	1	1	-1	-1	-1	-1	1	-1	2
6	1	-1	1	1	1	1	-1	-1	1	1	-1	1	2
7	-1	-1	-1	1	-1	1	-1	1	1	1	1	-1	5
8	-1	-1	1	1	-1	1	1	-1	-1	-1	-1	1	5
9	1	-1	-1	-1	-1	1	-1	1	-1	1	1	1	4
10	1	1	1	-1	-1	1	1	-1	1	1	-1	-1	4
11	-1	-1	1	-1	1	-1	1	1	1	1	-1	-1	4
12	-1	-1	-1	-1	1	-1	1	-1	1	1	1	1	5
13	-1	1	-1	1	-1	1	1	1	1	-1	-1	1	2
14	1	1	-1	-1	-1	-1	1	-1	1	-1	1	1	2
15	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	3
16	1	-1	-1	1	1	-1	1	1	-1	-1	-1	-1	4
17	-1	1	-1	1	1	1	1	-1	-1	1	1	-1	3
18	1	-1	1	1	-1	-1	-1	-1	1	-1	1	-1	3
19	1	-1	1	-1	1	1	1	1	-1	-1	1	1	3
20	1	1	-1	-1	1	1	-1	1	1	-1	-1	-1	5

	A	B	C	D	E	F	G	H	J	K	L	M	Total
Block	0.4	1.7	0.4	0.4	0	1.3	0.4	0.8	0.8	0.8	0.4	0.8	8.8

Table 3.12: Best $\mathrm{NOA}_{II}(20, 2^{12}\, 5^1, 2)$ and non-orthogonality table.

Run	A	B	C	D	E	F	G	H	J	K	L	M	N	Block
1	1	1	-1	-1	-1	-1	1	-1	1	-1	1	1	1	1
2	1	-1	-1	1	1	-1	1	1	-1	-1	-1	-1	1	1
3	-1	1	-1	1	-1	1	1	1	1	-1	-1	1	1	1
4	-1	-1	1	-1	1	-1	1	1	1	1	-1	-1	1	1
5	1	-1	1	-1	1	1	1	1	-1	-1	1	1	-1	2
6	1	1	1	1	-1	-1	1	1	-1	1	1	-1	-1	3
7	-1	1	1	-1	-1	-1	-1	1	-1	1	-1	1	1	4
8	-1	1	-1	1	1	1	1	-1	-1	1	1	-1	1	4
9	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	2
10	-1	1	1	-1	1	1	-1	-1	-1	-1	1	-1	1	3
11	1	1	-1	-1	1	1	-1	1	1	-1	-1	-1	-1	4
12	1	1	1	-1	-1	1	1	-1	1	1	-1	-1	-1	5
13	-1	-1	-1	1	-1	1	-1	1	1	1	1	-1	-1	2
14	1	-1	1	1	-1	-1	-1	-1	1	-1	1	-1	1	4
15	-1	1	1	1	1	-1	-1	1	1	-1	1	1	-1	5
16	-1	-1	1	1	-1	1	1	-1	-1	-1	-1	1	-1	5
17	1	-1	1	1	1	1	-1	-1	1	1	-1	1	1	2
18	-1	-1	-1	-1	1	-1	1	-1	1	1	1	1	-1	3
19	1	-1	-1	-1	-1	1	- 1	1	-1	1	1	1	1	3
20	1	1	-1	1	1	- 1	-1	-1	-1	1	-1	1	-1	5

	A	B	C	D	E	F	G	H	J	K	L	M	N	Total
Block	0	1.3	0.4	0.4	0	0.4	1.3	0.4	0.4	0.4	1.3	0.4	2.2	9.3

Table 3.13: Best $\mathrm{NOA}_{II}(20, 2^{13}\, 5^1, 2)$ and non-orthogonality table.

Chapter 4

Comparison

In Chapters 2 and 3, we studied the two approaches for constructing the best non-orthogonal blocked factorial designs when orthogonal blocking is not achievable. The first approach allows non-orthogonality between treatment factors while the second approach allows non-orthogonality between treatment factors and block effects. This chapter compares the two approaches in terms of design efficiency and ease of obtaining the best designs.

4.1 Design Efficiency

Efficiency is a crucial concept in the optimal design of experiments. Optimal designs provide better estimation of model parameters by minimizing the variances of estimators. The optimal design problem is to choose a design among all competing designs which minimizes the variances of estimated parameters.

One of the most popular is D-optimality criterion that aims at minimizing the determinant of the variance-covariance matrix of estimators, i.e minimizing $det[Var(\hat{\beta})]$, which is proportional to the volume of a confidence ellipsoid for β, under normality assumptions.

