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UTILIZING DESIGN STRUCTURE FOR IMPROVING DESIGN SELECTION AND ANALYSIS

A Dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy at Virginia Commonwealth University.

by

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List of Abbreviations

2FIs Two-factor Interactions

AIC Akaike Information Criteria

BIC Bayesian Information Criterion

DOE Design of Experiment

EC Estimation Capacity

FFDs Fractional Factorial Designs

GALP Generalized Alias Length Pattern

GR Generalize Resolution

MDS Minimal Dependent Set

MEs Main Effects

PEC Projection Estimation Capacity

PIC Projection Information Capacity

SBT Separate Block Technique

Abstract

UTILIZING DESIGN STRUCTURE FOR IMPROVING DESIGN SELECTION AND ANALYSIS

By Ahlam Ali Alzharani

A Dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy at Virginia Commonwealth University.

Virginia Commonwealth University, 2020.

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Recent work has shown that the structure for a design plays a role in the simplicity or complexity for data analysis. To increase the knowledge of research in these areas, this dissertation aims to utilize design structure for improving design selection and analysis. In this regard, minimal dependent sets and block diagonal structure are both important concepts that are relevant to the orthogonality of the columns of a design. We are interested in finding ways to improve the data analysis especially for active effect detection by utilizing minimal dependent sets and block diagonal structure for a design.

We introduce a new classification criterion for minimal dependent sets to enhance existing criteria for design selection. The block diagonal structure of certain nonregular designs will also be discussed as a means of improving model selection. In addition, the block diagonal structure and the concept of parallel flats will be utilized to construct three-quarter nonregular designs.

Based on the literature review on the effectiveness for the simulation study for

slight the light on the success or failure of the proposed statistical method, in this dissertation, simulation studies were used to evaluate the efficacy of our proposed methods. The simulation results show that the minimal dependent sets can be used as a design selection criterion, and block diagonal structure can also help to produce an effective model selection procedure. In addition, we found a strategy for constructing three-quarters of nonregular designs which depend on the orthogonality of the design columns. The results indicate that the structure of the design has an impact on development the data analysis and design selections. On this basis, it is recommended that analysts consider the structure of the design as a key factor in order to improve the analysis. Further research is needed to determine more concepts related to the structure of the design, which could help to improve data analysis.

CHAPTER 1

INTRODUCTION

Section 1.1 desribes the background of this dissertation.

1.1 Motivation

The area of experimental design is an open and monumental area for research. It has many applications in our lives, such as in the areas of economics, education, manufacturing and medicine. In this situation, the existing area of study needs to improve in order to keep pace with the requirements of the time and new research. The areas of constructing and analyzing the design are active research areas in the experimental design field. Until now, researchers have not come to an agreement on the best way to do the analysis and constructing designs. Therefore, new approaches and methods are still needed to develop these areas.

To avoid the complexity of the design analysis, the experimenter should be very careful in choosing a design in the first step. Screening designs are widely used in the first stage of an experiment to determine which of many factors have an impact on a response variable. Usually, there are a large number of factors, but only a few of them believed to be active. This fact refers to the concept of the effects' sparsity (Box and Meyer, 1986, and Hamada and Wu, 2000). Having prior knowledge of active factors has a big impact on reducing the cost and resources for the experiments, such that the inactive factors will be removed, while the active factors will be focused in further follow-up experiments. Furthermore, this step is very important since it provides information about the final model or the follow up experiment. Most of the time, this

screening experiment does not provide the final model due to ambiguities between the columns of the effects for the design, such as the aliasing, or the confounding between the effects.

The aliasing which is confounding between the columns of effects can not be ignored. In fact, it makes the analysis more difficult. However, several researchers advise to utilize these ambiguities (aliasing) to aid in the data analysis. Hamada and Wu, 1992, and Chipman et al., 1997, advocated for utilizing the complex aliasing of the Placket-Burman design for proposing an analysis strategy that turns this complex aliasing into advantages for the Placket-Burman design (Plackett and Burman, 1946). In fact, the structure of the design, which includes the orthogonality of the columns, run sizes, the number of factors, number of center runs and the replication runs, etc, having a big impact on the appearance of the aliasing. Thus, understanding the structure of a design helps with understanding the aliasing relation, which carries implications for both design choice and data analysis. So, improving our understanding of the structure and the properties of screening designs is actual, important for a design based analysis.

Thus, this dissertation investigates how to improve the analysis of the design, how to construct a new type of design, and how to provide a new model selection by utilizing and understanding the structure of the design. We proceed with these research questions with the following specific goals as outline below.

1.1.1 Classification of Minimal Dependent Sets for Design Selection and Analysis

In the design of experiment (DOE) literature, we found that minimal dependent sets (MDSs) help to understand model resolvability/discrimination and its impact on active effect detection; they can be used as criterion for design selection. Based on that, one of the primary goals of this dissertation is to explore the effect of MDSs on design analysis. Especially, we are focusing on study the relation between the MDSs and active effects detection. To accomplish that, first we are looking for a method to classify the MDSs for a design based on the characteristics of each MDS, such as size and number of factors. Next, we investigate the impact of the classification of MDSs on design selection and analysis. Based on selected designs for a specific run size and a number of factors, we perform a simulation study to evaluate our MDSs classification. Orthogonal and non-orthogonal designs will be considered.

1.1.2 Constructing Three-Quarter Nonregular Designs

Omitting a quarter of run size has been soundly investigated for regular design, however less research has been devoted to this technique of construction of nonregular designs. We are interested in constructing three-quarter designs of fractional factorial nonregular design by using the blocking technique. Based on the work of John, 1964, not all factorial effects allow for splitting the nonregular design into 4 equal blocks. We will investigate which factorial effects allow for splitting non-regular designs into 4 equal blocks, which then allows the construction of three-quarter designs, and which factorial effects do not. Moreover, we tend to study the properties of constructed three-quarters design based on the concept of MDSs and the number of flats, also, the criterion for ranking designs, such as the generalized resolution, estimation capacity and aliasing length pattern will be discussed.

1.1.3 Utilizing the Block Diagonal Structure of Nonregular Designs for Data Analysis

The fact that the factorial effects that belong to different blocks are uncorrelated led to create a block diagonal structure for a design. This structure is an interesting feature of a design, especially for estimating different models. Some studies have found that the structure of the design is used explicitly in the design analysis. Based on that, we utilize this structure for the experimental design to propose a new model selection strategy. Via a simulation study, the proposed method is applied over a number of parallel flats designs. We also consider a comparison for the performance of the proposed method and the usual standard model selection procedures.

1.2 Dissertation Outline

The rest of this dissertation is organized as follows. Chapter 2 provides a review of needed background and fundamental topics that are used in this dissertation. Chapters 3, 4, and 5 are the distinct research topics on construction and analysis screening design by utilizing the structure of the screening design. Each of these chapters contains a literature review of the topic relevant to that chapter. Furthermore, the contents for each chapter will be as follows: Chapter 3 is an in-depth exploration of MDSs which are considered as a specific criteria for a screening design. In this chapter, we provide additional background and literature review for this topic. As well, we present the methodology used to catalog MDSs. This chapter also contains a simulation study protocol, the results of the simulation and a conclusion for this topic.

Chapter 4 introduces the second topic for this dissertation, which is construction of three-quarters designs. This chapter also includes an additional background and literature reviews relevant to the covered topic. In addition, we provide the methodology used for the construction of three-quarters designs. This chapter also provides several theorems, with proofs, that related to the constructed design.

Chapter 5 provides the third topic, which is utilizing the blocks diagonal design for data analysis. As with the previous chapters, this chapter includes additional background information and literature review for the covered topic. Also, we present a simulation study protocol and the results. Finally, Chapter 6 provides the final concluding comments and discussion of future work.

CHAPTER 2

BACKGROUND AND LITERATURE REVIEW

In this chapter we provide a review of needed background and fundamental topics that are used in this dissertation. The purpose of this chapter is to introduce the reader to factorial designs, and provide general guidance on how to construct, analyze, and evaluate factorial designs. First, we present the basic information about two-level full factorial designs and fractional factorial designs. Then, we provide a summary of the criteria that are used for ranking and evaluating screening designs. Next, there is a brief section on the classic model selection procedures.

2.1 Two-level Full and Fractional Factorial Designs

Screening an experiment is the first step for the experiment. It sheds light on the important factors that impact the response. Effects that have influence on the response are called *active effects*, and factors that are involved in one or more active effects are called *active factors*. Having prior knowledge of active factors, has a big impact on reducing the cost and resources of the experiment, since these active factors will be the focus of the follow up experiment. Usually, two-level factorial designs are widely used for screening an experiment.

Two-level factorial designs are represented as 2^k , where k indicates the factors for the experiment. It requires 2^k treatment combinations. In this case, a design that contains all the treatment combinations is called a full factorial design (Fisher, 1936). These types of designs are the most common designs, because it is easier to analyze and construct. With two-level designs, each factor is investigated at two

levels. Often, the notation (-1) indicates the low level and (+1) indicates the high level. For example, an experiment runs to test the effects for temperature (A), and time (B) on the surface of copper, such that A has two levels: 80 in low level and 100 in high level. Also, factor B has two levels, 5 minutes in low level and 10 minutes in high level. For this experiment we have k=2 factors A and B. The two-level full factorial design for this experiment is represented as 2^2 , which has 4 treatment combinations. In fact, all experimental points are represented by a matrix which is called a design matrix and it is denoted by \mathcal{D} . The number of the rows in the design matrix is the number of the run size (n), and each row represents one-treatment combination, and each column represents one-factor (Montgomery, 2017). The Full factorial design matrix for the example above is shown in Table 1.

Table 1.: Full factorial design matrix 2^2

$$\begin{bmatrix}
A & B \\
-1 & -1 \\
-1 & 1 \\
1 & -1 \\
1 & 1
\end{bmatrix}$$

The design matrix is actually the design that is being used by the experimenter to run the experiment, which tells nothing about the model. With 2^k full factorial design, there is a $2^k - 1$ degree of freedom which is the number of the independent variables that a model can be estimated. The regression model contains k main effects (MEs), $\binom{k}{2}$ two-factor interactions (2FIs), $\binom{k}{3}$ three-factor interactions, $\binom{k}{n}$ n-factor interactions, and one term of k-factor interactions. The model matrix is a matrix that includes all the columns of effects that are involved in the desirable model with

an additional column for the intercept (Montgomery, 2017). For example, the first order model for the design matrix to the above example is

$$y_i = \beta_0 + \beta_1 A + \beta_2 B + e_i, \tag{2.1}$$

where y_i is the response at the observation i, β_1 , β_2 are the parameters, and e_i is the error. The model matrix for this model is shown in Table 2.

Table 2.: Model matrix for first order model

$$\begin{bmatrix}
1 & -1 & -1 \\
1 & -1 & 1 \\
1 & 1 & -1 \\
1 & 1 & 1
\end{bmatrix}$$

If we want to include the 2FIs in the model we do the first order model with the interactions which has the equation

$$y_i = \beta_0 + \beta_1 A + \beta_2 B + \beta_{12} A B + e_i \tag{2.2}$$

. Then, the model matrix for this model is shown in Table 3

Table 3.: Model matrix for first order model with 2FIs

$$\begin{bmatrix}
1 & -1 & -1 & 1 \\
1 & -1 & 1 & -1 \\
1 & 1 & -1 & -1 \\
1 & 1 & 1 & 1
\end{bmatrix}$$

In practice, there are limitations for the time and the resources that control

the experiment. When k (number of factors) is too large it takes too long to run all treatment combinations. This makes the full factorial design not desirable. For example, in 2^8 full factorial design, there will be 256 treatment combinations, and there are 255 degrees of freedom for estimating the effects. MEs have 8 degrees of freedom,2FIs have 28 degrees of freedom, three-factor interactions have 56 degrees of freedom, and the remaining high order interactions have 163 degrees of freedom, which are most likely negligible. Therefore, by this scenario, full factorial design involves a waste of resource (Gunst and Mason, 2009). Instead of the full factorial design, the best and acceptable design to use for solving this problem is a fractional factorial designs (FFDs).

2.1.1 Two-Level Fractional Factorial Designs

Box and Hunter, 1961, introduced the idea of FFDs, which uses a fraction of the runs needed. FFDs are denoted by 2^{k-p} such that $\frac{1}{2^p}$ is the fraction of the 2^k full factorial design, and p is the number of columns to be generated from the basic columns of the design matrix. So, with FFDs we have basic factors and generator factors. The number of the basic factor is k-p, and the number of generator factors is p. The generator's p determines, the defining relation for a design, which states the relation between the effects. The run size for FFDs is equal to 2^{k-p} . To construct FFDs, we begin with full factorial in the basic factors, then we used these factors to generate the additional factors. For example, 2^{4-1} is a $\frac{1}{2}$ of the 2^4 . Clearly, we have k=4, p=1, and, n=8, which calculated from $2^{4-1}=2^3=8$. With 2^{4-1} , there is one generator p=1, and three basic factors which are A, B, and C, and we need to generate D, which could be the high order interactions to the other factors, such as D=ABC. Thus, in this case, the defining relation is I=ABCD (Montgomery, 2017). The design matrix for 2^{4-1} is shown in Table 4.

Table 4.: Design matrix for 2^{4-1}

2.1.2 Aliasing

The trade-off by using the FFDs is the appearance of aliasing (bias) between the effects. With FFDs, the degree of freedom for estimating the effects will be decreased, then some effects are aliased with each other. So, when two columns of a design are identical, the corresponding effects are aliased. For example, consider 2^{4-1} , with four MEs denoted by A, B, C, and D, such that D = ABC. The defining relation is I = ABCD, where I is the intercept. Thus, the alias structure for 2^{4-1} is D = ABC, A = BCD, A = ACD, C = ABD, A = CD, A = BCD, A = BCD.

Table 5.: Design matrix for 2^{4-1} with aliasing relation D = ABC

From the design matrix in Table 5, clearly, the column for D is identical to column ABC, hence D is aliasing with ABC. This aliasing doesn't mean to imply that the effect of D is the same as the interaction of ABC on the response. However, the experiment cannot distinguish the ME, D, from the interaction, ABC. There are two types of aliasing: fully aliasing or partial aliasing. Fully aliasing occurs in both regular and non-regular designs, while, partial aliasing, occurs only in nonregular designs (Wass, 2010).

2.1.2.1 Aliasing for Regular Design

Regular design has a simple aliasing structure. This aliasing is constructed from the defining relation for 2^{k-p} design, as shown earlier. The aliasing chains demonstrate the correlation between any two effects. In the regular design, the aliasing between any two effects is fully confounding or orthogonal. If any two effect are fully confounding, that means the correlation between these effects are either +1 or -1. In this case,

it is impossible to separate the impact of these effects on the response, which makes the analysis more difficult. On the other hand, if any two effect are orthogonal, that means the correlation between these effects is 0, i.e., each effect has its own impact on the response without any dependency from other effect (Deng et al., 2000). For example, consider 2^{5-2} design. This design has 5 MEs, denoted by A, B, C, D, E. Since p=2, two of these MEs are generated by the other MEs. They are generated as D=AB and E=AC. Thus, the defining relation for this design is I=ABD=ACE=BDCE. The term BDCE is the product of ABD, and ACE such that $ABD*ACE=A^2BDCE=BDCE$, ($A^2=1$). The aliasing structure is A=BD=CE=ABDCE, B=AD=ABCE=DCE, C=ABCD=AE=BDE, D=AB=ACDE=BCE, E=ABDE=AC=BDC, etc. We can see from the aliasing structure that A=BD, so the correlation amount between A and ABD is 1. Thus, A is fully confounding with BD. Figure 1 shows the correlation between the effects for this design. We can see that the effects are either fully confounding (red cube) or orthogonal.

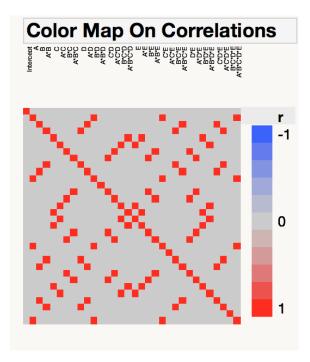


Fig. 1.: Correlation for regular design 2^{5-2}

2.1.2.2 Aliasing for Nonregular Design

Nonregular design has a complex aliasing structure, since a partial aliasing between the effects is produced. In this case, the correlation between effects might be equal to a fraction between 0, and ± 1 . Figure 2 shows the correlation of the effects for non-regular design (Placket-Burmun with n=12). With the partial aliasing, the correlated effects are shared the impact on the response. Also, the impact of correlated effects on the response can not be separated, but the level of the confounding is less than the full confounding. For example, consider a design 2^{5-2} , such that generators are D=0.5(AB) and E=0.5(AC), so that the defining relation will be I=0.5(ABD)=0.5(ACE)=0.25(BDCE). By multiplying the defining relation by A, B, C, D, E, we will have the aliasing chains for the MEs as follows:

$$A = 0.5BD = 0.5CE = 0.5ABCDE$$

$$B = 0.5AD = 0.5CE = 0.25DCE$$

 $C = 0.5ABDC = 0.5AE = 0.25BDE$
 $D = 0.5AB = 0.5ACED = 0.25BCE$
 $E = 0.5ABDE = 0.5AC = 0.25BDC$.

From the aliasing chains we can see that the MEs have a partial aliasing with the 2FIs. For instance, A = 0.5BD, so the correlation amount here is 0.5, so A is partial aliasing with BD.

Because of the complex aliasing in the nonregular design, it seems that this type of design is not desirable, especially when there are some 2FIs which are potentially are important. However, several researches have shown an interesting attention for nonregular design. Hamada and Wu, 1992, represented that some interactions could be detected by considering fractional nonregular design. Lin and Draper, 1992, and Wang and Wu, 1995, investigated the projection properties of some small Placket-Burman designs. Moreover, Wu, 1993, and Lin, 1993, constructed supersaturated design by using the Hadmard matrix, which is relies heavily on partial aliasing.

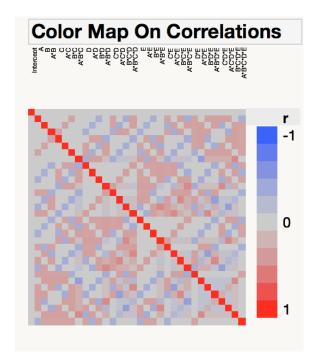


Fig. 2.: Correlation for nonregular design (Placket-Burman design)

2.2 Criteria for Ranking the Designs

In design of experiment (DOE) literature review, there are criteria for selecting and ranking designs under a number of factors and run sizes. We will talk briefly about some of these criteria in this section, due to the usefulness in using these criteria to evaluate and rank the factorial designs.

2.2.1 Resolution

The complete defining relation for a design contains all the columns for a design that are equal to the identity. Each term in this defining relation I is called a word. Each word has a number of letters, which is defined to be the length or size for this word. In fact, the generators are considered to be the foundation for the defining relation. To get the complete defining relation, we should consider the words in the defining relation and the generalized interaction for these words. So,

for a particular design, a defining relation will always have $2^p - 1$ words without including I. The length of the words in defining relation determine the resolution of the design. So, the resolution for a design is defined as the length for the shortest word in the defining relation (Box and Hunter, 1961). For example, consider a 2^{6-2} , such that the generators are defined as E = ABC, and D = BCF. So, the complete defining relation for this design is I = ABCE = BCDF = ADEF. The last word in this defining relation, ADEF, is the product of the first two words, so $(ABCE)*(BCDF) = AB^2C^2EDF = AEDF$. Consequently, the resolution for this design is IV since the length of shortest word in the defining relation is 4 (Montgomery, 2017).

The FFDs have been classified by Box and Hunter, 1961, according to the design's ability for separating MEs and 2FIs as follows:

- Resolution III designs. The MEs in these designs are not confounded with other MEs, however, they are confounded with 2FIs.
- 2. Resolution IV designs. The MEs are clear of the other MEs and 2FIs, however, the 2FIs are confounded with the other 2FIs.
- 3. Resolution V designs. Both MEs and 2FIs are confounded only with the high-order interactions.

Clearly, the choice of generators affects the aliasing structure, which consequently affects the resolution for a design. So, it is important to select the generators p, such that we obtain a design with highest resolution. For instance, consider 2^{6-2} design with the generators E = ABC, F = BCD, the defining relation is I = ABCE = BCDF = ADEF, so, this generators produce a design of resolution IV. If we select the generators such as E = ABC, and F = ABCD, in this case, the defining relation

is I = ABCE = ABCDF = DEF, and this defining relation determine a design of resolution III (Montgomery, 2017).

High resolution is an attractive feature for a design. Thus, resolution V design is the most desirable design, because both MEs and 2FIs are confounding with three or higher order interactions, which are usually considered as negligible effects in the analysis. Back to the previous example, the design that has defining relation I =ABCE = ABCDF = DEF has resolution III. We can see, that the shortest word DEF, has length 3. Clearly from this word DEF, the MEs are not confounded to other MEs, but it confounded with 2FIs, so D = EF, E = DF, F = DE. While the defining relation, I = ABCE = BCDF = ADEF, is determined to be a resolution IV design, so with this design, 2FIs are confounded with the other 2FIs. For instance, from a word ABCE, we have AB = CE, BC = AE, BE = AC. In fact, some time the resolution is insufficient to distinguish between the designs. If we have that all candidate designs have the same resolution, in this case we need to consider the word length pattern for the defining relation to each design. Let $A_i(\mathcal{D})$ be the number of word of length i, that involved the defining relation of design \mathcal{D} . Then, $W(D) = A_1, A_2, A_3, ..., A_k$ is called word length pattern. The design that minimizes the number of words, which are of minimum length, is the desirable design, and it is called a minimum aberration design (Montgomery, 2017).

2.2.2 Strength and Generalized Resolution

Tang and Deng, 1999, introduced strength in context with the orthogonality for a design, such that the orthogonality implies that for every two columns of a design matrix, a 2^2 occurs equally. The treatment combinations for 2^2 are represented by (++), (-+), (+-), and (-,-). In general, let OA(n,k,t) represent an orthogonal array containing symbols of +1 and -1, with n run size, k factors, and t strength.

Strength t means in every set of t columns of the design matrix, a full factorial 2^t occurs equally. A design with strength 3 implies independent estimation of the MEs from the 2FIs, while a design with strength 2 implies independent estimation for the MEs from other MEs. Therefore, a design with resolution, r, has a strength t = r - 1. Note that the run size for a strength, t, design has to be divisible by 2^t . Thus, a design with 16, 20, 28, and 32 runs all have strength 2, but a design with 24 runs either has strength 2 or strength 3 because it is divisible by $2^2 = 4$ and $2^3 = 8$. Note that the concept of strength can be extended to the non-orthogonal designs. In this case, the strength for these designs is less than 2 (Tang and Deng, 1999), (Mee et al., 2017).

Let \mathcal{D} represent a regular design, then j-interaction column is denoted as the product for j main effects. The sum for this column is either $\pm n$ or 0. If the sum is n, that means this column forms a full aliasing word, which means it is difficult to estimate this column. However, if the sum is 0, that corresponds to the orthogonality, which allows for estimating this column independently from other columns. For non-regular design, this sum may take different values than $\pm n$ or 0, which indicates partial aliasing among the columns of the design. Let J represent the absolute value for the maximum number of the sum of j-interaction columns. Generalized resolution is defined as $GR(\mathcal{D}) = t + (2 - J/n)$, such that t is the strength of the design, and n is the run size. According to generalized resolution, $GR(\mathcal{D})$, a design with high $GR(\mathcal{D})$ is preferred (Deng and Tang, 1999), (Tang and Deng, 1999), (Mee et al., 2017).

2.2.3 Estimation Capacity

Estimation capacity, EC, was first introduced by Cheng et al., 1999. Cheng et al., 2002, defined the estimation capacity as the total number of models containing all the MEs, k, and g 2FIs. Mee et al., 2017, defined EC as a vector,

 $(EC_1, EC_2, EC_3..., EC_g)$, of the proportions of estimable models with all the k, MEs and 1, 2, ..., g 2FIs. Jones et al., 2009, illustrated that the estimation capacity is the key characteristic of the supersaturated designs. They defined estimation capacity for supersaturated designs, EC_g , as

number of estimable g-terms main-effect models total number of g-term main-effect models

such that $EC_g = 1$, indicates that all models with all k MEs, and g 2FIs are estimable. It is desirable for a design to have large values of all entries of the vector EC. For example, consider 2^{6-2} design with the generators E = ABC, F = BCD that was shown earlier. The estimation capacity vector for this design equals

$$(EC_1, EC_2, EC_3, EC_4, EC_5, EC_6) = (1, 0.9143, 0.7473, 0.5275, 0.3037, 0.1279)$$

. This vector indicates the following: every possible model with k=6 and one 2FI is estimable since $EC_1=1$; there are 105 possible models with six MEs and two 2FIs, 9 of these model are not estimable since EC_2 equals 0.9143; there are 910 possible models with six MEs and three 2FIs, 229 of these model are not estimable since EC_3 equals 0.7473; there are 8190 possible models with six MEs and four 2FIs, 3870 of these model are not estimable since EC_4 equals 0.5275; there are 72072 possible models with six MEs and five 2FIs, 50184 of these models are not estimable since EC_5 equals 0.3037; there are 5460 possible models with six MEs and six 2FIs, 4762 of these models are not estimable since EC_6 equals 0.1279.

2.2.4 Projection Estimation Capacity (PEC), and Projection Information Capacity (PIC)

Loeppky et al., 2007 defined projection estimation capacity as $\rho_k(D)$ for a design, \mathcal{D} , to be the number of estimable models containing k MEs and their associated

2FIs. So, it could be represented as a sequence, PEC $(\rho_1, \rho_2, ..., \rho_g)$, where ρ_i is the proportion of estimable models that contain i MEs and their associated 2FIs. Li and Aggarwal, 2008, defined the PEC as an integer q, such that the second order model is estimable for every subset of q factors. The design that has large values for all the entries in the sequence is desirable. So, for comparing candidate designs, we should select the design that is maximizing the entries $(\rho_1, \rho_2, ..., \rho_g)$. The maximum value for ρ_i is 1 which means every possible model with iMEs and associated2FIs are estimable. For example, consider two designs 2^{6-2} , the first one with the generators (E = ABC, F = BCD). We denote this design as 16.6.1. The second one has the generators (E = ABC, F = ABCD), and we denote it as 16.6.2 (we showed these designs earlier). The projection estimation capacity for these design is shown in Table 6.

Table 6.: The projection estimation capacity *PEC* for designs 16.6.1, and 16.6.2

Designs	ρ_1	ρ_2	$ ho_3$	$ ho_4$	$ ho_5$	ρ_6
16.6.1	1	1	1	0.8	0	0
16.6.2	1	1	0.9500	0.7333	0.1667	0

Clearly from Table 6, we can see that design 16.6.1 outperforms design 16.6.2 with respect to PEC. The third entry of the PEC for 16.6.1 is 1, which is a larger than the third entry for 16.6.2. That means every possible model with k=3 MEs and associated 2FIs is estimable for design 16.6.1.

Sun, 1994, Li and Nachtsheim, 2000, and Mee et al., 2017 defined the Projection Information Capacity (PIC) as augmenting EC with the mean D-efficiency across all models of equal size.

2.2.4.1 Generalized Alias Length Pattern

Generalized Alias Length Pattern, GALP, was first produced by Cheng et al., 2008, as a measure of aliasing for 2FIs to strength 3 arrays. Mee, 2013, defined this criterion as the main diagonal of the matrix $(X'X/n)^2$, where X is the model matrix for the 2FIs model. The minimum values for GALP is 1, which indicates that the *ith* element column of the matrix (X'X/n) is uncorrelated with other columns of (X'X/n).

2.2.5 Minimal Dependent Sets

A minimal dependent set, or MDS, is a set of linearly dependent effects, such that if one of these effects is removed, all the effects in the resulting subset become linearly independent. Miller and Tang, 2012, defined the size of a MDS as the number of effects that are contained in the MDS. For example, consider a fractional factorial design with 6 factors and 16 runs. It is denoted as 2^{6-2} , such that the generators define as

$$E = (1/2)[AD + BD + ACDBCD], F = (1/2)[ADBD + CD + ABCD].$$

This design has 3, 10, 5, 8, and 4 MDSs of size 5, 6, 7, 8, and 9, respectively. One of the MDS of size 5 is $\{AD, AF, BD, BF, CE\}$. Based on the definition of MDS, a model containing all these effects is not estimable, but if we remove one of these effects, for example, if we remove AD, then a model containing $\{AF, BD, BF, CE\}$ is estimable. In this dissertation, in chapter 3, we will expand and investigate the concept of the MDSs in more details.

2.3 Model Selection

Model selection is an essential statistical technique, that simplifies the process of selecting the best model from a set of candidate models. The basic and simple model for data of observations y_i , n > k is given by

$$y_i = \beta_0 + \sum_{j=1}^m \beta_j x_{ij} + \varepsilon_i$$

where i = 1, 2, 3, ..., n, j = 1, 2, 3, ..., k, such that n is the run size, and k is the number of factors. x_{ij} represents the level of the factor x_j at the run i and β_j is the parameter of factor x_j , and it is assumed to not equal zero.

Various model selection procedures are founded. For example, all subset-selection procedure, step wise regression which include forward selection and backward elimination, and dantzig selection. These model selections follow specific criteria for model determination. For instance, R^2 , which defined as

$$R^2 = 1 - \frac{RSS}{TSS}$$

, where $RSS = (y - (X\hat{\beta})^T)(y - (X\beta)^T)$ is the residual sum of squares, and $TSS = \sum (y_i - \bar{y})^2$ is the total sum of squares, which measure the variation in the data. R^2 is not an appropriate criterion, since it is increasing as the number of variables included in the model is increasing. An alternative criterion is adjusted R^2 (Wherry, 1931). Adjusted R^2 is given by

$$R^{2} = 1 - \frac{RSS/(n-h-1)}{TSS/(n-1)}$$

, where n is the total number of observations, and h is the number of variables that are included in the model. The difference between R^2 and adjusted R^2 is the degree of freedom (n-h-1) in the numerator, and (n-1) in denominator. So, adjusted R^2

considers the reduction in the degrees of freedom for estimating the residual variance.

Another commonly used criterion is the C_p statistic (Mallows, 1973), which defines as

$$C_p = \frac{RSS}{s^2} - (n - 2p)$$

, where RSS is the residual sum of squares for a model, that contains p regression coefficients, with the intercept term β_0 , and s^2 is the mean square error for the full factorial model. Furthermore, two commonly used criteria, are Bayesian Information Criterion Schwarz et al., 1978, and Asymptotic Information Criterion Akaike, 1974. They are defined as

$$AIC = n \ln(RSS/n) + 2p$$

and

$$BIC = n \ln(RSS/n) + p \ln(n)$$

where, again, RSS is the residual sum of squares for a model, and p is the number of regression coefficients in the model. These criteria (AIC and BIC) are the most commonly criteria used in the stepwise regression (Wu and Hamada, 2011).

2.3.1 All Subset-Selection Procedure

All subset-selection procedure is one of the classical model selection procedures. It aims to evaluate every possible subset of factors. For example, if we have three independent variable x_1 , x_2 , and x_3 for a dependent variable Y which is the response, all possible simple linear models are as follows:

$$Y = \beta_0 + \varepsilon$$

$$Y_1 = \beta_0 + \beta_1 x_1 + \varepsilon_1$$

$$Y_2 = \beta_0 + \beta_2 x_2 + \varepsilon_2$$

$$Y_{3} = \beta_{0} + \beta_{3}x_{3} + \varepsilon_{3}$$

$$Y_{12} = \beta_{0} + \beta_{1}x_{1} + \beta_{2}x_{2} + \varepsilon_{12}$$

$$Y_{13} = \beta_{0} + \beta_{1}x_{1} + \beta_{3}x_{3} + \varepsilon_{13}$$

$$Y_{23} = \beta_{0} + \beta_{2}x_{2} + \beta_{3}x_{3} + \varepsilon_{23}$$

$$Y_{123} = \beta_{0} + \beta_{1}x_{1} + \beta_{2}x_{2} + \beta_{3}x_{3} + \varepsilon_{123}$$

For three predictors, we have $8 = 2^3$ models. In general, for h predictors, we have 2^h possible models.

2.3.2 Stepwise Regression

In fact, with a larger number of factors, the method of fitting a model for every subset of factors is impossible. Stepwise is alternative procedure, which, depends on sequentially adding or deleting the predictor (independent variable) x_i to the given model under a statistical value for the predictor, like mean squared error. The basic idea is to compare a current model with the new model, that is obtained by adding or deleting a predictor. Usually, the comparing of these two models conducts by calculating the F-statistic, which is define by

$$\frac{RSS_{\text{current mode}} - RSS_{\text{new model}}}{RSS_{\text{new model}}/\nu}$$

where, RSS is the residual sum of squares, and ν is the degree of freedom of the RSS of the new model. Stepwise regression has two main approaches: forward selection and backward elimination. Wu and Hamada, 2011

2.3.2.1 Forward Selection Procedure

Forward selection procedure is a stepwise regression, which starts with a model containing only the intercept, then sequential steps are started by adding one variable at a time. The added variable is the best choice based on a statistical criteria, which could be lowest p-value, lowest AIC, highest adjusted R^2 , largest F statistic, etc. After each step, a test is conducted on the new model for a selected statistical criterion, and these steps are repeated until this criterion stops improving. In the end, the selected variables will be the best selection for the final model (Wu and Hamada, 2011).

2.3.2.2 Backward Elimination Procedure

Backward elimination procedure is the opposite of forward selection. Instead of starting with a small number of variables, which is the intercept with forward selection, backward elimination starts with the full model that contains all the variables. Then, one insignificant variable is eliminated at a time, based on chosen criterion, and then this process repeats until no more variable can be dropped (Wu and Hamada, 2011).

2.3.3 Dantzig Selection Procedure

Dantzig selector is a shrinkage estimator. It was introduced by Candes, Tao, et al., 2007, as an estimator for model parameters for supersaturated design, where the number of run size n is less than the number of factors, k. For Dantzig selector, it should be assumed, that the true regression coefficients are sparse. Suppose we have observations $Y = X_1\beta + e$, for k factors, n run size, K_1 is the model matrix, K_2 is K_3 unknown parameter, and K_4 is K_4 unknown parameter, and K_4 is a solution to the K_4 -regularization problem

$$min \|\tilde{\beta}\|_{\ell_1}$$

, such that $\tilde{\beta} \in R^k$ subject to

$$||X_1 * r||_{\ell_{\infty}} \le (1 + t^{-1})\sigma$$

where r is the residual vector $Y - X_1 \tilde{\beta}$, and t is a positive scalar.

Berk, 2008, showed the following formulation for dantzig selector

$$\hat{\beta} = \min \sum_{j=1}^{k} |\beta|$$

subject to

$$\sum_{i=1}^{n} |x_{ij}r_i|$$

for j=1,2,...,k Berk, 2008, illustrated that the Dantzig selector uses the sum of the absolute values of the regression coefficients as an argument. The formula provided by Berk, 2008 aimed to minimizing the sum of the absolute values of the regression coefficients, such that if this sum is equal to zero, the associated predictors are removed from the analysis. Berk, 2008 advocated to restrict the amount $\sum_{i=1}^{n} |x_{ij}r_i|$ to a value λ . The main idea from restricted the amount $\sum_{i=1}^{n} |x_{ij}r_i|$ is, that this amount could captures any relation between the residual and each predictor. So, when $\sum_{i=1}^{n} |x_{ij}r_i| = 0$, that means the predictor has no relation to the residual, while if $\sum_{i=1}^{n} |x_{ij}r_i| > 0$, it means the predictor has relation with the residual and that will introduced a bias. By restricted the amount $\sum_{i=1}^{n} |x_{ij}r_i|$ to the value of λ , one can introduce different levels of the relation between the predictors and the residuals, as well different levels of bias for the estimated regression parameters Berk, 2008.

2.3.4 Group Lasso Procedure

Group lasso procedure introduced by Yuan and Lin, 2006 in order to allow for selection of group of active effects. Consider the general regression problem with K

factors:

$$Y = \sum_{j=1}^{K} X_k \beta_k + \epsilon,$$

where Y is a $n \times 1$ vector, $\epsilon \sim N(0, \sigma^2 I)$, X_k is a $n \times p_k$ matrix corresponding to the kth factor and β_k is a coefficient vector. The group lasso defined as the solution to

$$\frac{1}{2} \|Y - \sum_{k=1}^{J} X_k \beta_k \|^2 + \lambda \sum_{k=1}^{K} \|\beta_k\|_{K_k},$$

where $\lambda \geq 0$ is a tuning parameter, K_k is a positive definite matrices, and K is the number of positive definite matrices.

CHAPTER 3

CLASSIFICATION OF MINIMAL DEPENDENT SETS FOR DESIGN SELECTION AND ANALYSIS

3.1 Introduction

A minimal dependent set (MDS) for a fractional factorial design is a set of linearly dependent factorial effects, where if any one effect is removed from this set, the factorial effects in the resulting subset are linearly independent. Previous work has shown that the size of an MDS may have an impact on model discrimination and, thus, can be utilized to develop criteria for design selection; MDS-resolution and MDS-aberration are two examples. In this chapter, we investigate a new classification of MDSs and its impact on design selection and analysis. Both orthogonal and non-orthogonal designs will be considered. Via a simulation study, we see that as the number of factors in an MDS increases, power for active effect detection also increases.

A screening experiment is often an important first step in experimentation in order to determine which of many factors have an impact on a response variable of interest. Factorial effects (such as main effects MEs), and two-factor interactions (2FIs) that have a large impact on the response are called *active effects* and factors that are involved in one or more active effects are called *active factors*.

Two-level fractional factorial designs (FFDs) are widely used for screening experiments. Regular 2^{k-p} FFDs (Box and Hunter, 1961; Fries and Hunter, 1980) are easily the most common choice for screening experiments. These designs are straightforward to construct and have an aliasing structure that is well understood, in that any two factorial effects are either orthogonal or fully aliased. Nonregular designs, on

the other hand, have a more "complex" aliasing structure as factorial effects may be partially aliased (neither fully confounded or orthogonal). Despite this, nonregular designs offer considerable run size flexibility and have been shown to estimate more models than regular designs (Wu and Hamada, 2011).

The analysis of screening designs is typically guided by three empirical principles or regularities:

- 1. Effect sparsity: only a few of the many candidate factorial effects are truly active,
- 2. Effect hierarchy: MEs are more likely to be active than 2FIs, and 2FIs are more likely to be active than the three-factor interaction, and so forth,
- 3. Effect heredity: it is uncommon for an interaction to be active unless at least one of the factors involved is an active ME. Strong heredity indicates that a 2FI will be active only if both of its parent MEs are active. Weak heredity allows for an active 2FI to have at least one parent ME that is active (Chipman, 1996).

Numerous criteria exist for ranking and selecting screening designs; for a review, see Mee et al., 2017. One such criteria is based on the concept of minimal dependent sets (MDSs). An MDS is a set of linearly dependent effects, such that if one of the effects is removed, the remaining effects are estimable. Miller and Tang, 2012 showed a set of vectors, $V_1, V_2, ... V_m$ is an MDS if and only if V_m can be written as

$$V_m = a_1 V_1 + a_2 V_2 + \dots a_{m-1} V_{m-1}$$

where $a_1, a_2, ... a_{m-1}$ are nonzero constants. As an example, consider a 2^{6-2} nonregular design with generators E = (1/2)[AD + BD + ACD - BCD] and F = (1/2)[AD - BD + CD + ABCD] (Johnson and Jones, n.d.). This design has 30 MDSs involving

MEs and 2FIs; 3 MDS of size 5, 10 of size 6, 5 of size 7, 8 of size 8, and 4 of size 9. One MDS of size 5 is $\{D, AE, AF, BE, BF\}$. A model containing these five effects is not estimable. However, if we remove, say, BE, then a model containing the MEs and $\{D, AE, AF, BF\}$ is now estimable.

The concept of MDSs was first introduced by Miller and Sitter, 2004 and was used to evaluate partial aliasing of nonregular designs. Lin et al., 2008 also use MDS to assess nonorthogonal foldover designs. Moreover, Edwards, 2011 compare and rank semifoldover plans for orthogonal factorial designs based on the concept of MDSs. Miller and Tang, 2012 compare designs based on the size of an MDS (i.e. the number of factorial effects contained in an MDS). Miller and Tang, 2013 used MDSs to find optimal supersaturated designs.

Miller and Sitter, 2005 illustrated that difficulties in distinguishing between models can be determined by the form of the linear dependencies among effects. For more clarification, consider a 12-run nonorthogonal foldover design in 6 factors from Miller and Sitter, 2005. One of the MDS for this design is $\{AB, AC, BF, CF\}$ with the form of the linear dependency given by $cAB - cAC + cBF - cCF = \mathbf{0}$, where c is a scalar and $\mathbf{0}$ is a vector of zeros. Miller and Sitter, 2005 showed that if AB and AC are active effects and the coefficients for these effects have same size but opposite signs, then it may be difficult to distinguish a model containing $\{AB, AC\}$ from a model containing $\{BF, CF\}$. To see this, Miller and Sitter, 2005 illustrated a model of the form $y = 25 + 2A + 2B + 2C + 2F + \beta_{AB}AB + \beta_{AC}AC + \epsilon$, where $\epsilon \sim N(0, 1)$. Three scenarios for the coefficients β_{AB} , and β_{AC} were considered: (a) $\beta_{AB} = 2, \beta_{AC} = 2$; (b) $\beta_{AB} = 2, \beta_{AC} = -4$; and (c) $\beta_{AB} = 2, \beta_{AC} = -2$. It was shown that for (a) and (b), a model that involves $\{AB, AC\}$ is superior to other two-factors models that were considered. For scenario (c), however, the model involving $\{AB, AC\}$ has R^2 equals to 0.975 while a model involving $\{BF, CF\}$ has R^2 equals to 0.974. Thus, it

is difficult to distinguish between these two models.

In addition, Miller and Sitter, 2004 studied the difficulty of model discrimination through the concept of MDSs. For example, consider Placket-Burman design with n=12 and k=5 from Miller and Sitter, 2004. The MDSs for this design are as follows:

$$D + E + AB - AC - BD - CE,$$

$$C - D - AB - AD + BE + CE,$$

$$C + E - AC - AD - BD + BE,$$

$$B - C + AD + AE - BE - CD,$$

$$B - D - AB + AE - CD + CE,$$

$$B + E - AC + AE - BD - CD,$$

$$A - E + AC - BC + BD - DE,$$

$$A + D + AB - BC - CE - DE,$$

$$A + C - AD - BC + BE - DE,$$

$$A + B + AE - BC - CD - DE.$$

Miller and Sitter, 2004 showed that the following five pair of 2FIs: (AB, CE), (AC, BD), (AD, BE), (AE, CD), and (BC, DE) occur in 4 MDSs. Thus, if the true model involves one of these pairs, then it may be difficult to distinguish it from four other models. While, if the true model involves a pair of 2FIs that isn't one of these five pairs, then it may be difficult to distinguish it from only one other model. For instance, a model containing $\{AB, CE\}$ is difficult to distinguish from a model containing (AC, BD), a model containing (AD, BE), a model containing (AB, CE) is a model containing (AB, DE) is

difficult to distinguish from a model containing (BC, CE). In this case, MDSs help to narrow down the set of the candidate models to identify the true model.

Lin et al., 2008 explored the relationship between MDS and resolvability, and they showed that MDS for design provides a clearer assessment of the design's ability to distinguish computing models compared to resolvability. Lin et al., 2008 showed that as the size of an MDS increases, its impact on model discrimination decreases.

The size of an MDS for a regular design is always 2. The factorial effects contained in this MDS are fully confounding, thus, the correlation for these effects is either -1 or 1. In this case, this MDS may make a pair of models that could be impossible to distinguish between. On the other hand, the size of an MDS for a nonregular design differs from 2. The correlation for the factorial effects in this MDS is ± 1 or ranges in values between -1 and +1, which indicates partial aliasing. In this case, the MDS tends to spread the correlation among the effects, which leads to an increase in the design's ability for estimating models. For example, consider this design where k=6, and n=16, shown in Table 7.

Table 7.: Design with k=6 factors, and n=16

This design has six MDS for the 2FI model. These MDSs are:

$$A - BE,$$

$$B - AE,$$

$$E - AB,$$

$$D + AD + BD - 2CF - DE,$$

$$C + AC + BC - CE - 2DF$$
,
 $F + AF + BF - 2CD - EF$.

Clearly, three of these MDSs are of size 2 and three are of size 5. In Figure 3, there are three off-diagonal elements corresponding to the following pairs of effects: (A, BE), (B, AE), (E, AB). Obviously, the factorial effects in each of these pairs are fully aliasing; consequently, three MDSs of size 2. With, for example, the MDS $\{A, BE\}$, by MDS definition, a model containing the MEs and these effects is not estimable. However, if we remove, say, A, then a model containing the MEs and BE is now estimable. Thus, this MDS identifies two models that are indistinguishable. Back to Figure 1, the remaining 12 off-diagonal elements correspond to three alias sets. Each set involves one ME and four2FIs, such as (D, AD, BD, CF, DE). Therefore, three MDSs of size 5 are produced. An MDS of size 5 identifies 5 models, each containing one effect, where one might have a problem in distinguishing between two models as shown earlier.

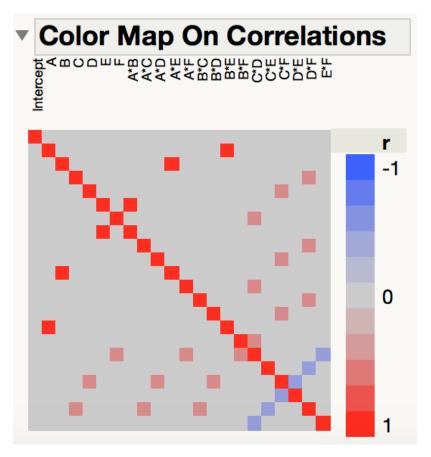


Fig. 3.: MDSs of size 2, and 5 for the design in Table 7

Each MDS has its own special characteristics for the size and number of factors involved. The question that arises is whether the number of factors that are involved in the MDS has an impact on active effects detection. Mee et al., 2017 compared the Estimation Capacity (EC), for two different designs with k=7 based on the concept of MDSs. They showed that the superior design has 3 MDSs of size 8, such that 2 of these MDSs involve 7 factors. In contrast, the other design has 3 MDSs of size 6, where 2 of these MDSs involve only 5 factors. This work shows that there is a difference between MDSs. This difference relates to the number of factors in the MDS, which has an impact on the design's ability for estimating models. Thus, in this article, we suggest a new classification criterion for MDSs and investigate the ability

of this criterion to distinguish designs with respect to their ability to identify active effects. This criterion could be considered as a measurement for the design's ability of active effects detection, which aims to improve the design selection and analysis. The remainder of this chapter is organized as follows. In Section 3.2, we provide a review of the MDSs-criteria, which are MDS-word length pattern, MDS-resolution, and MDS-aberration. In Section 3.3, we provide a new suggested classification for MDSs that incorporates specific information regarding the number of factors and effects in each MDS. Section 3.4 presents a simulation study and the results. Section 3.5 concludes the chapter.