The model used for the analysis of a blocked factorial design having design matrix $X = (X_1, X_2, \ldots, X_k)$ is given by

$$Y = \mu\, 1_n + X\,\beta + \mathcal{Z}\,\gamma + \epsilon \tag{4.1}$$

where Y is the vector of observations, 1_n is a vector of n ones, μ is the grand mean, β is a vector of treatment main effects, $\mathcal{Z} = (\mathcal{Z}_1, \mathcal{Z}_2, \ldots, \mathcal{Z}_{q-1})$ are orthogonal block contrasts, γ

is the vector of block parameters and ϵ is the vector of random error terms such that

$$E(\epsilon) = 0_n \text{ and } Var(\epsilon) = \sigma^2 I_n. \tag{4.2}$$

To estimate β, the following theorem is used.

Theorem 4.1 *Consider the linear model in (4.1) under the assumptions in (4.2). Then β is estimable if and only if $X^T X - X^T P_{\mathcal{Z}} X$ is invertible, in which case the best linear unbiased estimator (BLUE) for β is given by*

$$\hat{\beta} = (X^T X - X^T P_{\mathcal{Z}} X)^{-1} (X - P_{\mathcal{Z}} X)^T Y$$

because X and $\mathcal{Z}$ are all orthogonal to 1_n and has

$$Var(\hat{\beta}) = \sigma^2 \ (X^T X - X^T P_{\mathcal{Z}} X)^{-1}$$

where $P_{\mathcal{Z}}$ is projection matrix onto the linear subspace spanned by the columns of $\mathcal{Z}$, and has an explicit form of

$$P_{\mathcal{Z}} = \mathcal{Z}(\mathcal{Z}^T \mathcal{Z})^{-1} \ \mathcal{Z}^T. \tag{4.3}$$

As a functional of information matrix,

$$M = \sigma^2 (Var(\hat{\beta}))^{-1} = X^T X - X^T P_{\mathcal{Z}} X,$$

the D-optimality criterion aims at maximizing $\det[M] = \det[X^T X - X^T P_{\mathcal{Z}} X]$. If the design $\mathcal{D}$ is such that the design matrix X (treatment factors) has orthogonal columns and columns of X are orthogonal to $\mathcal{Z}$ (block factors), then $M = n\, I$ and thus, $\det(M) = n^k$ where k is the number of treatment factors. In this case, we have that

$$\det(M) = \det[X^T X - X^T P_{\mathcal{Z}} X] = n^k.$$

Therefore,

$$D_{\mathit{eff}} = \frac{\det[X^T X - X^T P_{\mathcal{Z}} X]^{\frac{1}{k}}}{n} = 1.$$

For a non-orthogonal blocked factorial design, the value of D_{eff} will be smaller than one. The D-efficiency as given by D_{eff} will be used to assess blocked factorial designs. The higher the efficiency, the better the design.

4.2 Results for Two Classes of Blocked Designs

We first give an example to illustrate the calculation of D-efficiency using NOA$(12, 2^5\, 3^1, 2)s$. Table 4.1 shows the best design obtained using Approach I that allows for non-orthogonality between treatment factors while maintaining orthogonality between treatment factors and block effects.

Run	A	B	C	D	E	Block
1	1	1	-1	-1	-1	1
2	1	1	1	1	1	1
3	-1	-1	-1	-1	1	1
4	-1	-1	1	1	-1	1
5	1	-1	-1	-1	-1	2
6	1	-1	1	1	1	2
7	-1	1	1	-1	-1	2
8	-1	1	-1	1	1	2
9	1	-1	-1	1	-1	3
10	1	1	1	-1	1	3
11	-1	1	-1	1	-1	3
12	-1	-1	1	-1	1	3

Table 4.1: Best NOA$_I(12, 2^5\, 3^1, 2)$

Since the treatment factors and blocks are orthogonal, we have that $\mathcal{Z}^T X = 0$. In such case, the D-efficiency D_{eff} reduces to

$$D_{\mathit{eff}} = \frac{\det[X^T X]^{\frac{1}{k}}}{n}.$$

Thus,

$$D_{\mathit{eff}} = \frac{\det[X^T X]^{\frac{1}{5}}}{12} = 0.9767.$$

The design obtained using Approach II allowing non-orthogonality between treatment factors and blocks while maintaining orthogonality between treatment effects is shown in Table 4.2. To obtain the D-efficiency D_{eff} of this design, we first need to find its projection matrix $P_{\mathcal{Z}}$.