3.2 Current MDSs Criteria

Lin et al., 2008 used the concept of MDSs to introduce MDS-resolution and MDS-aberration. Edwards, 2011 compared and ranked semifoldover plans for orthogonal designs based on MDS-resolution and MDS-aberration. To understand these criteria, Lin et al., 2008 introduced MDS-word length pattern (MDS-wlp) $(A_1, A_2, ... A_k)$ where A_i represents the number of MDSs of size i. For example, if we have MDS-word length pattern (0,0,0,2,5,4), this indicates a design has no MDSs of size 1, 2, and 3, but it has 2 MDSs of size 4, 5 MDSs of size 5 and 4 MDSs of size 6. MDS-resolution is defined to be the smallest size MDS of a design. For instance, MDS-resolution for a design with MDS-word length pattern represented by (0,0,0,2,5,4) is 4. MDS-aberration depends on sequential minimization of the entries for MDS-word length pattern. For example, if two designs have sequences of MDS-word length pattern, as follows:

$$(A_{1_1}, A_{2_1}, A_{3_1}, ..., A_{j_1}, ..., A_{m_1}),$$

$$(A_{1_2}, A_{2_2}, A_{3_2}, ..., A_{j_2}, ..., A_{m_2}),$$

where $A_{j_{1,2}}$ is the number of MDSs of size j for design 1 and 2, respectively, then the design that has smallest entry, A_j , is a less MDS-aberration design. In contrast, a design is said to have a minimum MDS-aberration if there is no design which has less MDS-aberration than this design. For example, if we consider MDS-word length pattern as follows (0,0,1,0,2), and (0,0,1,1,3), both of these MDS-word length patterns represent designs which have MDS-resolution 3. However, the fourth entry in the first sequence is less than the fourth entry for the second sequence. Therefore, the design with the first MDS-word length pattern is the best based on the MDSaberration.

From the work of Mee et al., 2017, consider orthogonal and nonorthogonal designs with k=7 and n=20 that are shown in Table 8. Orthogonal designs denote as 20.7.1, 20.7.2, and 20.7.3, and nonorthogonal designs denote as 20.7BayesD, 20.7PEC, and 20.7MEPI. Design 20.7BayesD is Bayesian D-optimal design with k=7 and n=20 (DuMouchel and Jones, 1994). 20.7PEC is projection estimation capacity optimal design with k=7 and n=20, which seek, to optimize evaluation of models with all the MEs and all the 2FIs in subsets of factors (Smucker and Drew, 2015). 20.7MEPI is the ME plus interaction optimal design with k=7 and n=20, which tends to optimize evaluation of models with all the MEs and a number of selected 2FIs (DuMouchel and Jones, 1994; Smucker and Drew, 2015).

Table 8.: Orthogonal and non-orthogonal designs

			20.7.1								20.7.2	:					:	20.7.3	;		
$\Gamma - 1$	-1	-1	-1	-1	-1	-17	Г	-1	-1	-1	-1	-1	-1	-17	$\Gamma - 1$	-1	-1	-1	-1	-1	-17
-1	-1	-1	-1	-1	1	1		-1	-1	-1	-1	-1	1	1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	1	-1	1	- 1	-1	-1	-1	-1	1	-1	1	-1	-1	-1	-1	1	1	1
-1	-1	1	1	-1	-1	1	- 1	-1	-1	1	1	-1	-1	1	-1	-1	1	1	-1	-1	1
-1	-1	1	1	1	1	-1		-1	-1	1	1	1	1	-1	-1	-1	1	1	1	1	-1
-1	1	-1	1	-1	-1	1	- 1	-1	1	-1	1	-1	-1	-1	-1	1	-1	1	-1	1	1
-1	1	-1	1	1	1	-1	-	-1	1	-1	1	1	1	-1	-1	1	-1	1	1	-1	-1
-1	1	1	-1	-1	1	-1	- 1	-1	1	1	-1	-1	1	1	-1	1	1	-1	-1	1	1
-1	1	1	-1	1	-1	-1	- 1	-1	1	1	-1	1	1	-1	-1	1	1	-1	1	1	-1
-1	1	1	1	1	1	1	İ	-1	1	1	1	1	-1	1	-1	1	1	1	1	-1	1
1	-1	-1	1	-1	1	-1	i	1	-1	-1	1	-1	1	-1	1	-1	-1	1	-1	1	-1
1	-1	-1	1	1	-1	-1	i	1	-1	-1	1	1	-1	1	1	-1	-1	1	1	1	1
1	-1	1	-1	-1	1	-1	ı	1	-1	1	-1	-1	1	-1	1	-1	1	-1	-1	1	1
1	-1	1	-1	1	1	1	- 1	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	-1	1
1	-1	1	1	1	-1	1	1	1	-1	1	1	1	1	1	1	-1	1	1	1	-1	-1
1	1	-1	-1	1	-1	-1	1	1	1	-1	-1	1	-1	-1	1	1	-1	-1	1	-1	1
1	1	-1	-1	1	1	1	- 1	1	1	-1	-1	1	1	1	1	1	-1	-1	1	1	-1
1	1	-1	1	-1	1	1	- 1	1	1	-1	1	-1	1	1	1	1	-1	1	-1	-1	1
1	1	1	-1	-1	-1	1		1	1	1	-1	-1	-1	1	1	1	1	-1	-1	-1	-1
L 1	1	1	1	-1	-1	-1	L	. 1	1	1	1	-1	-1	-1	L 1	1	1	1	-1	1	-1

$20.7 \mathrm{BayesD}$	20.7PEC	20.7MPEI
Γ 1 1 -1 -1 -1 -1 -17	Γ 1 -1 -1 1 -1 1 17	$\lceil 1 1 1 -1 -1 1 1 \rceil$
1 -1 1 1 1 1 -1	$\begin{vmatrix} -1 & 1 & -1 & 1 & -1 & 1 & -1 \end{vmatrix}$	$\begin{vmatrix} -1 & -1 & -1 & -1 & -1 & -1 \end{vmatrix}$
	1 1 1 1 1 1 -1	-1 1 1 -1 1 -1 -1
-1 -1 1 1 -1 -1	1 -1 1 1 1 -1	-1 -1 1 -1 1 1 1
1 -1 1 -1 1 -1	1 1 1 -1 -1 1 1	1 1 -1 1 -1 -1
1 1 -1 1 1 -1 1		
$\begin{bmatrix} -1 & 1 & -1 & 1 & -1 & 1 & -1 \end{bmatrix}$	$\begin{bmatrix} -1 & 1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix}$	1 -1 1 -1 1 -1 1
	1 1 -1 -1 1 -1	1 -1 1 -1 1 -1
	$\begin{bmatrix} -1 & 1 & 1 & -1 & -1 & -1 \end{bmatrix}$	$\begin{vmatrix} -1 & 1 & 1 & -1 & -1 & 1 \end{vmatrix}$
1 -1 -1 1 -1 1	$\begin{vmatrix} -1 & -1 & -1 & -1 & 1 & -1 \end{vmatrix}$	-1 -1 1 1 -1 -1 1
$\begin{vmatrix} -1 & -1 & -1 & -1 & 1 & -1 \end{vmatrix}$	$\begin{vmatrix} -1 & -1 & -1 & 1 & 1 & -1 & 1 \end{vmatrix}$	$\begin{vmatrix} -1 & -1 & -1 & 1 & 1 & 1 & -1 \end{vmatrix}$
1 1 -1 -1 1 1	1 1 1 1 -1 -1 1	1 -1 1 1 1 -1 -1
-1 1 1 1 1 -1	1 -1 -1 1 -1 -1	-1 1 -1 1 1 -1 1
1 1 1 -1 1 -1	-1 -1 -1 1 1 1 -1	1 -1 -1 -1 1
-1 1 1 1 -1 -1 1	1 1 -1 1 1 -1 -1	
$\lfloor -1 1 -1 -1 1 1 -1 \rfloor$		$\lfloor -1 1 -1 -1 1 -1 \rfloor$

The MDS-word length pattern, and the MDS-resolution for designs in Table 8 are given in Table 9. For the orthogonal designs, both design 20.7.1 and 20.7.2 outperform design 20.7.3 based on MDS-resolution. They both have maximum value for MDS-resolution, which equals to 8. In this case, we need to look for MDS-aberration for these designs, since MDS-resolution does not help to distinguish these designs. Based on MDS-aberration, design 20.7.1 is the best, since it has the least number of MDSs of size 8. On the other hand, design 20.7PEC has the maximum value for MDS-resolution among non-orthogonal designs. Thus, it is the winning design among other non-orthogonal designs and also, among all the designs (orthogonal and non-

orthogonal). Although, 20.7PEC is the best design based on the MDS-resolution but it may not be the best design for detection the active effects, Mee et al., 2017 showed that 20.7.1 is the recommended design on detective the active effects.

Table 9.: MDS word length pattern, and MDS-resolution for the designs in Table 8

Design	MDS word length pattern	MDS-resolution
20.7.1	(0, 0, 0, 0, 0, 0, 0, 1, 0, 6, 4, 26, 45, 118, 286, 1001, 3327, 326, 71776, 372469)	8
20.7.2	(0, 0, 0, 0, 0, 0, 0, 3, 0, 2, 2, 22, 30, 97, 297, 912, 3286, 14472, 73360, 428009)	8
20.7.3	(0, 0, 0, 0, 0, 4, 0, 11, 2, 29, 12, 112, 220, 762, 1718, 5657, 20072, 65300, 221300)	6
20.7 BayesD	(0, 0, 0, 0, 0, 0, 0, 0, 1, 2, 5, 5, 20, 56, 138, 376, 1338, 5330, 23829, 129439)	9
20.7MPEI	(0, 0, 0, 0, 0, 10, 0, 5, 2, 17, 8, 17, 21, 32, 51, 201, 605, 2235, 7157, 22235)	6
20.7PEC	(0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 2, 4, 9, 15, 39, 112, 338, 1405, 6593, 38654, 301524)	10

Not in all cases of comparison between designs, MDS-resolution and MDS-aberration are able to distinguish between designs. Consider the following situation: if we have two designs with MDS word-length pattern, as shown below:

$$(A_{1_1}, A_{2_1}, A_{3_1}, ..., A_{j_1}, ..., A_{m_1}),$$

$$(A_{1_2}, A_{2_2}, A_{3_2}, ..., A_{j_2}, ..., A_{m_2}),$$

where, $A_{j_1} = A_{j_2}$, such that A_{j_1} , and A_{j_2} is the number of MDSs of size j for design 1, and 2 respectively. Then, the question that arises is, which design is better? Thus, there is still a need to explore and develop new features for MDSs. It seems useful to explore the number of factors in MDSs, especially when comparing designs that have minimum MDS aberrations. Lin et al., 2008 showed that the small MDS has a destructive impact on the model discrimination, more than the large MDS. Investigating the influence of the number of factors that are involved in each MDS of a design can easily lead to similar thoughts. What is the difference between an MDS which has a greater number of factors, and another MDS which has fewer factors? In particular, what effect does this difference have on active effect detection? These questions led to the establishment of a new classification for MDSs that incorporates

specific information regarding the number of factors and effects in an MDS. The next section provides the new suggested classification of MDSs.

3.3 Classification Suggested for the MDSs

Our purpose in this chapter is to suggest a new classification criterion for MDSs and investigate the ability of this criterion to distinguish designs with respect to their ability to identify active effects. To achieve this aim, we provide a classification for the MDSs that focuses on the appearance of the factors at each MDS. We only consider MDSs that involve MEs and 2FIs, since they are the most important effects. Our classification tends to divide an MDS into 2 subsets. The first subset contains only MEs, and the second subset contains only 2FIs. Then, we count the common factors among MEs and 2FIs subsets, the unique factors that appeared at the MEs subset, and the unique factors that appeared at the 2FIs subset. Thus, an MDS can be represented as h: (l, m, f), where

- 1. h represents the size of an MDS.
- 2. *l* represents the number of common factors that appear in the MEs and 2FIs subsets.
- 3. m represents the number of factors that appear only in MEs subset.
- 4. f represents the number of factors that appear only in 2FIs subset.

For example: consider design 20.7.1, shown in Table 2. One of its MDSs of size 12 is $\{A, B, C, G, AD, BC, BE, CF, DG, EF, EG, FG\}$. Clearly, this MDS contains two subsets. The first one is $\{A, B, C, G\}$, which represents the MEs subset, and the second one is $\{AD, BC, BE, CF, DG, EF, EG, FG\}$, which represents the 2FIs subset. The MEs subset contains 4 factors, while the 2FIs subset contains 7 factors. There

are four common factors between the MEs and 2FIs subsets $\{A, B, C, G\}$. There is no factor that showed up only at the MEs subset. There are 3 factors that appeared only at 2FIs subset $\{D, E, F\}$. Thus, this MDS of size 12 represented as 12: (4,0,3). Also, consider another MDS for design 20.7.3 of size 6 $\{AE, AG, BF, BG, CE, CF\}$. This MDS does not have MEs. All the factorial effects are 2FIs. Therefore, there are no common factors between the MEs and 2FIs subsets. The number of factors that show up only at the MEs subset is zero, and the number of factors that show up only at the 2FIs subset is 6. Thus, this MDS represented as 6: (0,0,6). For orthogonal and non-orthogonal designs, introduced earlier in Section 2, there are a variety of MDS sizes and types. Tables 10 and 11 list the MDSs classifications of these designs, respectively. We used R software to generate code for MDSs classification which is shown in the Appendix section for this chapter. In this regards, we used the circuits function in the software 4ti2 team, n.d. to generate the MDSs for the MEs and 2FIs for a design.

Table 10.: The categorization for MDSs to orthogonal designs that are shown in Table $8\,$

	20.7.1		20.7.2		20.7.3
h:(l,m,f) 8:(2,0,5) 10:(2,0,5) 10:(4,0,1) 11:(0,1,5) 11:(1,0,6) 11:(4,0,2) 12:(0,0,6) 12:(3,0,4) 12:(4,0,3) 12:(4,0,3) 12:(4,1,2) 13:(1,0,6) 13:(2,0,5) 13:(3,0,4) 13:(4,0,3) 13:(4,0,3) 13:(4,0,3) 13:(6,0,1) 14:(0,1,6) 14:(0,1,6) 14:(0,1,6) 14:(2,0,5) 14:(3,0,4) 14:(4,0,3)	20.7.1 number of h:(l,m,f) 1 2 1 2 1 2 1 4 4 4 4 4 1 8 8 8 1 2 2 1 4 4 4 4 2 3 5 40 20	h:(1,m,f) 8:(2,0,5) 10:(4,0,1) 11:(0,1,6) 11:(4,0,2) 12:(0,0,7) 12:(1,0,6) 12:(2,0,5) 12:(4,0,3) 12:(4,1,2) 13:(1,0,6) 13:(2,0,5) 13:(3,0,4) 13:(5,0,2) 14:(2,0,5) 14:(2,0,5) 14:(3,0,4) 14:(4,0,3) 14:(4,1,2) 14:(4,0,3) 14:(4,0,3)	20.7.2 number of h:(l,m,f) 3 2 1 1 3 6 8 4 1 4 8 6 8 2 2 2 16 8 18 39 1 14 1	h:(l,m,f) -6:(0,0,6) 8:(0,0,6) 8:(2,0,5) 9:(2,0,5) 10:(0,0,7) 10:(2,0,5) 10:(4,0,1) 11:(2,0,5) 12:(0,0,6) 12:(0,0,6) 12:(2,0,5) 12:(3,0,4) 13:(2,0,5) 13:(2,0,5) 13:(2,0,5) 13:(2,0,5) 13:(2,0,5) 13:(2,0,5) 13:(2,0,5) 13:(3,0,4) 13:(4,0,3) 14:(4,0,3) 14:(4,0,3) 14:(4,0,3) 14:(4,0,3) 14:(4,0,3) 14:(4,0,3) 14:(4,0,3) 14:(4,0,3)	20.7.3 number of h:(l,m,f) 4 3 8 2 6 20 3 112 6 6 70 8 222 120 4 46 50 248 87 4 30 238
14: (4, 1, 2) 14: (5, 0, 2) 14: (6, 0, 1) 14: (7, 0, 0) 15: (0, 0, 7) 15: (1, 0, 6) 15: (2, 0, 5) 15: (3, 0, 4) 15: (5, 0, 1) 15: (5, 0, 2) 15: (5, 0, 1) 15: (7, 0, 0) 16: (1, 0, 6) 16: (2, 0, 5) 16: (2, 1, 4) 16: (3, 0, 4) 16: (4, 0, 2) 16: (4, 0, 3) 16: (4, 1, 2) 16: (6, 0, 0) 16: (6, 0, 0) 16: (6, 0, 0) 16: (7, 0, 0) 16: (7, 0, 0) 16: (8, 0, 0) 16: (9, 0, 0) 16: (9, 0, 0) 16: (9, 0, 0) 16: (9, 0, 0) 16: (9, 0, 0) 16: (9, 0, 0) 16: (9, 0, 0) 17: (9, 0, 0)	1 12 6 2 2 2 11 30 90 89 2 2 29 2 23 8 9 83 4 338 2 319 2 167 2 63 4 8 2 33 33 4 33 4 34 35 36 37 38 48 48 57 57 57 57 57 57 57 57 57 57	15:(1,0,6) 15:(2,0,5) 15:(2,1,4) 15:(3,0,4) 15:(3,1,3) 15:(4,0,3) 15:(5,0,2) 15:(6,0,1) 16:(1,0,6) 16:(2,0,5) 16:(3,0,4) 16:(4,0,2) 16:(4,0,2) 16:(4,0,2) 16:(4,1,2) 16:(5,0,2) 16:(6,0,1) 16:(7,0,0) 17:(1,0,6) 17:(2,0,4) 17:(4,0,2) 17:(4,0,3) 17:(4,0,3) 17:(4,0,3) 17:(5,0,1) 17:(5,0,1) 17:(5,0,1)	25 68 2 82 2 80 36 2 16 99 224 2 352 2 160 53 4 22 4 308 850 2 1078	14:(4, 1, 2) 14:(4, 2, 1) 14:(5, 0, 2) 14:(6, 0, 1) 15:(0, 0, 7) 15:(2, 0, 5) 15:(2, 1, 4) 15:(3, 0, 4) 15:(3, 1, 3) 15:(4, 1, 2) 15:(5, 0, 2) 15:(6, 0, 1) 15:(7, 0, 5) 16:(2, 1, 4) 16:(3, 1, 3) 16:(4, 1, 2) 16:(5, 0, 2) 16:(5, 1, 1) 16:(6, 0, 1) 16:(6, 0, 1) 17:(2, 0, 5) 17:(2, 0, 5) 17:(2, 0, 5) 17:(2, 0, 5)	4 2 108 41 24 398 4 260 4 704 4 314 4 2 638 4 808 20 2310 24 1522 8 272 51 6 794 8
17: (1, 0, 6) 17: (1, 1, 1, 5) 17: (2, 0, 4) 17: (2, 0, 4) 17: (2, 0, 4) 17: (3, 0, 4) 17: (3, 0, 4) 17: (3, 0, 3) 17: (4, 0, 3) 17: (4, 0, 3) 17: (5, 0, 1) 17: (5, 0, 2) 17: (5, 1, 1) 17: (6, 0, 1) 17: (6, 0, 0) 18: (1, 0, 6) 18: (2, 0, 5) 18: (3, 0, 4) 18: (4, 0, 3) 18: (5, 0, 1) 18: (5, 0, 1) 18: (6, 0, 1) 18: (7, 0, 0) 19: (1, 0, 6) 19: (2, 0, 5) 19: (3, 0, 4) 19: (4, 0, 3) 19: (4, 0, 3) 19: (4, 0, 3) 19: (5, 0, 1) 19: (5, 0, 1)	33 1 4 130 2 646 4 1300 2 648 75 18 270 2 32 12 314 2000 4736 4 4686 4 1890 6 272 48 798 5892 4	17:(6, 0, 1) 17:(6, 0, 1) 17:(7, 0, 0) 18:(1, 0, 6) 18:(2, 0, 5) 18:(3, 0, 4) 18:(3, 1, 3) 18:(4, 0, 3) 18:(4, 0, 3) 18:(5, 0, 1) 18:(5, 0, 1) 18:(5, 1, 1) 18:(6, 0, 1) 18:(7, 0, 0) 19:(1, 0, 6) 19:(2, 0, 5) 19:(3, 0, 4) 19:(4, 0, 2) 19:(4, 0, 3) 19:(4, 0, 3) 19:(4, 1, 2) 19:(5, 0, 1) 19:(5, 0, 1) 19:(6, 0, 0) 19:(7, 0, 0) 20:(2, 0, 5) 20:(2, 0, 5) 20:(3, 0, 4)	234 2 12 26 630 2448 4 4548 8 4 4497 20 2094 4 189 12 994 6556 4 18318 8 4 27698 68 17344 20 2334 362 15172	17:(3, 0, 4) 17:(3, 1, 3) 17:(4, 0, 3) 17:(4, 1, 2) 17:(5, 0, 2) 17:(5, 0, 1) 17:(5, 0, 2) 17:(6, 0, 1) 17:(6, 0, 1) 17:(7, 0, 0) 18:(2, 0, 5) 18:(3, 0, 4) 18:(4, 0, 2) 18:(4, 1, 2) 18:(5, 0, 1) 18:(5, 0, 1) 18:(6, 0, 0) 18:(7, 0, 0) 19:(4, 0, 3) 19:(4, 1, 2) 19:(5, 0, 1) 19:(5, 0, 1) 19:(6, 0, 0) 19:(6, 0, 0) 19:(6, 0, 0) 19:(6, 0, 0)	1846 12 6678 100 36 7480 88 88 2694 22 308 926 2136 12 12048 152 12 27822 248 12 18310 134 3488 18512 80 12 75936 396 60 90242
19: (4, 0, 2) 19: (4, 1, 2) 19: (5, 0, 1) 19: (5, 0, 2) 19: (5, 0, 1) 19: (6, 0, 1) 19: (6, 0, 1) 19: (7, 0, 0) 20: (1, 0, 6) 20: (2, 0, 5) 20: (3, 0, 4) 20: (4, 1, 2) 20: (5, 0, 1) 20: (5, 0, 1) 20: (5, 0, 1) 20: (6, 0, 0) 20: (6, 0, 1) 20: (6, 0, 1) 20: (6, 0, 1) 20: (7, 0, 0)	18040 12 4 27561 57 16034 16 3310 48 2132 16006 64470 5 1 133252 119 1 121517 158 34760	20: (4, 0, 3) 20: (4, 1, 2) 20: (5, 0, 1) 20: (5, 0, 2) 20: (5, 1, 1) 20: (6, 0, 0) 20: (6, 0, 1) 20: (6, 1, 0) 20: (7, 0, 0)	79630 8 4 152914 162 15 134511 210 45021	19:(6, 1, 0) 19:(7, 0, 0)	588 35474

Table 11.: The categorization for MDSs to non-orthogonal designs that are shown in Table 3

20	0.7 BayesD	I	20.7PEC		20.7MEPI
h:(l,m,f) 9:(2,0,5) 10:(2,0,5)	number of $h:(l,m,f)$ 1	h:(l,m,f) 10:(2, 0, 5)	number of h:(l,m,f)	h:(l,m,f) 6:(0,0,6)	number of h:(l,m,f)
10:(2, 0, 5) 11:(1, 0, 6)	2 1	10:(2, 0, 5) 11:(0, 0, 7) 11:(2, 0, 5)	1 1	8:(0, 0, 6) 8:(0, 0, 7)	$\begin{bmatrix} 1 \\ 4 \\ 2 \end{bmatrix}$
10:(2, 0, 3) 11:(1, 0, 6) 11:(2, 0, 5) 11:(4, 0, 2) 11:(4, 0, 3) 12:(2, 0, 5) 12:(3, 0, 4) 12:(3, 1, 3)	1 1 2	12:(0, 0, 6) 12:(0, 0, 7)	1 1	8:(0,0,7) 9:(0,0,7) 10:(0,0,6)	2
12:(2, 0, 5)	2 3 2 1	12:(2, 0, 5) 12:(4, 0, 3) 13:(2, 0, 5)	1 1	10:(0, 0, 7) 11:(0, 0, 7)	15 8 2
12:(3, 1, 3)	1 1	13:(3, 0, 3)	6 1 1	12:(0, 0, 6) 12:(0, 0, 7) 12:(4, 0, 3)	14 1
12: (3, 0, 4) 12: (3, 1, 3) 12: (4, 0, 2) 12: (4, 0, 3) 13: (2, 0, 5) 13: (3, 0, 4) 13: (4, 0, 3)	4	13:(5, 0, 2)	1 1 12	13:(0, 0, 7)	20 1
13:(3, 0, 4) 13:(4, 0, 3)	3 8 5 2 2	13: (4, 0, 3) 13: (5, 0, 2) 14: (2, 0, 5) 14: (2, 1, 4) 14: (4, 0, 3)	1 1	14:(0, 0, 7)	18 13
13:(5,0,2) 13:(6,0,1)	2 2	14:(5, 0, 2)	1 14	14:(5, 0, 2) 15:(0, 0, 7)	1 4
13: (3, 0, 4) 13: (4, 0, 3) 13: (5, 0, 2) 13: (6, 0, 1) 14: (2, 0, 5) 14: (3, 0, 4)	8 24 20	14: (5, 0, 2) 15: (2, 0, 5) 15: (3, 0, 4) 15: (4, 0, 3)	6	15:(4, 0, 3)	42 5
14:(4, 0, 3) 14:(5, 0, 1)	1 3	15: (3, 0, 4) 15: (4, 0, 3) 15: (5, 0, 2) 16: (0, 0, 7) 16: (2, 0, 5) 16: (3, 0, 4)	17 2 1	16:(5, 0, 2)	156 45
15:(0, 0, 7) 15:(2, 0, 5)	1 9	16:(2, 0, 5) 16:(3, 0, 4) 16:(4, 0, 3)	27 28 42	17:(4, 0, 3) 17:(5, 0, 2) 17:(5, 1, 1)	491 107 1
14: (5, 0, 1) 14: (5, 0, 2) 15: (0, 0, 7) 15: (2, 0, 5) 15: (3, 0, 4) 15: (4, 0, 3)	36 58	16:(5, 0, 2) 16:(6, 0, 1)	12 2 45	17:(6, 0, 1) 18:(4, 0, 3)	6 1408
15:(4, 0, 3) 15:(5, 0, 2) 15:(6, 0, 1)	29 5	17:(2, 0, 5) 17:(3, 0, 4)	45 83	18:(5, 0, 2) 18:(5, 1, 1)	654
16:(1,0,6) 16:(2,0,5)	1 18	17:(4, 0, 3)	126 67	18:(6, 0, 1)	171 2858
16:(3, 0, 4) 16:(4, 0, 2)	90 3 128	17:(6, 0, 1) 17:(7, 0, 0)	16 1	19:(5, 0, 2) 19:(5, 1, 1) 19:(6, 0, 1)	2011
16:(4, 0, 3) 16:(4, 1, 2) 16:(5, 0, 2)	1 1 108	18:(2, 0, 5) 18:(3, 0, 4)	67 281 521	19:(6, 0, 1) 20:(5, 0, 2) 20:(5, 1, 1) 20:(6, 0, 1)	2277 4036
16:(6, 0, 1) 16:(7, 0, 0)	26 1	18:(4, 0, 3) 18:(5, 0, 2) 18:(6, 0, 1)	402 125	20:(6, 0, 1)	21 18178
15: (5, 0, 2) 15: (6, 0, 1) 16: (1, 0, 6) 16: (2, 0, 5) 16: (3, 0, 4) 16: (4, 0, 2) 16: (4, 0, 3) 16: (4, 1, 2) 16: (5, 0, 1) 16: (7, 0, 0) 17: (1, 0, 6) 17: (2, 0, 5) 17: (3, 0, 4) 17: (4, 0, 3) 17: (4, 0, 3) 17: (4, 1, 2)	3 46	18: (6, 0, 1) 18: (7, 0, 0) 19: (2, 0, 5) 19: (3, 0, 4)	9 129		
17:(3,0,4) 17:(4,0,2)	236 1	19:(3, 0, 4) 19:(4, 0, 2) 19:(4, 0, 3)	782 1		
17:(4,0,3) $17:(4,1,2)$	452 2 2	19:(5, 0, 2)	2098 2455		
17:(4, 0, 3) 17:(4, 1, 2) 17:(5, 0, 1) 17:(5, 0, 2) 17:(5, 1, 1)	443 6	19:(6, 0, 1) 19:(6, 1, 0) 19:(7, 0, 0) 20:(2, 0, 5)	980 2		
	2 129	1 20.(3 0 4)	146 197 2167		
17:(6, 0, 1) 17:(6, 1, 0) 17:(7, 0, 0) 18:(1, 0, 6)	$\begin{array}{c} 2\\14\end{array}$	20: (4, 0, 3) 20: (4, 1, 2) 20: (5, 0, 2) 20: (5, 1, 1)	8507 2		
18:(2, 0, 5)	6 112	20:(5, 0, 2) 20:(5, 1, 1) 20:(6, 0, 1)	14817 6		
18:(3, 0, 4) 18:(3, 1, 3)	694	20:(6, 0, 1)	10633 11		
18:(3, 1, 3) 18:(4, 0, 3) 18:(4, 1, 2) 18:(5, 0, 2)	1524 5 1861	20:(7, 0, 0) 21:(2, 0, 5) 21:(3, 0, 4)	2314 164		
18:(5, 1, 1) 18:(6, 0, 1)	10 977	21:(4,0,3)	4084 31539 96215		
18:(6, 1, 0) 18:(7, 0, 0)	5 134	21:(5, 0, 2) 21:(5, 1, 1) 21:(6, 0, 0)	96215 17 4		
19:(1, 0, 6) 19:(2, 0, 5) 19:(3, 0, 4)	12 252	21:(6, 0, 1)	120194 59		
19:(3, 0, 4) 19:(3, 1, 3) 19:(4, 0, 3)	1854	21:(6, 1, 0) 21:(7, 0, 0)	49248		
19:(4, 0, 3) 19:(4, 1, 2)	5831 10				
19:(4, 1, 2) 19:(5, 0, 2) 19:(5, 1, 1) 19:(6, 0, 1)	8728 14 5916				
19:(6, 1, 0) 19:(7, 0, 0) 20:(1, 0, 6)	16 1194				
20:(1,0,6) 20:(2,0,5)	46 882				
20:(2, 0, 5) 20:(3, 0, 4) 20:(4, 0, 3) 20:(4, 1, 2)	6526 24285				
20:(5, 0, 1)	5 3				
20:(5, 0, 2) 20:(5, 1, 1)	44434 43				
20:(6, 0, 0) 20:(6, 0, 1) 20:(6, 1, 0)	7 39602 67				
20:(6, 1, 0) 20:(7, 0, 0)	13539				

3.4 Simulation Study and the Results

Power is defined as the average proportion of correctly identified active effects. It can be used as a measurement for the effectiveness of screening designs. It is a very useful tool for comparing the performance of designs on detecting the active effects. The usual method that uses the power as a tool for comparing designs is through employing a simulation study to conduct it.

In this section, with consideration of our MDSs classification, we report simulations for comparing selected MDSs of a 7-factor design with 20 runs, a 6-factor design with 16 and 20 runs, and a 5-factor design with 20 runs. The 7-factor designs with 20 runs are the orthogonal and nonorthogonal designs that were shown earlier in Table 8. All the remaining designs that were used in the simulation are displayed in the Appendix section.

For our simulation, we use forward selection as a procedure for selecting models. It has a simple implementation and it is available in many software packages like R. Forward selection procedure is a stepwise regression, which starts with the model containing just an intercept, and then, sequentially, steps start by adding one variable at a time. The added variable is the best choice based on some criteria which could be lowest p-value, lowest AIC, highest adjusted R^2 , largest F statistic, etc. Then, these steps repeat by adding one variable at a time until the criteria stop improving. In the end, the selected variables are the best selection for the final model.

3.4.1 The Methodology for the Simulation

For each MDS under comparison, the methodology for the simulation study is applied as follows. In each of 1000 iterations:

1. Consider a matrix M of k MEs columns and g 2FIs columns, which are corre-

- sponding columns to the 2FIs for the k MEs.
- 2. Consider a sub matrix, M_1 , from the matrix M, which represents the columns for the factorial effects, that involved the selected MDS.
- 3. Let X be the matrix which contains columns that are randomly selected from M_1 , so that X is corresponding to the matrix of active effects.
- 4. The number of active effects is starting from 3 until the size for the selected MDS. So, if we have an MDS of size p, such that p > 3, the number of selected active effects from M_1 starts from 3 effects up to p.
- 5. The response vector is generated as $y = X\beta + \epsilon$, where $\epsilon \sim N(0, 1)$.
- 6. The coefficients, β , for the active effects are obtained by randomly sampling (with replacement) values from the set $\{-3, -2, -1, 1, 2, 3\}$.
- 7. The set of significant effects is chosen by using forward selection procedure.
- 8. At the end of 1000 iterations, the power (the average proportion of correctly identified active effects, that include both MEs and 2FIs), power for MEs (the average proportion of correctly identified active MEs), and power for 2FIs (the average proportion of correctly identified active 2FIs) are recorded.

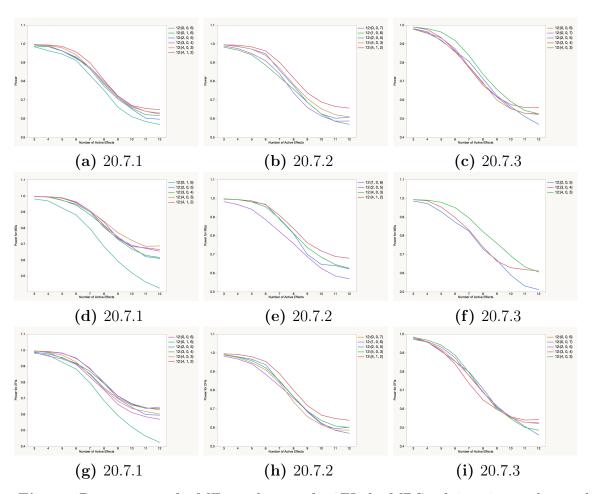
3.4.2 Simulation Results

3.4.2.1 Orthogonal designs with k=7, n=20

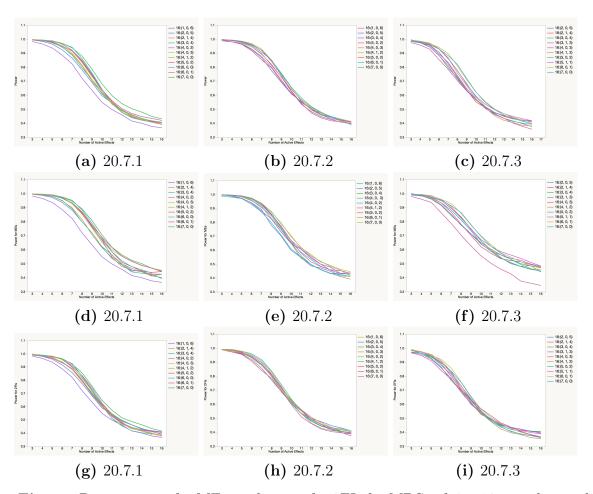
Section 3.3 showed the classification of MDSs for orthogonal and nonorthogonal designs that were shown in Table 2. Due to the wide variety of MDS sizes and types, we randomly selected MDSs with sizes 12 and 16 for these designs to employ the simulation. For instance, for design 20.7.1, the selected MDSs are as follows: 12:(0,

0, 6), 12:(0, 1, 6), 12:(2, 0, 5), 12:(3, 0, 4), 12:(4, 0, 3), 12:(4, 1, 2), 16:(1, 0, 6), 16:(2, 0, 5) 16:(2, 1, 4), 16:(3, 0, 4), 16:(4, 0, 2), 16:(4, 0, 3), 16:(4, 1, 2), 16:(5, 0, 2) 16:(6, 0, 0), 16:(6, 0, 1), 16:(6, 1, 0), and 16:(7, 0, 0). Based on our simulation protocol, we display the results of simulations for these designs in Figures 4, 5, 6, and 7. In Figure 4, X-axes for the plots represent the number of active effects. The Y-axes represents power in sub figures (a), (b), and (c) while it represents power for MEs in sub figures (d), (e), and (f), and it represents power for 2FIs in sub figures (g), (h), and (i) to 20.7.1, 20.7.2, and 20.7.3 respectively. Each color line represents a type of MDS of size 12.

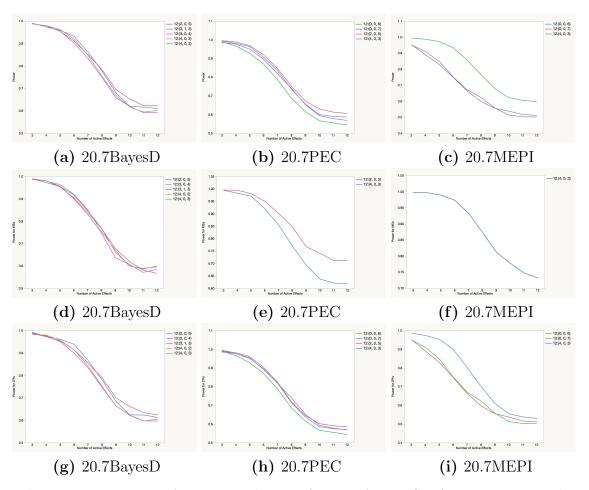
Figure 5 is organized in the same way as Figure 4 but for MDSs of size 16. The results of the simulation for nonorthogonal designs are displayed in Figures 6 and 7 for MDSs of size 12 and 16, respectively. In Figure 6, X-axes for the plots represent the number of active effects. In sub figures (a), (b), and (c), the Y-axes represent power while in sub figures (d), (e), and (f), the Y-axes represent power for MEs, and in sub figures (g), (h), and (i) the Y-axes represent power for 2FIs to 20.7BayesD, 20.7PEC, and 20.7MEPI, respectively. Again, each color line represents a type of MDS of size 12. Also, Figure 7 is organized in the same way as Figure 6 but for MDSs of size 16.



 $\bf Fig.~4.:~$ Power, power for MEs, and power for 2FIs for MDSs of size 12 to orthogonal designs in Table 2



 $\bf Fig.~5.:~$ Power, power for MEs, and power for 2FIs for MDSs of size 16 to orthogonal designs in Table 2



 $\bf Fig.~6.:~$ Power, power for MEs, and power for 2FIs for MDSs of size 12 to nonorthogonal designs in Table 2

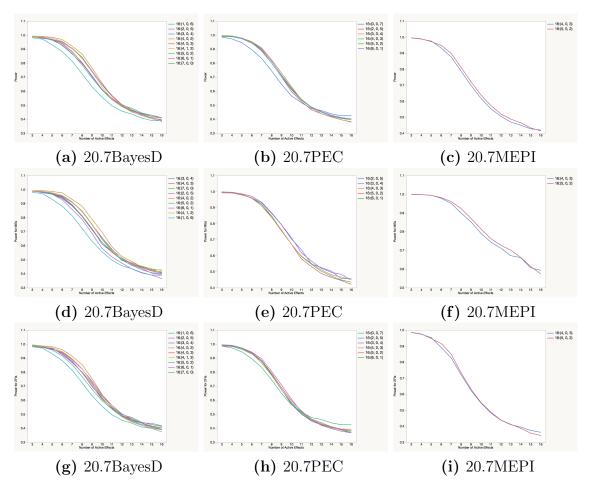


Fig. 7.: Power, power for MEs, and power for 2FIs for MDSs of size 16 to nonorthogonal designs in Table 2

Overall, our classification of MDSs showed a significant impact on the active effect detection of the designs that under were consideration. The MDS that has a large number of factors exhibits more power, power for MEs, and power for 2FIs. Our comments for the simulation results as follows:

- 1. For all designs and types of MDSs, as the number of active effects increases, the power, power for MEs, and power for 2FIs are decreasing.
- 2. It is worth noting that the value of l in the MDSs classification affects power, power for MEs, and power for 2FIs, especially for orthogonal designs. As can

- be seen from Figures 2 and 3, the simulation results show that the MDS with a larger l exhibit better power, power for MEs, and power for 2FIs.
- 3. We see some benefit from the value of m. Both design 20.7.1, and 20.7.2 have two MDSs with the same value l 12: (4, 0, 3) and 12: (4, 1, 2). Both of these types of MDS have 4 common factors between MEs and 2FIs subsets, but they have a different number of factors, which are present in only MEs and 2FIs subsets. By considering the power for MEs to test which MDS performance is better, 12:(4, 1, 2) exhibits better power for MEs than 12:(4, 0, 3), especially for design 20.7.2 (Figure 4(b), and 4(e)). Obviously, 12: (4, 1, 2) has a larger m, which is the number of factors that only appear in MEs subset.
- 4. For the two sizes of MDSs of design 20.7BayesD, there is no dramatic difference between the classification of MDSs. However, with MDSs of size 16, it is obvious that the type of MDS with the least l 16: (1, 0, 6) exhibits the worst power, power for MEs, and power for 2FIs.
- 5. For design 20.7PEC, MDS of type 12:(2, 0,4) exhibits better power, power for MEs, and power for 2FIs than 12:(4, 0, 2), which is unexpected. However, as the case of design 20.7BayesD, it is clear that MDS of type 12:(0, 0, 6) gives the worst power.
- 6. For design 20.7MEPI, it is obvious that the performance of an MDS with a larger l is better for power, power for MEs and power for 2FIs.
- 7. According to our simulation study, it can be said that the type of MDS with a larger l is more preferred than the type of MDS with less l. Therefore, for the designs comparison, it can be said that the design with more of these MDSs (the type of MDS with a larger l) could be recommended for active effect detection.

3.4.2.2 k=6, n=16, 20

The classification of the MDSs for the orthogonal designs with k=6, and n=20, 16 that were used in the simulation are shown in Table 12. We denote to these designs as 16.6 and 20.6. For these design, we randomly selected MDSs of size 6 for design 16.6.1, and MDSs of size 14 for design 20.6.1. The result of the simulation of these design are displayed in Figure 8. In Figure 8, X-axes for the plots represent the number of active effects. The Y-axes represents power in sub figures (a) and (b) while it represents power for MEs in sub figures (d) and (e), and it represents power for 2FIs in sub figures(g) and (h) to 16.6 and 20.6, respectively. Again, each color line represents a type of MDS.

Table 12.: The classification for MDSs to orthogonal designs with k=6, and n=16, and 20

	16.6.1	20.6.1				
h:(l, m, f)	number of $h:(l,m,f)$	h:(l, m, f)	number of $h:(l, m, f)$			
5:(2, 0, 3)	3	10:(0, 0, 6)	1			
6:(0,0,6)	4	10:(4, 0, 1)	2			
6:(2,0,3)	4	12:(2, 0, 4)	4			
6:(2,0,4)	2	13:(4, 0, 2)	1			
7:(2,0,4)	4	14:(2, 0, 4)	2			
7:(2,1,3)	1	14:(4, 0, 2)	3			
8:(2, 0, 4)	6	(, - , ,				
8:(2, 1, 3)	2					
9:(2, 0, 4)	2					

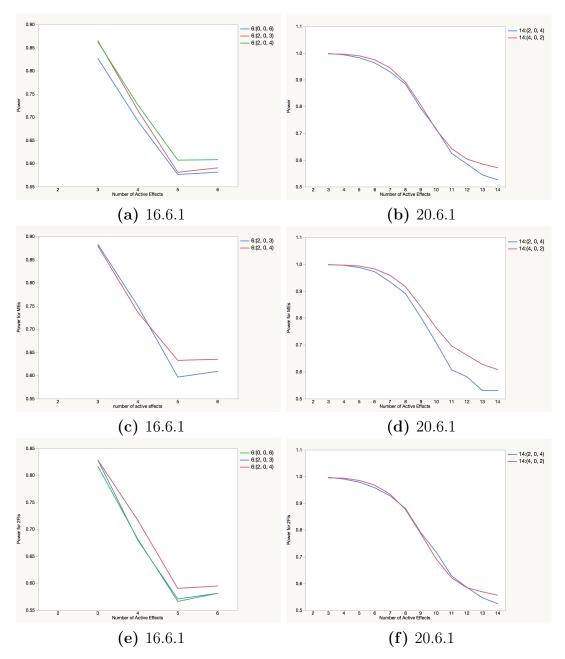


Fig. 8.: Power, power for MEs, and power for 2FIs to orthogonal designs with k=6, and n=16, 20

Our comments on the displayed results are as follows:

1. As with the seven-factor case, the MDS with a larger l provides better performance with respect to power, power for MEs, and power for 2FIs.

2. It is obviously recommended to consider MDS of type 6: (2, 0, 4) and 14: (4, 0, 2) of design 16.6 and 20.6, respectively, for active effect detection. Thus, we prefer to see more of these types of MDSs than another type of MDS.

3.4.2.3 Other Run Sizes

The reported simulation result for designs with k=7, n=20, and k=6, n=20, 16 show a pattern that repeated for other cases. Generally, MDSs that involve a large number of factors most likely exhibit more power than the other MDS. This finding highlights the differences between the MDSs of the designs and can be used as a measure of the effectiveness of candidate designs.

3.5 Conclusion

In this chapter, we have investigated the structure for a design by considering the minimal dependent sets, MDSs, for this design, which could be used as a criterion for design selection. We focused on discovering the effect of the number of factors for an MDS on the ability for a design to identify the active effects. We accomplished that, by providing a classification for the MDSs of a design. This classification is focused on counting the number of factors in MEs and 2FIs that are involved in an MDS. Then, we conducted a simulation study, which aimed to test the effectiveness of our classification of MDSs on power for active effect detection. For MDSs that have the same size, it was seen that when the number of common factors between MEs and 2FIs is increasing, the power to detect the active effects is increasing, too, especially for orthogonal design. This aspect of the research suggested that, for comparison between designs, a design that has a greater number of MDSs, which involve a large number of common factors between MEs and 2FIs, is preferable.

Our classification for the MDSs of a design focused on the appearance of factors

in MEs and 2FIs. There are many ways to classify the MDSs for a design, which have not been explored yet. It will be important that future research investigate the comparison between different size of MDSs with respect to power or another statistical concept, for instance, false discovery rate, estimation capacity, generalize aliasing length, etc. Also, our classification was tested with respect to the power. Future research could continue to explore the impact of this classification for another statistical concept, such as false discovery rate.