Let $\mathcal{Z}_1$ and $\mathcal{Z}_2$ be two mutually orthogonal block contrasts. Then $\mathcal{Z} = (\mathcal{Z}_1, \mathcal{Z}_2)$. The projection matrix $P_{\mathcal{Z}}$ is obtained by substituting the matrix $\mathcal{Z}$ in equation 4.3. Thus, the

Run	A	B	C	D	E	Block
1	-1	-1	-1	-1	-1	0
2	-1	-1	-1	1	1	1
3	-1	1	1	-1	1	1
4	1	-1	1	1	-1	1
5	1	1	1	1	-1	0
6	1	1	-1	1	1	2
7	-1	1	-1	-1	-1	2
8	-1	1	1	1	-1	2
9	-1	-1	1	1	1	0
10	1	1	-1	-1	1	0
11	1	-1	-1	1	-1	1
12	1	-1	1	-1	1	2

Table 4.2: Best $\text{NOA}_{II}(12, 2^5\, 3^1, 2)$

D-efficiency of the design in Table 4.2 is

$$D_{\mathit{eff}} = \frac{\det[X^T X - X^T P_{\mathcal{Z}} X]^{\frac{1}{k}}}{n} = 0.9641.$$

Efficiency Comparison between Best $\mathbf{NOA}_I(n, 2^k\, q^1, 2)$s and $\mathbf{NOA}_{II}(n, 2^k\, q^1, 2)$s

Tables 4.3 and 4.4 show the values of D-efficiency of the best nearly-orthogonal designs of 12 and 20 runs obtained using approach I and II.

Design	Approach I	Approach II
$\text{NOA}(12, 2^5\, 3^1, 2)$	0.9767	0.9641
$\text{NOA}(12, 2^6\, 3^1, 2)$	0.9614	0.9394
$\text{NOA}(12, 2^7\, 3^1, 2)$	0.9507	0.9210
$\text{NOA}(12, 2^8\, 3^1, 2)$	0.9428	0.9018

Table 4.3: D-efficiency for designs of 12 runs in three blocks.

It is evident from the tables that the values of D_{eff} of 12 and 20 runs designs obtained using approach I are closer to 1, which means they are less non-orthogonal as compared to the designs obtained using approach II. Thus, it can be said that approach I gives us a better class of designs that have minimal non-orthogonality and are more efficient.

Design	Approach I	Approach II
$\mathrm{NOA}(20, 2^9\, 5^1, 2)$	0.9216	0.8909
$\mathrm{NOA}(20, 2^{10}\, 5^1, 2)$	0.8634	0.8500
$\mathrm{NOA}(20, 2^{11}\, 5^1, 2)$	0.8185	0.8050
$\mathrm{NOA}(20, 2^{12}\, 5^1, 2)$	0.7829	0.7949

Table 4.4: D-efficiency for designs of 20 runs in five blocks.

4.3 Complexity in Construction of the Best Designs

Approach I involves adding another treatment factor $k + 1$ to the best non-orthogonal design with k factors such that it satisfies the three conditions mentioned in Section 2.2. For example, to obtain the best $\mathrm{NOA}_I(12, 2^7\, 3^1, 2)$, we add a treatment factor to the best $\mathrm{NOA}_I(12, 2^6\, 3^1, 2)$. More generally, we should consider simultaneously adding three columns (treatment factors) to the $\mathrm{OA}(12, 2^4\, 3^1, 2)$, which is bit complex. To obtain $\mathrm{NOA}_{II}(n, 2^k\, q^1, 2)$ using approach II , we just need to add a q-level blocking factor to the orthogonal n-run non-regular design with k factors (that is easily available in any software like R). Thus, finding the best $\mathrm{NOA}(n, 2^k\, q^1, 2)$ is more straightforward by approach II as it is by approach I.

Chapter 5

Summary

In this project, non-orthogonal blocking of non-regular designs is studied. In non-regular designs, orthogonal blocking is possible for up to a certain number of factors. When orthogonal blocking is not possible, we need to construct non-orthogonal blocked designs that are as orthogonal as possible. To do so, we have to allow either non-orthogonality between treatment factors or non-orthogonality between treatment factors and blocks.

Two approaches are discussed to construct the best non-orthogonal blocked factorial designs. Chapter 2 introduced the first approach that allows for non-orthogonality between treatment factors. It also discussed a measure of non-orthogonality to compare and determine the best designs among all competing ones. Best non-orthogonal blocked designs i.e $\mathrm{NOA}_I(n, 2^k\, q^1, 2)$ for 12 runs in three blocks and 20 runs arranged in five blocks, found by our method, are computed and tabulated.

The second approach that allows for non-orthogonality between treatment factors and blocks while maintaining orthogonality between treatment factors is discussed in Chapter 3. The non-orthogonality in the design is measured by summing over the variability in the frequencies of all the level combinations between a two-level treatment factor and the q-level block factor. Using our method, the best 12-run and 20-run designs arranged in three and five blocks respectively, are tabulated.

Both approaches give useful designs, but it's important to find out which approach is the better one to use. The comparison is done in terms of design efficiency using D-optimality criterion and in terms of complexity in construction. While approach I gives rise to more efficient designs, approach II is easier to implement computationally.

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