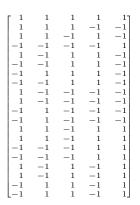
3.6 Appendix

Table 13.: Orthogonal design with k=6 factors, and n=16

Table 14.: Orthogonal design with k=6 factors, and n=20

Γ 1	1	1	1	1	1-
1	1	-1	-1	-1	-1
1	-1	1	1	-1	-1
-1	1	1	1	-1	-1
-1	-1	1	-1	1	-1
-1	-1	-1	1	-1	1
-1	1	1	-1	-1	1
1	1	-1	1	1	-1
1	-1	-1	-1	1	1
1	1	1	1	-1	1
-1	-1	1	1	1	1
-1	1	-1	-1	1	-1
-1	1	-1	-1	-1	1
-1	-1	-1	1	1	-1
1	-1	-1	-1	-1	1
1	1	1	-1	1	-1
-1	-1	1	-1	-1	-1
-1	1	-1	1	1	1
1	-1	-1	1	-1	-1
1	-1	1	-1	1	1_

Table 15.: Orthogonal design with k=5 factors, and n=20



3.6.1 R Code for MDSs Classification

```
#inputs:
#X: MDSs matrix for MEs and 2FIs (coded as +/-1 and 0)
#"Getting MDSs matrix by use 4ti2 software"
#output:
#matrix for MDSs classification;
#columns: MDS, (h,l,m,f)

library(stringr)
library(rlist)
library(stringi)
X<-as.data.frame(X)
k=ncol(X)
X<-simplify2array(
apply(
    X[1:k], 1,</pre>
```

```
function(x) paste(naMEs(X[1:k])[x != 0], collapse = "\")
)
\mathbb{E} \left\{ -\mathbf{function}(\mathbf{x}) \right\}
  h < -(str_count(x, "\setminus w+"))
  b<-str_split(x, "_")
  c<-as.list(strsplit(x, '\\s+')[[1]])
  g < -list.sort(nchar(c))
  splited \leftarrow split(c, f = g)
  d1<-splited$'1'
  d2<-splited$'2'
  d12 \leftarrow unlist(d1) \#MEs \ subset
  n1 < -length (d12)
  s13 \leftarrow paste (d12, sep=""", collapse=""")
  vf1<-rawToChar(unique(charToRaw(s13)))
  a1 < -vf1
  d22 \leftarrow \mathbf{unlist} (d2) \#2FIs \ subset
  n2 < -length (d22)
  s3<-paste (d22, sep="", collapse="")
  vf2<-rawToChar(unique(charToRaw(s3)))
  b1<-vf2
  pasteOccurrence <- function(x){</pre>
  ave(x, x, FUN=function(x) paste0(x, seq_along(x)));
```

```
all<-paste(collapse=',',
  substr(setdiff(pasteOccurrence(strsplit(a1, '')
  [[1L]]), pasteOccurrence(strsplit(b1, '')[[1L]])),
  1L, 1L)
  b11<-paste(collapse=',',
  substr(setdiff(pasteOccurrence(strsplit(b1, '')
  [[1L]]), pasteOccurrence(strsplit(a1, '')[[1L]])),
  1L, 1L)
  m<-nchar (a11)
  f<-nchar (b11)
  a <- unlist(strsplit(vf1,""))
  b <- unlist(strsplit(vf2,""))
  l < -sum(!is.na(pmatch(a,b)))
  return(as.matrix(c(h, l, m, f), ncol=1))
\mathbf{q} \leftarrow \mathbf{lapply}(X, E)
q1 < -as \cdot array(q)
q2 < -as \cdot data \cdot frame (q1)
result <-cbind(X, q2)
df <- apply(result, 2, as.character)
```

}

write.csv(df, file = "result.csv")

CHAPTER 4

CONSTRUCTING THREE-QUARTER NONREGULAR DESIGNS

4.1 Introduction

Omitting a quarter of run size from a complete 2^k factorial design produces a three-quarter design. Research has shown that a three-quarter from a regular 2^k could be able to estimate all the main effects (MEs) and two-factor interactions (2FIs). In this paper, we investigate the construction and theoretical properties of three-quarter design of regular and nonregular design. Via blocking technique on a pair of factorial effects we provide three-quarter designs that have impressive values for ranking designs criteria. Through the use of indicator function and parallel flats designs, general properties of constructed three-quarter design will be discussed.

A screening experiments is often conducted in the early stage of experimentation in order to determine the few important factors from a larger set of candidate factors. The two-level fractional factorial designs (FFDs) are the most popular designs used for screening experiments. Regular 2^{k-p} FFDs (Box and Hunter, 1961; Fries and Hunter, 1980) are the common choice for screening experiments. These designs are straightforward to construct and have a simple aliasing structure, in which any two factorial effects are either orthogonal or fully aliased. Nonregular design, on the other hand, have a more complex aliasing structure in that factorial effect may be partially aliased (neither fully aliased or orthogonal). Nonetheless, the nonregular designs offer run size flexibility and high ability to estimate more models than the regular design (Wu and Hamada, 2011).

The three-quarter design is a fractional factorial design, which can be obtained by

omitting one quarter of the full run size of a design. This design aims to improve run size economy without too much sacrifice in the estimability of low-order effects. The easiest way to construct a three-quarter design is to divide a design into four blocks of equal size, and then eliminate any block so that the final design has three blocks of run size. Mee (2009) shows an example for three-quarter design that constructed by partitioning the 2^4 into four blocks using blocking technique on the effects ABC and ABD as shown in Table 16. Mee, 2009 illustrates that the three-quarter of 2^4 is able to estimate all MEs and 2FIs, which is shown in Table 17.

Table 16.: Partition 2⁴ into 4 blocks

A	В	С	D	ABC	ABD
-1	-1	-1	-1	-1	-1
-1	1	1	1	-1	-1
1	1	-1	-1	-1	-1
1	-1	1	1	-1	-1
-1	-1	-1	1	-1	1
1	1	-1	1	-1	1
-1	1	1	-1	-1	1
1	-1	1	-1	-1	1
-1	1	-1	1	1	-1
1	-1	-1	1	1	-1
1	1	1	-1	1	-1
-1	-1	1	-1	1	-1
1	1	1	1	1	1
-1	-1	1	1	1	1
-1	1	-1	-1	1	1
1	-1	-1	-1	1	1

Table 17.: Three-quarter design of 2^4

A	В	С	D
-1	-1	-1	-1
-1	1	1	1
1	1	-1	-1
1	-1	1	1
-1	-1	-1	1
1	1	-1	1
-1	1	1	-1
1	-1	1	-1
-1	1	-1	1
1	-1	-1	1
1	1	1	-1
-1	-1	1	-1

The first block of run for 2^4 (first four runs in Table 16) has the defining relation

$$I = ABC = -ABD = CD.$$

With a 2^4 there are 16 columns in the full factorial model. These columns defined by a principal group and co-sets. The principal group is the group containing the identity (i.e, the intercept), the terms in the defining relation I = -ABC = -ABD, and the generalized interaction of these terms. Thus, the principal group is I = -ABC = -ABD = CD, and clearly it has 4 effects. The remaining 12 effects are partitioned into 3 co-sets of size 4. Multiplying the principal group by A, B, and C, respectively, we obtain all the co-sets:

$$A = -BC = -BD = ACD,$$

$$B = -AC = -AD = BCD,$$

$$C = -AB = -ABCD = D.$$

Three-quarter design has a special structure for its information matrix, namely a block diagonal structure. With this structure, any two factorial effects belonging to different blocks are uncorrelated. It is a very attractive structure since it mitigates some of the aliasing complexity. Figure 9 shows the block diagonal structure for the three-quarter design of 2⁴ which was shown earlier in Table 17.

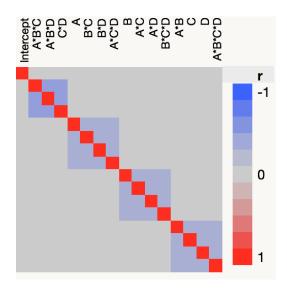


Fig. 9.: Block diagonal structure for three-quarter design of 2^4

There is a rich literature on the construction of three-quarter designs of regular 2^{k-p} . First of all, Davies et al., 1954 discusses three quarter design of regular 2^5 , where not all MEs and 2FIs are estimable. John, 1961 provides a three-quarter design of 2^4 and 2^5 by omitting a quarter of the run size, where the MEs and 2FIs can be estimated. In addition, Addelman, 1969 constructs three-quarter designs of regular designs by using two contrasts to divide the design into 4 blocks, then eliminating one of them. Addelman, 1961 proposes three-quarter designs of 2^k for up to 6 factors. For example, consider 2^{5-2} , which is defined by the defining relation I = ABC = ADE = BCDE. Addelman, 1961 shows that the treatment combinations of this design split into 4 quarters. Each quarter satisfies the following relations:

• $x_1 + x_2 + x_3 = 0 \pmod{2}$, $x_1 + x_4 + x_5 = 0 \pmod{2}$, $x_2 + x_3 + x_4 + x_5 = 0 \pmod{2}$,

- $x_1 + x_2 + x_3 = 0 \pmod{2}$, $x_1 + x_4 + x_5 = 1 \pmod{2}$, $x_2 + x_3 + x_4 + x_5 = 1 \pmod{2}$,
- $x_1 + x_2 + x_3 = 1 \pmod{2}$, $x_1 + x_4 + x_5 = 0 \pmod{2}$, $x_2 + x_3 + x_4 + x_5 = 1 \pmod{2}$,
- $x_1 + x_2 + x_3 = 1 \pmod{2}$, $x_1 + x_4 + x_5 = 1 \pmod{2}$, $x_2 + x_3 + x_4 + x_5 = 0 \pmod{2}$,

where the treatment combinations, x_i , is either 0 or 1 for i = 1, 2, 3, 4, 5. These four relations could be represented by the four defining relations:

$$I = -ABC = -ADE = BCDE,$$

 $I = -ABC = -ADE = BCDE,$
 $I = -ABC = ADE = -BCDE,$
 $I = -ABC = -ADE = BCDE.$

Each defining relation corresponds to a quarter. Addelman, 1961 showed that a three-quarter design of 2^{5-2} may be obtained by selecting any treatment combinations that occur in any three of the four quarters of 2^{5-2} . For instance, combining the treatment combinations that occur in I = -ABCDE = BCDE, I = -ABC = -ADE = BCDE, and I = -ABC = ADE = -BCDE represent a three-quarter design of 2^{5-2} .

John, 1962 points out that a set of fractions that correspond to blocks, where the defining relations for these fractions have the same terms but differ in the sign, is called a family of 2^{k-p} . Also, John, 1962 defines that a combination of three designs from the same family is called a $3(2^{k-p})$ design. Addelman, 1969 proposes a plan for designs with 6 to 11 factors that were all constructed by combining regular fractional

factorial designs from the same family.

Cheng et al., 2004 discusses blocked nonregular two-level fractional factorial designs. Also, Briggs, 2011 constructs three-quarter design from nonregular design Plackett-Burman. Based on the previous works, the goal of this paper is to focus on the construction of three-quarter designs of two-level fractional factorial regular and nonregular designs by using blocking technique on a pair of factorial effects to divide a design into 4 equal blocks, then eliminating a block (a quarter of the run size).

The rest of this chapter is organized as follows. In Section 4.2, we review needed background on indicator function, minimal dependent sets (MDSs), and parallel flats designs (PFDs). In Section 4.3, we discuss the construction of three-quarter designs of regular designs. In Section 4.4, we explain our method for constructing three-quarter designs of nonregular designs, and provide some theories related to the constructed designs. Next, in Section 4.5 we examine three-quarter designs with the concept of MDSs. Then, in Section 4.6, we provide a comparison between three-quarter designs of regular designs and three-quarter designs of nonregular designs, based on standard criteria for ranking the designs. Finally, Section 4.7 is the conclusion and ideas for future work.

4.2 Foundations

4.2.1 Indicator Function

 i = 1, 2, ...k). Consider \mathcal{D} to be a fractional factorial with n runs and k factors. The indicator function of \mathcal{D} is denoted as $F_{\mathcal{D}}$ which is defined as,

$$F_{\mathcal{D}}(x) = \begin{cases} a_x, & \text{if } x \in \mathcal{D} \\ 0, & \text{if } x \in \mathcal{F} \setminus \mathcal{D} \end{cases}$$

$$(4.1)$$

where a_x denotes the number of replicates of x in \mathcal{D} . Let's define $X_l(x) = \prod_{i \in l} x_i$ for $l \in P$, where P is the collection of all subsets of $\{1, 2, ..., k\}$. Then, the indicator function of \mathcal{D} has the following form

$$F_{\mathcal{D}}(x) = \sum_{l \in P} b_l X_l(x), \tag{4.2}$$

with coefficients

$$b_l = \frac{1}{2^k} \sum_{x \in \mathcal{D}} X_l(x). \tag{4.3}$$

The constant term of the indicator function $F_{\mathcal{D}}$ is the sum of the intercept column divided by 2^k , which is

$$b_{\odot} = n/2^k. \tag{4.4}$$

Each term in the indicator function is called a word. Cheng et al., 2004 mentioned that the value of b_l/b_{\odot} is the correlation between the two effects columns. For instance, consider \mathcal{D} which is a 2^{7-3} , with factors A - D and E = ABC, F = BCD, and G = EF, the indicator function for this design is

$$F_{\mathcal{D}} = 16 + 16x_1x_4x_7 + 16x_5x_6x_7 + 16x_1x_2x_3x_5 + 16x_1x_4x_5x_6$$

$$+16x_2x_3x_4x_6 + 16x_1x_2x_3x_6x_7 + 16x_2x_3x_4x_5x_7$$

$$(4.5)$$

From the word $(16x_1x_4x_7)$, the correlation between X_1 and X_4X_7 is given by $b_{147}/b_{\odot}=16/16=1$, (more examples in this scene will be presented on next sections).

4.2.2 Minimal Dependent Sets (MDSs)

MDS for a design is a set of linearly dependent effects, that has a special property, where if one of the effects from this set is removed, all the rest of the effects become linearly independent. For example, consider a 2^{6-2} , such that E = AC, F = 1/2[CD + ACD + BCD - ABCD] (Johnson and Jones, n.d.). This design has the following MDSs for MEs and 2FIs model:

$$E-AC$$
 $C-AE$
 $A-CE$
 $E+C+BC-BE-2DF$
 $F+AF-CD-DE$
 $D+AD-CF-EF$

For this design, there are 3, 2, and 1 MDSs of size 2, 4, and 5, respectively. One of these MDSs is $\{F, AF, CD, DE\}$. By the definition of MDS, a model contains all the effects in this MDS is not estimable, while, if one effect is removed, for instance, AF, then a model contains the rest of the effects $\{F, CD, DE\}$ is estimable.

The concept of MDSs was utilized first by Miller and Sitter, 2004 to rank designs based on their ability to identify active effects. Miller and Sitter, 2004 show that MDSs help to narrow down the set of candidate models. Also, Lin et al., 2008 investigate the effect of MDSs on model discrimination and develop criteria (MDS-resolution and MDS-aberration) to evaluate nonorthogonal foldover designs. In this case, a design with a larger MDS is preferable to a design with a smaller MDS, which means that MDS resolution (the number of smallest MDS size) is to be maximized; MDS-aberration ranks designs based on sequentially minimizing the number of small-

est MDS size.

4.2.3 Parallel Flats Designs

A regular 2^{k-m} fractional factorial design is called *single flat design*. The runs for fractional factorial design satisfy aliasing relations. This type of design can defined by the alias matrix \mathbf{A} , and consist of all treatment combinations $\mathbf{x} = (x_1, ..., x_k)'$ satisfying $\mathbf{A}\mathbf{x} = \mathbf{c}$, where \mathbf{A} is an $m \times k$ matrix of rank m, and, \mathbf{c} is an $m \times 1$ vector with two level ± 1 . Suppose $S_1, S_2, ..., S_f$ are single flat designs that defined by the same alias matrix \mathbf{A} , and $\mathbf{c}_1, \mathbf{c}_2, ..., \mathbf{c}_f$ respectively. Then parallel flats design (f-PFD) is the combining of these f single flats. Thus, a f-PFD could be determined by (\mathbf{A}, \mathbf{C}) , where, \mathbf{C} is an $m \times f$ matrix containing the vectors $\mathbf{c}_1, \mathbf{c}_2, ..., \mathbf{c}_f$. It is obvious that the run size for f-PFD is equal to $n = f \times 2^{k-m}$ (Liao and Chai, 2004). For example, consider a design 2^{6-2} , which is shown in Table 18.

Table 18.: Nonregular design with k=6 and n=16

A	В	С	D	Е	F
-1	-1	-1	-1	1	1
1	-1	-1	-1	1	-1
-1	1	-1	-1	-1	1
1	1	-1	-1	-1	1
-1	-1	1	-1	1	-1
1	-1	1	-1	-1	-1
-1	1	1	-1	1	1
1	1	1	-1	-1	-1
-1	-1	-1	1	-1	-1
1	-1	-1	1	-1	1
-1	1	-1	1	1	-1
1	1	-1	1	1	-1
-1	-1	1	1	-1	1
1	-1	1	1	1	1
-1	1	1	1	-1	-1
1	1	1	1	1	1

This design is determined by (A, C), where **A** and **C** are

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The number of columns for matrix \mathbf{C} determines the number of single flats for the design. So, this design is 8-PFD. Since the run size for this design is n=16, and it has 8 single flats, each flat has a run size equaling 16/8=2 runs. So, each flat represents a regular 2^{6-5} that satisfies $I=\pm A$, $I=\pm B$, $I=\pm C$, $I=\pm DE$, $I=\pm DF$.

Parallel flats designs were introduced by Connor and Young, 1961. Srivastava et al., 1984 provided general theories of parallel flats designs. One of these theories is that the information matrix of a parallel flats design is always expressed as a block diagonal matrix if $f \leq n$, where f is the number of flats, and n is the number of runs. The information matrix is X'X, which can be written as

$$X'X = \begin{bmatrix} X_1'X_1 & 0 & \dots & 0 \\ 0 & X_2'X_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \dots \\ 0 & 0 & \dots & X_g'X_g \end{bmatrix}$$

where **X** is the model matrix for a general linear model $y = \mathbf{X}\beta + \epsilon$, and $\epsilon \sim N(0, \sigma^2 I)$.

Each submatrix $\mathbf{X}_{j}'\mathbf{X}_{j}$ in the diagonal of the information matrix corresponds to an aliasing set, and g is the number of aliasing sets. All the off-diagonal are zero matrices, which indicates the orthogonality among the submatrices.

4.2.3.1 4-PFD

In this section, we will introduce four examples of 4-PFD. The first one is a non-regular design, 2^{6-2} , where n = 16 and k=6. We denote this design by 16.6.2, and display it in Table 19. Figure 10 shows the block diagonal structure of 16.6.2. Obviously, we can see that any two effects belonging to different blocks are uncorrelated, and we can see that there is a partial correlation between the effects within a block.

Table 19.: Nonregular design 16.6.2.

A	В	С	D	Е	F
-1	-1	-1	-1	1	-1
1	-1	-1	-1	-1	1
-1	1	-1	-1	-1	1
1	1	-1	-1	1	1
-1	-1	1	-1	1	1
1	-1	1	-1	-1	-1
-1	1	1	-1	-1	-1
1	1	1	-1	1	-1
-1	-1	-1	1	1	1
1	-1	-1	1	-1	-1
-1	1	-1	1	-1	-1
1	1	-1	1	1	-1
-1	-1	1	1	1	-1
1	-1	1	1	-1	1
-1	1	1	1	-1	1
1	1	1	1	1	1

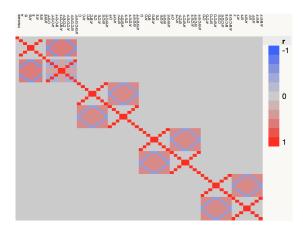


Fig. 10.: Block diagonal structure for 16.6.2.

The second 4-PFD design is 2^{6-1} with n=32 and k=6, such that F=0.5E(AB+AC+BD-CD). The columns of the full factorial model of 2^{6-1} appear in 8 co-sets of size 8. These co-sets are defined by the principal group, which is the set that contains the identity (i.e., intercept), and the interactions in the defining relation I=0.5EF(AB+AC+BD-CD), and generalized interactions. So the principal group for 2^{6-1} is

$$\{I, AD, BC, ABCD, ABEF, ACEF, BDEF, CDEF\},\$$

and the co-sets for this design is obtained by multiplying the principal group by A, B, E, F, AB, AE, and AF, such as, A co-set is

$$\{A, D, ABC, BCD, BEF, CEF, ABDEF, ACDEF\}.$$

If we arrange the columns of full factorial model for 2^{6-1} based on the principal group and the co-sets, we obtained a block diagonal structure with 8 blocks of size 8, where each block has rank 4. Thus, with 4-PFD, the maximum size of MDSs must be 5, since the rank for each block is 4.

Another example of 4-PFD with n=16, and k=7 is shown in Table 20. This design

was provided by Edwards, 2011. Edwards, 2011 provides a semifoldover plans for two-level orthogonal design. Semifolding technique is adding half of foldover fraction design as an alternative to foldover technique which require adding a fraction which has same size as the initial design. One of initial designs that Edwards, 2011 used is 4-PFD, which is in Table 20.

Table 20.: 4-PFD with n=16 and k=7

A	В	С	D	Е	F	G
1	1	1	1	1	1	1
1	1	1	-1	-1	-1	-1
1	1	-1	1	1	-1	-1
1	1	-1	-1	-1	1	1
-1	-1	-1	-1	-1	1	1
-1	-1	-1	1	1	-1	-1
-1	-1	1	-1	-1	-1	-1
-1	-1	1	1	1	1	1
1	-1	1	1	-1	1	-1
1	-1	1	-1	1	-1	1
1	-1	-1	1	-1	-1	1
1	-1	-1	-1	1	1	-1
-1	1	-1	-1	1	-1	1
-1	1	-1	1	-1	1	-1
-1	1	1	-1	1	1	-1
-1	1	1	1	-1	-1	1

The fourth example of 4-PFD design is 2^{7-1} where n=64 and k=7, such that G=0.5EF(AB+CD+AC-BD). The number of blocks for a 4-PFD is n/4. Figure 11, shows the block diagonal structure for this design, and it is clear there are 16 orthogonal blocks. We will focus deeply on the construction of three-quarter designs of 4-PFD using this design in Section 4.4.

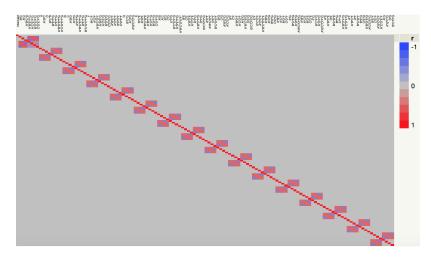


Fig. 11.: Block diagonal structure for 2^{7-1} .

4.3 Construct Three-Quarters Based on Regular Designs

In this section, we discuses a class of three-quarter design constructed by blocking a regular design using a pair of factorial effect. Consider a regular design 2^{6-2} , with generators E = ABC and F = ABD. The principal group for this design is $\{I, ABCE, ABDF, CDEF\}$. The full factorial model for 2^6 has 64 columns of effects, four of these effects appear in the principal group, and the remaining effects are partitioned into 15 co-sets of size 4. Multiplying the principal group by A, B, C, D, E, F, AB, AC, AD, BC, BD, CD, DE, BCD, and ACD, we obtain all the co-sets as follows:

 $\{A, BCE, BDF, ACDEF\},\$ $\{B, ACE, ADF, BCDEF\},\$ $\{C, ABE, ABCDF, DEF\},\$ $\{D, ABCDE, ABF, CEF\},\$ $\{E, ABC, CDF, ABDEF\},\$ $\{F, ABD, CDE, ABCEF\},\$

 $\{AB, CE, DF, ABCDEF\},\$ $\{AC, BE, BCDF, ADEF\},\$ $\{AD, BCDE, BF, ACEF\},\$ $\{BC, AE, ACDF, BDEF\},\$ $\{BD, ACDE, AF, BCEF\},\$ $\{CD, ABDE, ABCF, EF\},\$ $\{BCD, ADE, ACF, BEF\},\$ $\{ACD, BDE, BCF, AEF\}.\$

As we mentioned earlier, a common way to construct a three-quarter design is to divide the design into four blocks, using factorial effects for blocking, and then eliminate any block. In fact, the effects in the principal group of a regular design have one level either 1 or -1. In this case, we can't use any effects in the principal group of a regular design for blocking, since the columns of these effects form a matrix with one unique row. This doesn't allow for dividing the design into 4 equal blocks. Thus, we need to select a pair of factorial effects from co-sets (either within a co-set or two different co-sets), since these effects have two levels 1 and -1.

First, let's consider blocking the design 2^{6-2} by a pair of effects (BCD, ACD), where BCD and ACD belong to two different co-sets. The pair of effects (BCD, ACD) forms a matrix with four unique rows, (-1, -1), (-1, 1), (1, -1), and (1, 1), which results in dividing the design into four equal blocks as shown in Figure 12. So, if we remove any block (for example the fourth block), the resulting design is a three-quarter design with n=12. Table 21 shows this three-quarter design.

Α	В	С	D	E	F	BCD	ACD
-1	-1	-1	-1	-1	-1	-1	-1
1	1	1	-1	1	-1	-1	-1
-1	-1	1	1	1	1	-1	-1
1	1	-1	1	-1	1	-1	-1
-1	1	-1	1	1	-1	-1	1
1	-1	1	1	-1	-1	-1	1
-1	1	1	-1	-1	1	-1	1
1	-1	-1	-1	1	1	-1	1
1	-1	-1	1	1	-1	1	-1
-1	1	1	1	-1	-1	1	-1
-1	1	-1	-1	1	1	1	-1
1	-1	1	-1	-1	1	1	-1
-1	-1	1	-1	1	-1	1	1
1	1	-1	-1	-1	-1	1	1
-1	-1	-1	1	-1	1	1	1
1	1	1	1	1	1	1	1

Fig. 12.: Blocking the design 2^{6-2} on the pair (BCD, ACD).

Table 21.: Three-quarter design of 2^{6-2} .

A	В	С	D	Е	F
-1	-1	-1	-1	-1	-1
1	1	1	-1	1	-1
-1	-1	1	1	1	1
1	1	-1	1	-1	1
-1	1	-1	1	1	-1
1	-1	1	1	-1	-1
-1	1	1	-1	-1	1
1	-1	-1	-1	1	1
1	-1	-1	1	1	-1
-1	1	1	1	-1	-1
-1	1	-1	-1	1	1
1	-1	1	-1	-1	1

Second, let's consider another case where the pair of effects that are used for blocking are selected from the same co-set. For example, blocking the design 2^{6-2} by the pair of effects (DE, CF), where DE, and CF belong to the same co-set $\{DE, CF, ABEF, ABCD\}$. This pair of effects forms a matrix with two unique rows (-1, -1) and (1, 1), which results in dividing the design into two equal blocks as shown in Figure 13. Therefore, we can't construct a three-quarter design from the regular design 2^{6-2} by using this pair for blocking.

In fact, this case is equivalent to a case where one effect is selected from the principal group and the other effect is selected from any co-set. Since each effect in the principal group has only one level either 1 or -1, and the other effect in any co-sets has two level 1 and -1, using a pair of these effects for blocking forms a matrix with two unique rows. This creates two equal blocks. For instance, blocking 2^{6-2} by the pair (CDEF, DE), where CDEF belongs to the principal group, and DE belongs to the co-set $\{DE, CF, ABEF, ABCD\}$, divides the design into two equal blocks as shown in Figure 14. Thus, based on these examples, the only way to construct a three-quarter design from a regular design is to use a pair of factorial effects for blocking, where these effects belong to two different co-sets.

Α	В	С	D	E	F	DE	CF
1	1	1	-1	1	-1	-1	-1
1	1	-1	1	-1	1	-1	-1
1	-1	1	1	-1	-1	-1	-1
1	-1	-1	-1	1	1	-1	-1
-1	1	1	1	-1	-1	-1	-1
-1	1	-1	-1	1	1	-1	-1
-1	-1	1	-1	1	-1	-1	-1
-1	-1	-1	1	-1	1	-1	-1
-1	-1	-1	-1	-1	-1	1	1
-1	-1	1	1	1	1	1	1
-1	1	-1	1	1	-1	1	1
-1	1	1	-1	-1	1	1	1
1	-1	-1	1	1	-1	1	1
1	-1	1	-1	-1	1	1	1
1	1	-1	-1	-1	-1	1	1
1	1	1	1	1	1	1	1

Fig. 13.: Blocking the design 2^{6-2} on the pair (DE, CF).

A	В	С	D	E	F	CDEF	DE
1	1	-1	1	-1	1	1	-1
-1	1	-1	-1	1	1	1	-1
1	-1	1	1	-1	-1	1	-1
-1	-1	1	-1	1	-1	1	-1
1	1	1	-1	1	-1	1	-1
-1	1	1	1	-1	-1	1	-1
1	-1	-1	-1	1	1	1	-1
-1	-1	-1	1	-1	1	1	-1
-1	-1	1	1	1	1	1	1
1	-1	1	-1	-1	1	1	1
-1	1	-1	1	1	-1	1	1
1	1	-1	-1	-1	-1	1	1
-1	-1	-1	-1	-1	-1	1	1
1	-1	-1	1	1	-1	1	1
-1	1	1	-1	-1	1	1	1
1	1	1	1	1	1	1	1

Fig. 14.: Blocking the design 2^{6-2} on the pair (CDEF, DE).

The previous examples serve to illustrate the following results.

Theorem 1 Let \mathcal{D} be a n-run regular design. Blocking \mathcal{D} by using a pair of factorial effects, where these effects selected from two different co-sets of \mathcal{D} , divides \mathcal{D} into four equal blocks. By eliminating one block, we obtain a three-quarter design.

Theorem 2 Three-quarter design of regular design is always 3-PFD.

Proof. Let \mathcal{D} be an n-run regular design. From Theorem 1, blocking \mathcal{D} by a pair of effects were selected from two different co-sets, divides \mathcal{D} into four equal blocks. By the definition of PFDs, the terms in the principal group form a matrix with rows that are constant within each flat, while the terms in each co-set are not necessarily constant within a flat. Thus, since \mathcal{D} is a two-level orthogonal design, each effect of a co-set has two levels, -1 and 1, within a flat. Thus, the terms in two co-sets formed a matrix with four unique rows within a block. Since, \mathcal{D} is regular design which is 1-PFD, and it has four blocks, then a matrix formed by the terms in two co-sets has one unique row within each block. So, each block is corresponding to a single flat. Clearly, by removing one block, the resulting three-quarter design is 3-PFD.

4.4 Methodology to Construct Three-Quarter of Nonregular 4-PFD

In this section we are focusing on constructing three-quarter of 4-PFD. As we mentioned earlier, one strategy for constructing a three-quarter design is to use a pair of factorial effects to block a design. This results in dividing a design into four equal blocks; we then eliminate any block to get three-quarter of the design. Consider the 4-PFD which is 2^{6-1} , with the factor A-E and F=0.5(ABE+ACE+BDE-CDE), as shown earlier in Section 4.2. The principal group for this design is

$$\{I, AD, BC, ABCD, ABEF, ACEF, BDEF, CDEF\}.$$

Blocking this 4-PFD by the pair (BC, ABCD), and (AD, ABEF), where the factorial effects in these pairs belong to the principal group are shown in Figure 15.

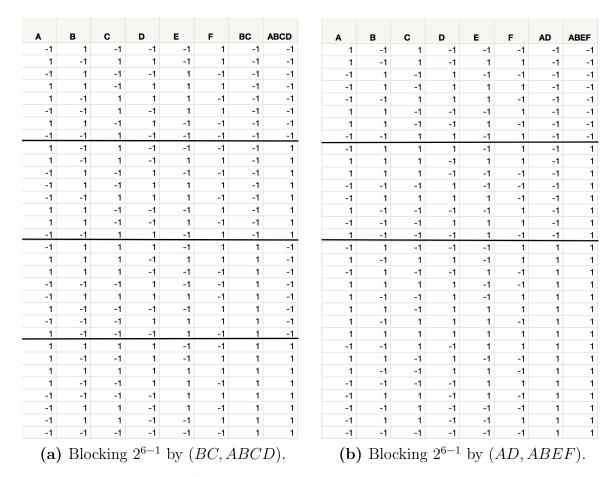


Fig. 15.: Blocking 2^{6-1} by factorial effects selected from the principal group.

The pair of factorial effects (BC, ABCD) divides the 4-PFD into four equal blocks while the pair (AD, ABEF) divides it into 3 unequal blocks as shown in Figure 15. Therefore, using (BC, ABCD) to block the 4-PFD can construct three-quarter. On the other hand, (AD, ABEF) cannot construct three-quarter. So, not all the pairs of effects that are selected from the principal group of a 4-PFD generate four blocks of the same size. By finding the correlation matrix between the effects columns in the principal group of the 4-PFD, we found that the uncorrelated effects can divide the design into 4 equal blocks, while the correlated effects cannot. Figure 16 shows the correlation matrix for the effects in the principal group of the 4-PFD that is 2^{6-1} .

	AD	BC	ABCD	ABEF	ACEF	BDEF	CDEF
AD	1.0000	0.0000	0.0000	0.5774	-0.5774	0.5774	0.5774
BC	0.0000	1.0000	0.0000	0.5774	0.5774	-0.5774	0.5774
ABCD	0.0000	0.0000	1.0000	-0.5774	0.5774	0.5774	0.5774
ABEF	0.5774	0.5774	-0.5774	1.0000	-0.3333	-0.3333	0.3333
ACEF	-0.5774	0.5774	0.5774	-0.3333	1.0000	-0.3333	0.3333
BDEF	0.5774	-0.5774	0.5774	-0.3333	-0.3333	1.0000	0.3333
CDEF	0.5774	0.5774	0.5774	0.3333	0.3333	0.3333	1.0000

Fig. 16.: The correlation matrix to the effects columns of the principal group for 2^{6-1} .

Theorem 3 Let \mathcal{D} be a two-level orthogonal n-run design. Let (U_1, U_2) be a pair of uncorrelated effects belonging to \mathcal{D} . Using (U_1, U_2) for blocking \mathcal{D} led to splitting \mathcal{D} into 4 equal blocks of size $\frac{n}{4}$. Then, omitting one of these blocks, the resulting design is a three-quarter design. In contrast, a pair of correlated effects doesn't allow for the construction of a three-quarter design, since it doesn't split the design into 4 equal blocks.

Proof. Let (U_1, U_2) represent a pair of uncorrelated effects that belong to \mathcal{D} . Since U_1 and U_2 are uncorrelated effects, it means the sum of the columns for each of these effects is equal to zero. By the definition of the indicator function, the columns of these effects will not appear in the indicator function of \mathcal{D} . Based on Kenny et al., 2003; and Cheng et al., 2004, two columns in \mathcal{D} can be used to generate 2^2 blocks of equal size if and only if no word of these columns appeared on the indicator function for \mathcal{D} . Thus, it follows that using a pair of uncorrelated effects is able to construct 2^2 =4 equal blocks, then, by omitting any block, we obtain a three-quarter design. In contrast, for a pair of correlated effects the sum of the columns for each of these effects doesn't equal zero, so these effects appear at the indicator function for \mathcal{D} . Using a pair of these effects, we would be unable to construct 2^2 equal blocks, hence, we can't construct a three-quarter design.

As we mentioned earlier 4-PFD has a block diagonal structure, so for this type of design, any two factorial effects from two different co-set are uncorrelated. This

means we can construct a three-quarter design by using two factorial effects that were selected from two different co-sets for blocking. In this context, correlated effects exist only within a co- set. Therefore, our methodology for selecting factorial effects which will be used for blocking 4-PFD is based on the following three different plans:

- 1. Select uncorrelated factorial effects from the principal group,
- 2. Select uncorrelated factorial effects, where one factorial effect is from the principal group and the other is from any co-set,
- 3. Select uncorrelated factorial effects, where these effects are from different cosets.

Note that selecting two effects from same co-set are equivalent to selecting one effect from the principal group and the other from any co-set, as shown in the examples of Section 4.3.

4.4.1 Both Effects from The Principal Group

Consider 4-PFD which is 2^{7-1} with n=64, and k=7, such that G=0.5(ABEF+CDEF+ACEF-BDEF). Again, the principal group is the group that contains the identity (i.e. intercept), the effects in the defining relation I=0.5G(ABEF+CDEF+ACEF-BDEF) and their generalized interactions. So, the principal group for this design is

$$\{I, ABEFG, CDEFG, ACEFG, BDEFG, BC, AD, ABCD\}.$$

With 2⁷, there are 128 columns for the full factorial model. The principal group contains 8 effects of them, so the remaining effects are partitioned into 15 co-sets,

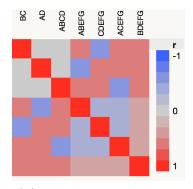
each of size 8. Multiplying the principal group by

A, B, F, G, E, AB, BE, BG, BG, EF, EG, FG, AE, AF, AG

we obtain all the co-sets for the design as follows:

- A co-set $\{A, D, ABC, BCD, BEFG, ACDEFG, CEFG, ABDEFG\}$,
- B co-set $\{B, C, ABD, ACD, AEFG, BCDEFG, ABCEFG, DEFG\},\$
- F co-set $\{F, BCF, ADF, ABCDF, ABEG, CDEG, ACEG, BDEG\}$,
- G co-set $\{G, BCG, ADG, ABCDG, ABEF, CDEF, ACEF, BDEF\}$,
- E co-set $\{E, BCE, ADE, ABCDE, ABFG, CDFG, ACFG, BDFG\}$,
- AB co-set $\{AB, AC, BD, CD, EFG, ABCDEFG, BCEFG, ADEFG\},$
- BE co-set $\{BE, CE, ABDE, ACDE, AFG, BCDFG, ABCFG, DFG\}$,
- BG co-set $\{BG, CG, ABDG, ACDG, AEF, BCDEF, ABCEF, DEF\}$,
- BF co-set $\{BF, CF, ABDF, ACDF, AEG, BCDEG, ABCEG, DEG\}$,
- EF co-set $\{EF, BCEF, ADEF, ABCDEF, ABG, CDG, ACG, BDG\}$,
- EG co-set {EG, BCEG, ADEG, ABCDEG, ABF, CDF, ACF, BDF},
- FG co-set $\{FG, BCFG, ADFG, ABCDFG, ABE, CDE, ACE, BDE\}$,
- AE co-set $\{AE, ABCE, DE, BCDE, BFG, ACDFG, CFG, ABDFG\}$,
- AF co-set $\{AF, ABCF, DF, BCDF, BEG, ACDEG, CEG, ABDEG\}$,
- AG co-set $\{AG, ABCG, DG, BCDG, BEF, ACDEF, CEF, ABDEF\}$.

Figure 17 shows the color map and the correlation matrix for the effects columns of the principal group. Based on the following pairs of uncorrelated effects: (BC, AD), (BC, ABCD), and (AD, ABCD), we can construct three-quarter designs of this 4-PFD. We evaluate these designs based on some criteria for ranking the designs, such as the number of MDSs, the number of flats, generalized resolution, the number of estimated MEs and 2FIs, and the orthogonality of MEs as shown in Table 22.





- (a) Color map of correlation for the effects of the principal group.
- (b) Correlation matrix of the effects for the principal group.

Fig. 17.: The correlation of the effects for the principal group.

Table 22.: Properties for constructed three-quarter designs from the principal group of 2^{7-1} .

Pairs of factorial effects	Number of MDSs	Number of flats	Generalized resolution	Number of estimate MEs and 2FIs	Orthognality of MEs
(BC, AD)	one MDS $\{AB, AC, BD, CD\}$	3	2.6667	7 MEs, 17 2FIs	not orthogonal of MEs
(BC, ABCD)	one MDS $\{AB, AC, BD, CD\}$	3	2.6667	7 MEs, 17 2FIs	not orthogonal of MEs
(AD, ABCD)	one MDS $\{AB, AC, BD, CD\}$	3	2.6667	7 MEs, 17 2FIs	not orthogonal of MEs

Theorem 4 Let \mathcal{D} be a two-level orthogonal n-run 4-PFD design. Let (U_1, U_2) be a pair of uncorrelated effects belonging to the principal group of \mathcal{D} . Then, using (U_1, U_2) for blocking \mathcal{D} , produce 4 equal blocks. By omitting any block, the resulting design is a three-quarter design which is 3-PFD.

Proof. Let \mathcal{D} be a two-level orthogonal n-run 4-PFD design, and (U_1, U_2) be a pair of uncorrelated effects belonging to the principal group of \mathcal{D} . By Theorem 3, using

 (U_1, U_2) for blocking \mathcal{D} divides \mathcal{D} into four equal blocks. By the definition of PFDs, the terms in the principal group are constant within each flat, while the terms in each co-set are not necessarily constant within each flat. Thus, since \mathcal{D} is a two-level orthogonal design, each effect of the principal group has one level, either 1 or -1, within each flat. Therefore, the terms of the principal group form a matrix with one unique row within a block. Since, \mathcal{D} has four blocks, then a matrix formed by the terms of the principal group has one unique row within each block, so each block for \mathcal{D} has one unique row. So, each block is corresponding to a single flats. It follows that removing one block corresponds to removing a single flat. Thus, the resulting three-quarter design is 3-PFD.

Example: Consider 4-PFD which is the nonregular 2^{7-1} that shown earlier. The principal group for this design is

$$\{I, ABEFG, CDEFG, ACEFG, BDEFG, BC, AD, ABCD.\}$$

Figure 18 shows that the effects in the principal group form a matrix with an unique row for each block which means each block corresponds to a single flat. Thus, for instance, blocking this 4-PFD by the pair of effects (AD, BC) will have one unique row (-1, -1) in first block, (-1, 1) in the second block, (1, -1) in the third block, and (1, 1) in the fourth block. By eliminating a block (for example, the fourth block), we will have three-quarter with 3 flats.

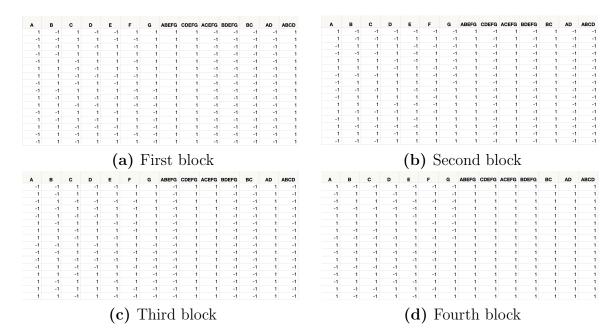


Fig. 18.: Principal group within all the blocks of design 2^{7-1} .

We now consider the proprieties of three-quarter designs which depend on the indicator function for the design. In this regard, the following lemma will be useful.

Lemma 1 (Lemma 3 in Edwards, 2014) Let $F_{\mathcal{A}}$ and $F_{\mathcal{B}}$ be indicator functions of two disjointed designs, \mathcal{A} and \mathcal{B} , respectively. The indicator function of design $\mathcal{A} \cup \mathcal{B}$ is then $F_{\mathcal{A} \cup \mathcal{B}} = F_{\mathcal{A}} + F_{\mathcal{B}}$.

Theorem 5 Let \mathcal{D}_{f_3} be an n-run, k-factor, and three-parallel flat design 3-PFD. Then, the correlation (or inner product) between any two factorial effect columns are either $0, \pm \frac{1}{3}$, or ± 1 .

Proof. Let S_1 , S_2 , and S_3 denote the flats that \mathcal{D}_{f_3} is composed with, respectively.

The indicator function of \mathcal{D}_{f_3} is given by $F_{\mathcal{D}_{f_3}} = F_{S_1} + F_{S_2} + F_{S_3}$, where

$$F_{S_1}(x) = \sum_{l \in P} b_l^1 X_l(x),$$

$$F_{S_2}(x) = \sum_{l \in P} b_l^2 X_l(x),$$

$$F_{S_3}(x) = \sum_{l \in P} b_l^3 X_l(x),$$

 $X_l(x) = \prod_{i \in l} x_i$ for $l \in P$, P is the collection of all subsets of $\{1, 2, ..., k\}$, and $b_l = \frac{1}{2^k} \sum_{x \in H_{f_3}} X_l(x)$. Then,

$$F_{\mathcal{D}_{f_3}} = \sum_{l \in P} b_l^1 X_l(x) + \sum_{l \in P} b_l^2 X_l(x) + \sum_{l \in P} b_l^3 X_l(x)$$
$$F_{\mathcal{D}_{f_3}} = \sum_{l \in P} (b_l^1 + b_l^2 + b_l^3) X_l(x).$$

Since \mathcal{D}_{f_3} is 3-PFD with n-run, by the definition of f-PFD, \mathcal{D}_{f_3} is the combination of three single flat of size $\frac{n}{3}$. Thus, any $b_l^j \neq 0$ will equal $\pm \frac{n}{3}/2^k$, since with regular design, the effects are either orthogonal or fully confounding, where j = 1, 2, 3, so $|b_l^1| = |b_l^2| = |b_l^3|$. Thus, it follows that $b_l^1 + b_l^2 + b_l^3$ equals $\pm n/2^k$, or $\pm \frac{n}{3}/2^k$.

The constant term of the indicator function is $b_{\odot} = n/2^k$. So, the correlation amount between any two factorial effect columns is as follows:

if
$$b_l^j = \pm n/2^k$$
, then, $b_l^j/b_{\oslash} = (\pm n/2^k)/(n/2^k) = \pm 1$,
if $b_l^j = \pm \frac{n}{3}/2^k$, then, $b_l^j/b_{\oslash} = (\pm \frac{n}{3}/2^k)/(n/2^k) = \pm \frac{1}{3}$.

Example: Consider 4-PFD with k=7 and n=64, such that G=0.5(ABEF+CDEF+ACEF-BDEF), which was shown earlier. Blocking this design by (AD,ABCD), where AD and ABCD belong to the principal group, generates four blocks of equal size, each block has run size equals n=16. The indicator function to each block as follows:

- 1. $F_{S_1}(x) = 1/2^7 (16 + 16x_1x_4 16x_2x_3 16x_1x_2x_3x_4 + 16x_1x_2x_5x_6x_7 + 16x_1x_3x_5x_6x_7 16x_2x_4x_5x_6x_7 16x_3x_4x_5x_6x_7),$
- 2. $F_{S_2}(x) = 1/2^7 (16 16x_1x_4 16x_2x_3 + 16x_1x_2x_3x_4 + 16x_1x_2x_5x_6x_7 16x_1x_3x_5x_6x_7 16x_2x_4x_5x_6x_7 + 16x_3x_4x_5x_6x_7),$
- 3. $F_{S_3}(x) = 1/2^7 (16 16x_1x_4 16x_2x_3 16x_1x_2x_3x_4 16x_1x_2x_5x_6x_7 + 16x_1x_3x_5x_6x_7 16x_2x_4x_5x_6x_7 + 16x_3x_4x_5x_6x_7),$
- 4. $F_{S_4}(x) = 1/2^7 (16 + 16x_1x_4 16x_2x_3 + 16x_1x_2x_3x_4 + 16x_1x_2x_5x_6x_7 + 16x_1x_3x_5x_6x_7 + 16x_2x_4x_5x_6x_7 + 16x_3x_4x_5x_6x_7).$

Fontana et al., 2000 propose and prove that if the absolute values of the nonzero coefficients for an indicator function are constant, then the associated design is regular. Otherwise, if the absolute values of the nonzero coefficients are not constant, then the associated design is nonregular design. In the example above, the absolute value of the coefficients to the words in all the indicator functions are constant, which means each indicator function corresponds to a regular design. Now, by omitting S_4 without loss of generality, we obtain a three-quarter design that is 3-PFD. The indicator function to this design, $\mathcal{D}_{3/4}$, is

$$F_{\mathcal{D}_{3/4}}(x) = 1/2^7 (48 - 16x_1x_4 - 16x_2x_3 - 16x_1x_2x_3x_4 + 16x_1x_2x_5x_6x_7 + 16x_1x_3x_5x_6x_7 - 48x_2x_4x_5x_6x_7 + 16x_3x_4x_5x_6x_7).$$

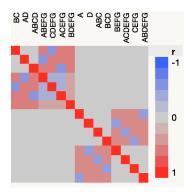
From the indicator function to $\mathcal{D}_{3/4}$, we can see that the correlation amount between X_1, X_4 is $(-16/2^7)/(48/2^7) = -1/3$, and the correlation between X_2X_4 and $X_5X_6X_7$ is $(-48/2^7)/(48/2^7) = -1$.

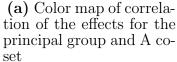
4.4.2 One Effect from the Principal Group and the Other from Any Co-Set

In this subsection, we consider the case in which one effect is selected from the principal group and the other effect is selected from any co-set. As the case of regular design, this case is equivalent to the case where two factorial effects are selected within the same co-set, as shown in Section 4.3. Figure 19 shows the color map correlation and the correlation matrix to the effects of the principal group and A co-set for the 4-PFD, that was shown in the previous subsection. Table 23 shows the pairs of uncorrelated effect that can be used to construct three-quarter designs of this 4-PFD, and the criteria associated with these designs, which are the same as those used in the previous subsection.

Table 23.: Properties for three-quarter designs constructed by blocking using effects from the principal group and A co-set.

Pairs of factorial effects	Number of MDSs	Number of flats	Generalized resolution	Number of estimate MEs and 2FIs	Orthogonality of MEs
(A, BC)	one MDS $\{B, C, AB, AC\}$	6	1.6667	5 MEs, and 19 2FIs	not orthogonal of MEs
(A, AD)	one MDS $\{I, A, D, AD\}$	6	1.6667	5 MEs, and 19 2FIs	not orthogonal of MEs
(A, ABCD)	No MDSs	6	1.6667	all MEs, and 2FIs	not orthogonal of MEs
(ABC, BC)	one MDS $\{B, C, AB, AC\}$	6	1.6667	5 MEs, and 19 2FIs	not orthogonal of MEs
(ABC, AD)	No MDSs	6	2.6667	all MEs, and 2FIs	not orthogonal of MEs
(ABC, ABCD)	No MDSs	6	1.6667	all MEs, and 2FIs	not orthogonal of MEs
(D, BC)	one MDS $\{B, C, BD, CD\}$	6	1.6667	5 MEs, and 17 2FIs	not orthogonal of MEs
(D, AD)	one MDS $\{I, A, D, AD\}$	6	1.6667	6 MEs, and 17 2FIs	not orthogonal ofMEs
(D, ABCD)	No MDSs	6	1.6667	all MEs, and 2FIs	not orthogonal of MEs
(BEFG,BC)	one MDS $\{B, C, AB, AC\}$	6	1.6667	5 MEs, and 19 2FIs	not orthogonal of MEs
(BEFG,AD)	No MDSs	6	2.6667	all MEs, and 2FIs	not orthogonal of MEs
(BEFG,ABCD)	No MDSs	6	1.6667	all MEs, and 2FIs	not orthogonal of MEs
(ACDEFG,BC)	one MDS $\{B, C, BD, CD\}$	6	1.6667	5 MEs, and 19 2FIs	not orthogonal of MEs
(ACDEFG,AD)	one MDS $\{I, A, D, AD\}$	6	1.6667	6 MEs, and 19 2FIs	not orthogonal of MEs
(ACDEFG,ABCD)	No MDSs	6	1.6667	all MEs, and 2FIs	not orthogonal of MEs
(CEFG,BC)	one MDS $\{B, C, AB, AC\}$	6	1.6667	5 MEs, and 19 2FIs	not orthogonal of MEs
(CEFG,AD)	one $MDS\{I, A, D, AD\}$	6	1.6667	6 MEs, and 19 2FIs	not orthogonal of MEs
(CEFG,ABCD)	No MDSs	6	1.6667	all MEs, and 2FIs	not orthogonal of MEs
(ABDEFG,BC)	No MDSs	6	1.6667	all MEs, and 2FIs	not orthogonal of MEs
(ABDEFG,AD)	No MDSs	6	2.6667	all MEs, and 2FIs	not orthogonal of MEs
(ABDEFG,ABCD)	No MDSs	6	1.6667	all MEs, and 2FIs	not orthogonal of MEs



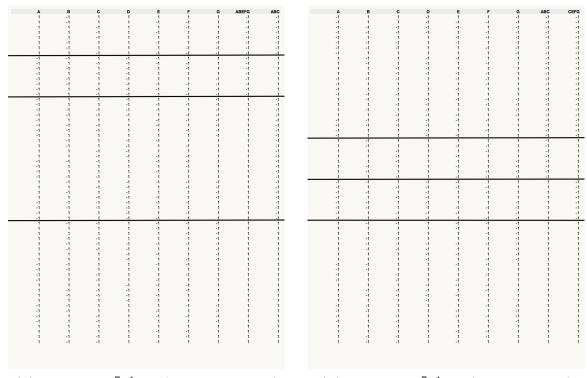




(b) Correlation matrix of the effects for the principal group and A co-set

Fig. 19.: The correlation among the effects for the principal group and A co-set

For this case, we notice that some cases of uncorrelated effects don't divide the design into 4 equal blocks. That is because they are equivalent to correlated effects, such that these effects are selected from the same co-set. For instance, we can see in Figure 19(a), ABC and ABEFG are uncorrelated effects, but we can see in Figure 20(a) they don't divide the 4-PFD into 4 equal blocks. In fact, the pair of effects (ABC, ABEFG) is equivalent to (ABC, CEFG), where both ABC and CEFG belong to the A co-set, and they are correlated effects. Figure 20(b) shows that these effects don't divide the 4-PFD into 4 equal blocks.



(a) Blocking 2^{7-1} by (ABEFG, ABC). (b) Blocking 2^{7-1} by (ABC, CEFG).

Fig. 20.: Blocking nonregular 2^{7-1} by (ABEFG, ABC), and (ABC, CEFG).

Theorem 6 Let \mathcal{D} be a two-level orthogonal n-run 4-PFD design. Let (U_1, U_2) be a pair of uncorrelated effects, where U_1 belongs to the principal group of \mathcal{D} , and U_2 belongs to a co-set of \mathcal{D} . Then, using (U_1, U_2) for blocking \mathcal{D} produce 4 equal block, by omitting any block. The resulting design is a three-quarter design which is 6-PFD.

Proof. Let \mathcal{D} be a two-level orthogonal n-run 4-PFD design, and (U_1, U_2) be a pair of uncorrelated effects, where U_1 belongs to the principal group of \mathcal{D} , and U_2 belongs to a co-set of \mathcal{D} . By theorem 3, using (U_1, U_2) for blocking \mathcal{D} divides \mathcal{D} into four equal blocks. By the definition of PFDs, the terms in the principal group are constant within each flat, while the terms in each co-set are not necessarily constant within each flat. Thus, since \mathcal{D} is a two-level orthogonal design, each effect of the principal group has one level, either 1 or -1 within each flat, however each effect of a co-set

has two levels, -1 and 1, within each flat. Therefore, the terms of the principal group and the co-set form a matrix with two unique rows within a block. Since \mathcal{D} has four blocks, then a matrix formed by the terms of the principal group and the co-set has two unique rows within each block. So, each block is corresponding to two single flats. Thus, it follows that removing one block corresponds to removing two-single flats. Thus, the resulting three-quarter design is 6-PFD.

Example: Consider the 4-PFD in the previous subsection. The principal group for this design is

$$\{BC, AD, ABCD, ABEFG, CDEFG, ACEFG, BDEFG\}$$

and the A co-set is

$$\{A, D, ABC, BCD, BEFG, ACDEFG, CEFG, ABDEFG\}.$$

Figure 21 shows the effects of the principal group and A co-set within each blocks for the 4-PFD. It is clear that the effects of the principal group and the A co-set form a matrix with two unique rows within each block, therefore, each block corresponds to two-single flat. Thus, blocking the 4-PFD by a pair of effects, such that one effect is selected from the principal group, and the other from the A co-set, means combining 8 single flat together. Figure 22 shows blocking the 4-PFD by (BC, ABC) where BC is from the principal group, and ABC is from the A co-set. We can see that the first block has two unique row (-1,1) and (-1,-1), which correspond to two flat with the following defining relations:

•
$$I = -A = -D = -AD = -BC = ABC = -BCD = -ACDEFG =$$

 $CDEFG = ABDEFG = -ACEFG = -BEFG = -BDEFG = CEFG =$
 $ABEFG = ABCD$,

• I = -A = -D = -AD = -BC = ABC = BCD = ACDEFG = CDEFG = -ABDEFG = -ACEFG = BEFG = -BDEFG = -CEFG = ABEFG = ABCD.

The second block has (-1,1) and (-1,-1), which correspond to two single flat with the following defining relations:

- I = -A = -D = AD = BC = ABC = BCD = -ACDEFG = CDEFG = ABDEFG = ACEFG = BEFG = -BDEFG = -CEFG = -ABEFG = -ABCD,
- I = A = D = AD = -BC = -ABC = -BCD = ACDEFG = CDEFG = -ABDEFG = ACEFG = -BEFG = -BDEFG = CEFG = -ABEFG = -ABCD.

In addition, the third block has (1, -1) and (1, 1), which correspond to two single flat with the following defining relations:

- I = -A = D = -AD = -BC = -ABC = BCD = ACDEFG = -CDEFG = ABDEFG = ACEFG = -BEFG = -BDEFG = -CEFG = ABEFG = -ABCD,
- I = A = -D = -AD = BC = ABC = -BCD = -ACDEFG = -CDEFG = -ABDEFG = ACEFG = BEFG = -BDEFG = CEFG = ABEFG = ABCD.

Thus, combining three blocks together will produce a three-quarters design of 6-PFD.

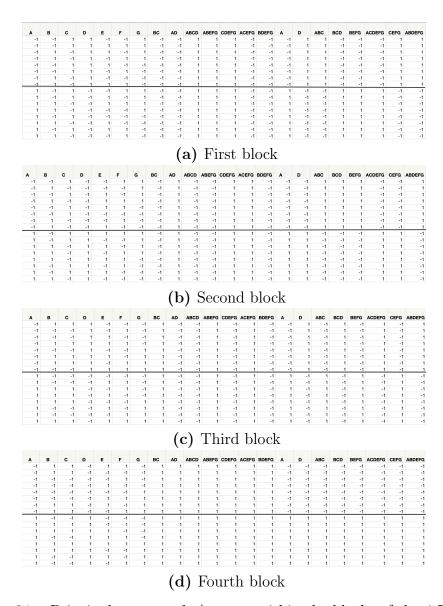


Fig. 21.: Principal group and, A co-set within the blocks of the 4-PFD.

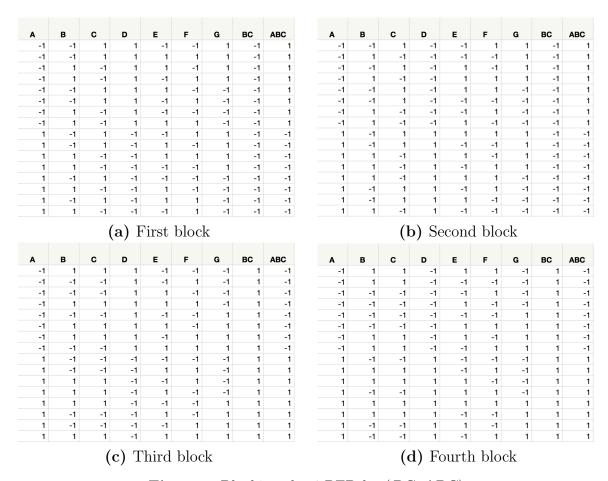


Fig. 22.: Blocking the 4-PFD by (BC, ABC).

Theorem 7 Let \mathcal{D}_{f_6} be an n-run, k-factor, and six-parallel flat design 6-PFD. Then, the correlation (or inner product) between any two factorial effect columns are either $0, \pm \frac{1}{3}, \pm \frac{2}{3}, \text{ or } \pm 1.$

Proof. Let $S_1, S_2, S_3,...,S_6$ denote the flats that \mathcal{D}_{f_6} is composed with, respectively.

The indicator function of \mathcal{D}_{f_6} is given by $F_{\mathcal{D}_{f_6}} = F_{S_1} + F_{S_2} + F_{S_3} + ... + F_{S_6}$, where

$$F_{S_1}(x) = \sum_{l \in P} b_l^1 X_l(x),$$

$$F_{S_2}(x) = \sum_{l \in P} b_l^2 X_l(x),$$

$$F_{S_3}(x) = \sum_{l \in P} b_l^3 X_l(x),$$

$$\vdots$$

$$F_{S_6}(x) = \sum_{l \in P} b_l^6 X_l(x),$$

 $X_l(x) = \prod_{i \in l} x_i$, for $l \in P$, where P is the collection of all subsets of $\{1, 2, ..., k\}$, and $b_l = \frac{1}{2^k} \sum_{x \in H_{f_6}} X_l(x)$.

Thus,

$$\begin{split} F_{\mathcal{D}_{f_6}} &= \sum_{l \in P} b_l^1 X_l(x) + \sum_{l \in P} b_l^2 X_l + \sum_{l \in P} b_{l_X}^3 X_l(x) + \ldots + \sum_{l \in P} b_l^6 X_l(x), \\ F_{\mathcal{D}_{f_6}} &= \sum_{l \in P} (b_l^1 + b_l^2 + b_l^3 + \ldots + b_l^6) X_l(x). \end{split}$$

Since \mathcal{D}_{f_6} is 6-PFD with an n-run, based on the definition of f-PFD, \mathcal{D}_{f_6} is the combination of six single flat of size $\frac{n}{6}$. Thus, any $b_l^j \neq 0$ will equal $\pm \frac{n}{6}/2^k$, since with regular design, the effects are either orthogonal or fully confounding, where j = 1, 2, 3, ..., 6. So, $|b_l^1| = |b_l^2| = |b_l^3| = ... = |b_l^6|$. Thus, it follows that $b_l^1 + b_l^2 + b_l^3 + b_l^4 + b_l^5 + b_l^6$ equals $\pm n/2^k$, $\pm (\frac{4n}{6})/2^k$, $\pm (\frac{2n}{6})/2^k$, or 0.

As in the previous theorem, the constant term of the indicator function of \mathcal{D}_{f_6} is $b_{\odot} = n/2^k$. The correlation amount between any two factorial effect columns as follows:

if
$$b_l^j = \pm n/2^k$$
, $b_l^j/b_{\odot} = (\pm n/2^k)/(n/2^k) = \pm 1$,
if $b_l^j = \pm \frac{4n}{6}/2^k$, $b_l^j/b_{\odot} = (\pm \frac{4n}{6}/2^k)/(n/2^k) = \pm \frac{2}{3}$,
if $b_l^j = \pm \frac{2n}{6}/2^k$, $b_l^j/b_{\odot} = (\pm \frac{2n}{6}/2^k)/(n/2^k) = \pm \frac{1}{3}$,
if $b_l^j = 0$, $b_l^j/b_{\odot} = 0$.

Example: Consider the 4-PFD with n=64, and k=7, such that G=0.5(ABEF+CDEF+ACEF-BDEF) that was shown earlier. Blocking this design by (ABCD, A), where ABCD is selected from the principal group, and A is selected from A co-set generates four blocks, each of size 16. Since, the effects that used for blocking are selected from the principal group and A co-set respectively, based on Theorem 7 each block corresponds to two single flats. So, all four blocks contain 8 single flat. Let $S_1, S_2, S_3, ..., S_8$ denotes to these flats, the indicator function of each flat as follows:

- 1. $F_{S_1}(x) = 1/2^7 (8 8x_1 + 8x_4 8x_1x_4 8x_2x_3 + 8x_1x_2x_3 8x_2x_3x_4 + 8x_1x_2x_3x_4 8x_2x_5x_6x_7 + 8x_3x_5x_6x_7 + 8x_1x_2x_5x_6x_7 8x_1x_3x_5x_6x_7 8x_2x_4x_5x_6x_7 + 8x_3x_4x_5x_6x_7 + 8x_1x_2x_4x_5x_6x_7 8x_1x_3x_4x_5x_6x_7),$
- 2. $F_{S_2}(x) = 1/2^7(8 8x_1 8x_4 8x_1x_4 8x_2x_3 8x_1x_2x_3 + 8x_2x_3x_4 + 8x_1x_2x_3x_4 + 8x_2x_5x_6x_7 8x_3x_5x_6x_7 + 8x_1x_2x_5x_6x_7 8x_1x_3x_5x_6x_7 8x_2x_4x_5x_6x_7 + 8x_1x_3x_4x_5x_6x_7 8x_2x_4x_5x_6x_7 + 8x_1x_3x_4x_5x_6x_7),$
- 3. $F_{S_3}(x) = 1/2^7(8 8x_1 8x_4 + 8x_1x_4 8x_2x_3 + 8x_1x_2x_3 + 8x_2x_3x_4 8x_1x_2x_3x_4 + 8x_2x_5x_6x_7 8x_3x_5x_6x_7 x_1x_2x_5x_6x_7 + 8x_1x_3x_5x_6x_7 8x_2x_4x_5x_6x_7 + 8x_3x_4x_5x_6x_7 + 8x_1x_2x_4x_5x_6x_7 8x_1x_3x_4x_5x_6x_7),$
- 4. $F_{S_4}(x) = 1/2^7(8 + 8x_1 + 8x_4 + 8x_1x_4 8x_2x_3 8x_1x_2x_3 8x_2x_3x_4 8x_1x_2x_3x_4 8x_2x_5x_6x_7 + 8x_3x_5x_6x_7 8x_1x_2x_5x_6x_7 + 8x_1x_3x_5x_6x_7 8x_2x_4x_5x_6x_7 + 8x_1x_3x_4x_5x_6x_7 8x_2x_4x_5x_6x_7 + 8x_1x_3x_4x_5x_6x_7),$
- 5. $F_{S_5}(x) = 1/2^7 (8 8x_1 + 8x_4 8x_1x_4 + 8x_2x_3 8x_1x_2x_3 + 8x_2x_3x_4 + 8x_1x_2x_3x_4 8x_2x_5x_6x_7 8x_3x_5x_6x_7 + 8x_1x_2x_5x_6x_7 + 8x_1x_3x_5x_6x_7 + 8x_2x_4x_5x_6x_7 8x_3x_4x_5x_6x_7 + 8x_1x_2x_4x_5x_6x_7 + 8x_1x_3x_4x_5x_6x_7),$
- 6. $F_{S_6}(x) = 1/2^7(8 + 8x_1 8x_4 8x_1x_4 + 8x_2x_3 + 8x_1x_2x_3 8x_2x_3x_4 8x_1x_2x_3x_4 + 8x_1x_2x_3 + 8x_1x_2x_3 8x_2x_3x_4 8x_1x_2x_3 + 8x_1x_2x_3 8x_2x_3x_4 8x_1x_2x_3 8x_1x$

 $8x_2x_5x_6x_7 + 8x_3x_5x_6x_7 + 8x_1x_2x_5x_6x_7 + 8x_1x_3x_5x_6x_7 - 8x_2x_4x_5x_6x_7 - 8x_3x_4x_5x_6x_7 - 8x_1x_2x_4x_5x_6x_7 - 8x_1x_3x_4x_5x_6x_7),$

- 7. $F_{S_7}(x) = 1/2^7 (8 8x_1 8x_4 + 8x_1x_4 + 8x_2x_3 8x_1x_2x_3 8x_2x_3x_4 + 8x_1x_2x_3x_4 8x_2x_5x_6x_7 8x_3x_5x_6x_7 + 8x_1x_2x_5x_6x_7 + 8x_1x_3x_5x_6x_7 + 8x_2x_4x_5x_6x_7 + 8x_3x_4x_5x_6x_7 8x_1x_2x_4x_5x_6x_7 8x_1x_3x_4x_5x_6x_7),$
- 8. $F_{S_8}(x) = 1/2^7(8 + 8x_1 + 8x_4 + 8x_1x_4 + 8x_2x_3 + 8x_1x_2x_3 + 8x_2x_3x_4 + 8x_1x_2x_3x_4 + 8x_2x_5x_6x_7 + 8x_3x_5x_6x_7 + 8x_1x_2x_5x_6x_7 + 8x_1x_3x_5x_6x_7 + 8x_1x_3x_5x_6x_7 + 8x_1x_3x_4x_5x_6x_7 + 8x_1x_3x_5x_6x_7 + 8x_1x_5x_6x_7 + 8x_1x_5x_6$

By removing a quarter of the run size, which is involved two single flat, we obtain a three-quarter design $\mathcal{D}_{3/4}$, that is six flat with indicator function given by:

$$F_{\mathcal{D}_{3/4}}(x) = 1/2^7 (48 - 16x_1x_2 - 16x_2x_3 - 16x_1x_2x_3x_4 + 16x_1x_2x_5x_6x_7 + 16x_1x_3x_5x_6x_7 - 48x_2x_4x_5x_6x_7 + 16x_3x_4x_5x_6x_7)$$

From the indicator function of $\mathcal{D}_{3/4}$, the correlation amount between X_2 , and X_3X_4 is $(-16/2^7)/(48/2^7) = -1/3$, and the correlation between X_2X_4 and $X_5X_6X_7$ is $(-48/2^7)/(48/2^7) = -1$.

4.4.3 Both Effects from Different Co-sets

With block diagonal structure design, any two effects belonging to different blocks are uncorrelated. In fact, these blocks are corresponding to the co-sets for a design. That means for 4-PFD, we are able to construct three-quarter designs from any two effects, where they are from two different co-sets. Figure 15 shows the correlation of the effects for A, and B co-sets for the 4-PFD that was shown in the previous subsection. Table 9 shows the properties of three-quarter designs, which were constructed by blocking the 4-PFD by a pair of effects where they were selected from A and B co-sets.

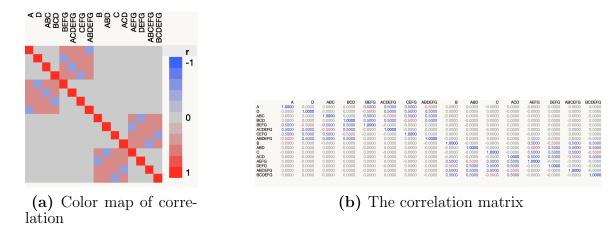


Fig. 23.: The correlation of the effects for A and B co-sets.

Table 24.: Properties for three-quarter designs constructed by blocking using effect from A and B co-sets.

Pairs of factorial effects	number of MDSs	Number of flats	Generalized resolution	Number of estimate MEs and 2FIs	Orthogonality of MEs
(A, B)	one MDS $\{I, A, B, AB\}$	12	1.6667	5 MEs, and 20 2FIs	not orthogonal to MEs
(A, C)	one MDS $\{I, A, C, AC\}$	12	1.6667	5 MEs, and 20 2FIs	not orthogonal to MEs
(A, ABD)	one MDS $\{B, D, AB, AD\}$	12	1.6667	5 MEs, and 19 2FIs	not orthogonal to MEs
(A, ACD)	one MDS $\{C, D, AC, AD\}$	12	1.6667	5 MEs, and 19 2FIs	not orthogonal to MEs
(A, AEFG)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(A, BCDEFG)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(A, ABCEFG)	No MDSs	12	1.6667	All MEs, and 2FIs	not orthogonal to MEs
(A, DEFG)	No MDSs	12	1.6667	All MEs, and 2FIs	not orthogonal to MEs
(D, B)	one MDS $\{I, B, D, BD\}$	12	1.6667	5 MEs, and 20 2FIs	not orthogonal to MEs
(D,C)	one MDS $\{I, C, D, CD\}$	12	1.6667	5 MEs, and 20 2FIs	not orthogonal to MEs
(D,ABD)	one MDS $\{A, B, AD, BD\}$	12	1.6667	5 MEs, and 19 2FIs	not orthogonal to MEs
(D,ACD)	one MDS $\{A, C, AD, CD\}$	12	1.6667	5 MEs, and 19 2FIs	not orthogonal to MEs
(D, AEFG)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(D, BCDEFG)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(D,ABCEFG)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(D,DEFG)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(ABC,B)	one MDS $\{I, B, D, BD\}$	12	1.6667	all MEs, and 20 FIs	not orthogonal toMEs
(ABC,C)	one MDS $\{I, C, D, CD\}$	12	1.6667	5 MEs, and 20 2FIs	not orthogonal toMEs
(ABC,ABD)	one MDS $\{A, B, AD, BD\}$	12	1.6667	5 MEs, and 19 2FIs	not orthogonal toMEs
(ABC,ACD)	one MDS $\{A, C, AD, CD\}$	12	1.6667	5 MEs, and 19 2FIs	not orthogonal toMEs
(ABC,AEFG)	No MDSs	12	1.6667	all MEs, and 2FI	not orthogonal to MEs
(ABC,BCDEFG)	No MDSs	12	1.6667	all MEs, and 2FI	not orthogonal to MEs
(ABC,ABCEFG)	No MDSs	12	1.6667	all MEs, and 2FI	not orthogonal to MEs
(ABC,DEFG)	No MDSs	12	1.6667	all MEs, and 2FI	not orthogonal to MEs
(BCD, B)	one MDS $\{C, D, BC, BD\}$	12	1.6667	5 MEs, and 19 2FIs	not orthogonal to MEs
(BCD, C)	one MDS $\{B, D, BC, CD\}$	12	1.6667	5 MEs, and 19 2FIs	not orthogonal to MEs
(BCD, ABD)	No MDSs	12	2.6667	all MEs, and 2FIs	not orthogonal to MEs
(BCD, ABD)	No MDSs	12	2.6667	all MEs, and 2FIs	not orthogonal to MEs
(BCD, ACD)	No MDSs	12	2.6667	all MEs, and 2FIs	not orthogonal to MEs
(BCD, AEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(BCD, BCDEFG)	No MDSs	12	1.8333	All MEs, and 2FIs	not orthogonal to MEs
(BCD, ABCEFG)	No MDSs	12	1.8333	All MEs, and 2FIs	not orthogonal to MEs
(BCD, DEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(BEFG, B)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(BEFG,C)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(BEFG,ABD)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(BEFG, ACD)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(BEFG, AEFG)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(BEFG,BCDEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(BEFG, ABCEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(BEFG, DEFG)	No MDSs	12 12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(CEFG, B)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(CEFG, C)	No MDSs	12	1.6667	all MEs, and 2FIs all MEs, and 2FIs	not orthogonal to MEs not orthogonal to MEs
(CEFG, ABD)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(CEFG, ACD) (CEFG, AEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(CEFG, AEFG) (CEFG, BCDEFG)	No MDSs No MDSs	12	1.8333 1.8333	all MEs, and 2FIs	not orthogonal to MEs
(CEFG, BCDEFG)	No MDSs No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(CEFG, DEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ACDEFG, B)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(ACDEFG, C)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(ACDEFG, ABD)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ACDEFG, ACD)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ACDEFG, AEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ACDEFG, BCDEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ACDEFG, ABCEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ACDEFG, DEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ABDEFG, B)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(ABDEFG, C)	No MDSs	12	1.6667	all MEs, and 2FIs	not orthogonal to MEs
(ABDEFG, ABD)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ABDEFG, ACD)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ABDEFG, AEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ABDEFG, BCDEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ABDEFG, ABCEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
(ABDEFG, DEFG)	No MDSs	12	1.8333	all MEs, and 2FIs	not orthogonal to MEs
	1		1		

Theorem 8 Let \mathcal{D} be a two-level orthogonal n-run 4-PFD design. Let (U_1, U_2) be a pair of uncorrelated effects, where U_1 and U_2 belong to different co-sets of \mathcal{D} . Then,

using (U_1, U_2) for blocking \mathcal{D} , produce 4 equal blocks by omitting any block. The resulting design is a three-quarter design which is twelve flats.

Proof. Let \mathcal{D} be a two-level orthogonal n-run 4-PFD design, and (U_1, U_2) be a pair of uncorrelated effects, where U_1 and U_2 belong to two different co-sets of \mathcal{D} . By Theorem 3, using uncorrelated (U_1, U_2) for blocking \mathcal{D} , divides \mathcal{D} into four equal blocks. By the definition of PFDs, the terms in the principal group are constant within each flat, while the terms in each co-set are not necessarily constant within each flat. Thus, since \mathcal{D} is a two-level orthogonal design, each effect of a co-set has two levels, -1 and 1, within each flat. Therefore, the terms of two different co-sets form a matrix with four unique row within a block. Since, \mathcal{D} has four blocks, then a matrix formed by the terms of two different co-sets has four unique row within each block. So, each block is corresponding to four-single flat. Thus, it follows that removing one block corresponds to removing four-single flat. Thus, the resulting three-quarter design is 12-PFD.

Example: Consider the 4-PFD with n=64, and k=7, such that G=0.5(ABEF + CDEF + ACEF - BDEF) as was shown earlier. The B and F co-sets of \mathcal{D} are

$$\{B,C,ABD,ACD,AEFG,BCDEFG,ABCEFG,DEFG\},$$

$$\{F, BCF, ADF, ABCDF, ABEG, CDEG, ACEG, BDEG\}$$

respectively. Since any two effects from B, and F are uncorrelated, then blocking the 4-PFD by a pair of effects, that selected from B and F, divides the 4-PFD into 4 blocks of size n=16. Figure 24 shows the effects of B and F co-sets within each block. It is clear that the effects for the co-sets B and F form a matrix with four unique rows for each block. So, using a pair of effects, for example, (ABD, ADF) to

block the 4-PFD such that ABD and ADF are selected from B and F, respectively, divides the 4-PFD into 4 equal blocks, each block has four single flats of size 4. Figure 25 shows the four blocks of the 4-PFD when using the pair of effects (ABD, ADF) for blocking. Thus, this 4-PFD is a combination of 16 single flats. By removing one block, which contains four single flats, the three-quarter design is twelve flats.

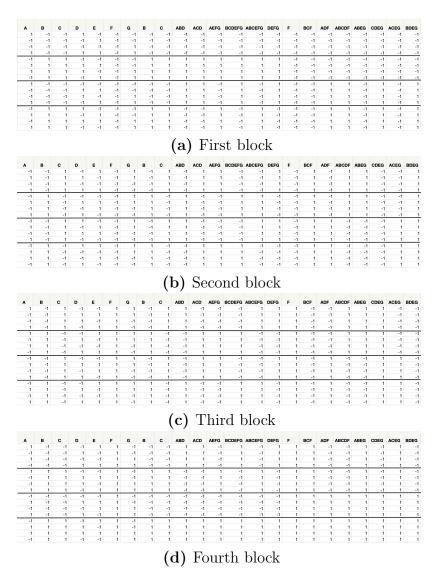


Fig. 24.: B, and F co-sets within the blocks for the 4-PFD.

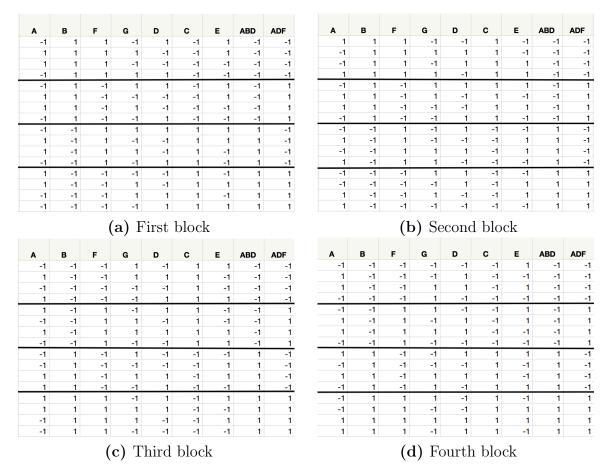


Fig. 25.: Blocking the 4-PFD by (ABD, ADF).

Theorem 9 Let $\mathcal{D}_{f_{12}}$ be an n-run, k-factor, and twelve-parallel flat design 12-PFD. Then, the correlation (or inner product) between any two factorial effect columns are either ± 1 , $\pm \frac{5}{6}$, $\pm \frac{2}{3}$, $\pm \frac{1}{2}$, $\pm \frac{1}{3}$, $\pm \frac{1}{6}$, or 0.

Proof. Let S_1 , S_2 , S_3 ,..., S_{12} denote the flats that $\mathcal{D}_{f_{12}}$ is composed with, respectively. The indicator function of $\mathcal{D}_{f_{12}}$ is given by $F_{\mathcal{D}_{f_{12}}} = F_{S_1} + F_{S_2} + F_{S_3} + F_{S_4} + ... + F_{S_{12}}$, where

$$F_{S_1}(x) = \sum_{l \in P} b_l^1 X_l(x),$$

$$F_{S_2}(x) = \sum_{l \in P} b_l^2 X_l(x),$$

$$F_{S_3}(x) = \sum_{l \in P} b_l^3 X_l(x),$$

$$\vdots$$

$$F_{S_{12}}(x) = \sum_{l \in P} b_l^{12} X_l(x)$$

where $X_l(x) = \prod_{i \in l} x_i$, for $l \in P$, where, P is the collection of all subsets of $\{1, 2, ..., k\}$, and $b_l = \frac{1}{2^k} \sum_{x \in \mathcal{D}_{f_{12}}} X_l(x)$.

Thus,

$$F_{\mathcal{D}_{f_{12}}} = \sum_{l \in P} b_l^1 X_l(x) + \sum_{l \in P} b_l^2 X_l + \sum_{l \in P} b_l^3 X_l(x) + \dots \sum_{l \in P} b_l^{12} X_l(x),$$

$$F_{\mathcal{D}_{f_{12}}} = \sum_{l \in P} (b_l^1 + b_l^2 + b_l^3 + \dots + b_l^{12}) X_l(x).$$

Since $\mathcal{D}_{f_{12}}$ is twelve flats with n-run, based on the definition of f-PFD, $\mathcal{D}_{f_{12}}$ is combination of twelve single flats of size $\frac{n}{12}$. Thus, any $b_l^j \neq 0$ will equal $\pm \frac{n}{12}/2^k$, since with regular design, the effects are either orthogonal or fully confounding, where j=1,2,3,...,12. So, $|b_l^1|=|b_l^2|=|b_l^3|=...=|b_l^{12}|$. Thus, it follows that $b_l^1+b_l^2+b_l^3+...+b_l^{12}$ equals $\pm n/2^k$, $\pm (\frac{10n}{12})/2^k$, $\pm (\frac{8n}{12})/2^k$, $\pm (\frac{6n}{12})/2^k$, $\pm (\frac{4n}{12})/2^k$, or 0.

As in the previous theorems, the constant term of the indicator function for $\mathcal{D}_{f_{12}}$ is $b_{\odot} = n/2^k$. The correlation amount will be as follows:

if
$$b_l^j = \pm n/2^k$$
, then $b_l^j/b_{\oslash} = (\pm n/2^k)/(n/2^k) = \pm 1$,
if $b_l^j = \pm \frac{10n}{12}/2^k$, $b_l^j/b_{\oslash} = (\pm \frac{10n}{12}/2^k)/(n/2^k) = \pm 5/6$,
if $b_l^j = \pm \frac{8n}{12}/2^k$, then $b_l^j/b_{\oslash} = (\pm \frac{8n}{12}/2^k)/(n/2^k) = \pm 2/3$,
if $b_l^j = \pm \frac{6n}{12}/2^k$, then $b_l^j/b_{\oslash} = (\pm \frac{6n}{12}/2^k)/(n/2^k) = \pm 1/2$,
if $b_l^j = \pm \frac{4n}{12}/2^k$, then $b_l^j/b_{\oslash} = (\pm \frac{4n}{12}/2^k)/(n/2^k) = \pm 1/3$,
if $b_l^j = \pm \frac{2n}{12}/2^k$, then $b_l^j/b_{\oslash} = (\pm \frac{2n}{12}/2^k)/(n/2^k) = \pm 1/6$.

Example: Consider the 4-PFD, which is 2^{7-1} , with the generators G = 0.5(ABEF + CDEF + ACEF - BDEF) that was shown earlier. By blocking this design by (ABC, ABEG), where they belong to A and F co-sets respectively, we obtain 4 blocks, each of size n=16. By removing the fourth block without loss the generality, we have a three-quarter design $\mathcal{D}_{3/4}$, with an indicator function as follows: $F_{\mathcal{D}_{f_{12}}}(x) = 1/2^7(48 - 16x_1 - 16x_4 - 16x_1x_4 - 16x_3x_5x_6x_7 + 32x_1x_2x_5x_6x_7 + 16x_1x_3x_5x_6x_7 - 32x_2x_4x_5x_6x_7 + 16x_3x_4x_5x_6x_7 - 16x_1x_3x_4x_5x_6x_7)$

The coefficient of the words in the indicator function of three-quarter design $\mathcal{D}_{3/4}$ is either ± 16 , or ± 32 . So, the correlation amount between any effects for this three-quarter design is either $\pm 1/3$, or $\pm 2/3$. For example, the correlation amount between X_1X_4 is $(\frac{-16}{64})/(\frac{48}{64}) = \frac{-1}{3}$, and the correlation between X_2 and $X_4X_5X_6X_7$ is $(\frac{-32}{64})/(\frac{48}{64}) = \frac{2}{3}$.

4.5 Three-Quarter Designs and MDSs

In the previous section, we found that some three-quarter designs produce an MDSs of size 4, while in some cases, three-quarter designs do not produce MDSs. For example, consider the AG co-set of the 4-PFD, which is 2^{7-1} that was shown earlier.

$$\{AG, ABCG, DG, BCDG, BEF, ACDEF, CEF, ABDEF\}.$$

From this co-set, we are able to construct three-quarter designs based on 12 pairs of uncorrelated effects, 6 of these pairs are producing one MDS of size 4, while the other 6 pairs are not. Table 25 shows the pairs of effects that are producing/not producing MDSs from the AG co-set.

Table 25.: Pairs of blocking effects that producing/not producing MDSs from AG co-set of the 4-PFD.

Pairs of factorial effects	MDSs
(AG, ABCG)	$\{AB, AC, BG, CG\}$
(AG, DG)	$\{I, AD, AG, DG\}$
(DG, BCDG)	$\{BD, BG, CD, CG\}$
(BEF,CEF)	AB, AC, BG, CG
(ACDEF, CEF)	$\{I, AD, AG, DG\}$
(ACDEF, ABDEF)	$\{BD, BG, CD, CG\}$
(AG, BCDG)	No MDSs
(ABCG, DG)	No MDSs
(ABCG, BCDG)	No MDSs
(CEF, ABDEF)	No MDSs
(BEF, ACDEF)	No MDSs
(BEF, ABDEF)	No MDSs

Consider Generalized Alias Length Pattern (GALP) to evaluate three-quarter designs that produce MDSs and those that do not. GALP was first produced by Cheng et al., 2008 as a measure of aliasing for 2FIs to strength 3 arrays. Mee, 2013 defined this criterion for strength 3 arrays as the main diagonal of the matrix $(X'X/n)^2$, where X is the model matrix for the 2FIs interaction model. Mee, 2013 noted that the minimum value for the *ith* element of $(X'X/n)^2$ is 1, which would indicates that the *ith* column is uncorrelated with every other column.

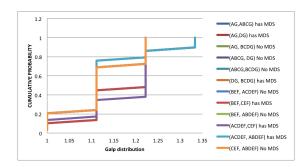


Fig. 26.: GALP distribution for three-quarter design that constructed from *AG* co-set of the 4-PFD.

Figure 26 shows GALP distribution for the three-quarter designs that were constructed by blocking the 4-PFD using a pair of effects that were selected from the AG co-set. The GALP distribution of three-quarter designs, that were constructed based on blocking the 4-PFD by the following pairs of effects:

$$(AG, BCDG), (ABCG, DG), (ABCG, BCDG),$$

 $(CEF, ABDEF)(BEF, ACDEF), (BEF, ABDEF)$

$$(4.6)$$

are overlapping, which is represented by the orange line in Figure 26. Table 25 shows that using one of these pairs for constructing three-quarter design of the 4-PFD doesn't produce an MDS. Thus, it seems reasonable that these pairs of effects have the same GALP distribution.

Also, the GALP distribution for three-quarter designs, that constructed by blocking on the following pairs: (DG, BCDG), (ACDEF, ABDEF) are overlapping, which represented by blue line in Figure 26. Each of these pairs provides a three-quarter design, that produces the same MDS, which is $\{BD, BG, CD, CG\}$ as shown in Table 25, which might be the reason to have same GALP distribution.

Moreover, the GALP distribution for three-quarter designs, that were constructed by blocking on the following pairs: (AG, ABCG), (BEF, CEF), are overlapping, which is represented by dark red line in Figure 18 and again they produce same MDS. Also, the purple line in Figure 18 represents the GALP distribution of three-quarter designs that were constructed by blocking the 4-PFDs on the pairs of uncorrelated effects (AG, DG), (ACDEF, CEF), and they produce the same MDS as shown in Table 25.

Based on the plot in Figure 26, the three-quarter designs that don't produce MDSs (orange line) have less distinct values of GALP than the other three-quarter designs. Also, the largest value for the GALP to these designs is 1.22, which is less

than the other three-quarter designs, which have 1.33. Also, the *GALP* for these designs have the lowest aliasing for MEs and 2FIs. Thus, our recommendation is that the three-quarter designs that don't produce MDSs are the best designs among the other three-quarter designs, especially, for identifying the active MEs and 2FIs.

4.6 Comparison between Three-Quarter of Regular Design and Three-Quarter of 4-PFD Design

In this section, we provide a comparison between three-quarter of a regular design and three-quarter of 4-PFD design. We will compare these designs based on the usual criteria for ranking designs, such as estimation capacity (EC), projection estimation capacity (PEC), projection information capacity (PIC), and generalized aliasing length pattern (GALP).

4.6.1 Projection Estimation Capacity PEC

Loeppky et al., 2007 defined a PEC as a sequence $(k_1, k_2, ..., k_r)$, where k_i is the proportion of estimable models for i MEs and their associated 2FIs. Li and Aggarwal, 2008 defined the PEC as an integer q, such that the 2FIs model is estimable for every subset of q factor. In this subsection, we will compare three-quarter design of regular/4-PFD design based on PEC. Let \mathcal{D}_{1r} denote a three-quarter design of regular design 2^{7-1} , with generator G = ABCDEF. Consider the 4-PFD which is a nonregular 2^{7-1} as was shown in Section 4.4. Let \mathcal{D}_{1f_3} denote a three-quarter design that was constructed by blocking the 4-PFDs using two effects from the principal group, \mathcal{D}_{1f_6} denotes a three-quarter design that was constructed by blocking the 4-PFD using two effects, where one effect is from the principal group and the other from any co-set, and $\mathcal{D}_{1f_{12}}$ denotes a three-quarter design that was constructed by blocking the 4-PFD, using two effects from different co-sets.

Table 26.: Projection estimation capacity criteria for three-quarter designs with k=7 and n=48

Design	PEC_1	PEC_2	PEC_3	PEC_4	PEC_5	PEC_6	PEC_7
\mathcal{D}_{1r}	1	1	1	1	1	1	1
\mathcal{D}_{1f_3}	1	1	1	0.9714	0.8571	0.5714	0
\mathcal{D}_{1f_6}	1	1	1	1	1	1	1
$\mathcal{D}_{1f_{12}}$	1	1	1	1	1	1	1

Table 26, shows that \mathcal{D}_{1r} , \mathcal{D}_{1f_6} , and $\mathcal{D}_{1f_{12}}$ have identical PEC. Based on the assumption of factor sparsity, by using these designs, the 2FIs model can be estimated for any subset of 1 to 7 factors. For instance, for design \mathcal{D}_{1f_6} , the two factor interaction model is estimable for any subset of 7 factor since $PEC_7=1$, while for design \mathcal{D}_{1f_3} , there is no 2FIs model that could be estimable for any subset of 7 factors because $PEC_7=0$ for this design. For the considered designs, we notice that PEC for three-quarter of regular design \mathcal{D}_{1r} is better than PEC for \mathcal{D}_{1f_3} , while, it is equivalent to \mathcal{D}_{1f_6} and $\mathcal{D}_{1f_{12}}$. This could suggest an equal efficiency for both three-quarter designs of regular/4-PFD designs, based on PEC of the considered designs.

Let \mathcal{D}_{2r} denote a three-quarter design of regular design 2^{6-1} , with generator F = ABCD. Consider the 4-PFD which is a nonregular design 2^{6-1} with n=32, and k=6, such that F = 0.5E(AB + AC + BD - CD) that was shown in Section 4.2. Let \mathcal{D}_{2f_3} denote a three-quarter design that was constructed by blocking this 4-PFD using two effects were selected from the principal group, \mathcal{D}_{2f_6} denote a three-quarter design that was constructed by blocking this 4-PFD using two effects, where one effect was selected from the principal group and the other from any co-set, and $\mathcal{D}_{2f_{12}}$ denote a three-quarter design that was constructed by blocking this 4-PFD, using two effects were selected from different co-sets. Table 27 shows the comparison of these designs

based on PEC.

Table 27.: Projection estimation capacity criteria for three-quarter designs with k=6 and n=24

Design	PEC_1	PEC_2	PEC_3	PEC_4	PEC_5	PEC_6
\mathcal{D}_{2r}	0.9809	0.9028	0.7680	0.5622	0.2978	0
\mathcal{D}_{2f_3}	1	0.9924	0.9803	0.8324	0.2978	0
\mathcal{D}_{2f_6}	0.9905	0.9771	0.9155	0.7327	0.2691	0
$\mathcal{D}_{2f_{12}}$	0.9953	0.9866	0.9660	0.9104	0.8075	0

In this example, we found that all three-quarters designs of 4-PFD design \mathcal{D}_{2f_3} , \mathcal{D}_{2f_6} , and $\mathcal{D}_{2f_{12}}$ are better than three-quarter deign of regular design \mathcal{D}_{2r} based on PEC. For design $\mathcal{D}_{2f_{12}}$ the two factor interaction model can be estimated around 14 out of the 15 four-factor projections, and for \mathcal{D}_{2f_3} the two factor interaction model can be estimated for 12 out of the 15 four-factor projections. Design \mathcal{D}_{2f_6} is slightly worse with around 11/15, while \mathcal{D}_{2r} is the worst among designs with around 8/15. Thus, $\mathcal{D}_{2f_{12}}$ is recommended design for estimating a large number of two factor interaction models.

4.6.2 Estimation Capacity (EC)

Estimation capacity (EC) is a vector, $(EC_1, EC_2, EC_3..., EC_g)$, of the proportions of estimable models with all k MEs and $\{1, 2, ..., g\}$ 2FIs. Jones et al., 2009 illustrated that the estimation capacity is the key characteristic of the supersaturated designs. Jones et al., 2009 defined estimation capacity, for supersaturated designs as

number of estimable g-term main-effect models total number of g-term main-effect models

such that $EC_g = 1$, which indicates that all models with k MEs, and g 2FIs are estimable. Table 28 shows this criteria for a three-quarter design of the regular design 2^{7-1} , and four cases of three-quarter design of the 4-PFD that we discussed in the previous subsection.

Table 28.: Estimation capacity for three quarters designs with k=7 and n=48

Design	EC_1	EC_2	EC_3	EC_4	EC_5	EC_6	EC_7
\mathcal{D}_{1r}	0.9524	0.9048	0.8571	0.8095	0.7619	0.7143	0.6667
\mathcal{D}_{1f_3}	1	1	1	0.9998	0.9992	0.9975	0.9942
\mathcal{D}_{1f_6}	1	1	1	1	1	1	1
$\mathcal{D}_{1f_{12}}$	1	1	1	1	1	1	1

From Table 28, we have two cases of three-quarter designs of 4-PFD \mathcal{D}_{1f_6} and $\mathcal{D}_{1f_{12}}$ having 100% for all the sequences of EC, which indicate high efficiency of these designs for estimating every possible model with k=7 MEs and g=7 2FIs. However, the three-quarter design of regular design \mathcal{D}_{1r} has around 95% for EC_1 , which means not all possible models of 7 MEs, and only 1 2FIs, are estimable. Thus, the EC of three-quarter design of 4-PFD is impressive, since it is guaranteed to find the true model for 7 MEs, and at most 7 2FIs, by using \mathcal{D}_{1f_6} or $\mathcal{D}_{1f_{12}}$.

Again consider the three-quarter design of regular design \mathcal{D}_{2r} which is 2^{6-1} , and the four cases of three-quarters design of the 4-PFD which is a nonregular design 2^{6-1} , that were shown in the previous subsection. Table 29 shows the comparison of these designs based on EC. The estimation capacity is excellent for all these designs. Design $\mathcal{D}_{2f_{12}}$ has the highest estimation capacity. As the previous example of comparing three-quarter design of regular/4-PFD design, all three quarter designs of 4-PFD design are superior to three-quarter of regular design. This comparing

indicates the effectiveness of these designs for estimation models with MEs and 2FIs.

Table 29.: Estimation capacity for three quarters designs with k=6 and n=24

Design	EC_1	EC_2	EC_3	EC_4	EC_5	EC_6
\mathcal{D}_{2r}	0.9333	0.8667	0.7934	0.7092	0.6117	0.5017
\mathcal{D}_{2f_3}	1	0.9714	0.9143	0.8293	0.7186	0.5870
\mathcal{D}_{2f_6}	1	0.9905	0.9692	0.9341	0.8831	0.8152
$\mathcal{D}_{2f_{12}}$	1	1	1	1	0.9997	0.9980

For the two cases designs with factors k=6 and 7, we note the highest EC associated with the 12-PFD. The reason of that is a design with a larger number of flats means fewer (but larger) aliasing sets than a design with a smaller number of flats. As a result, the MDSs of a 12-PFD are larger than a design with a smaller number of flats, which leads to increased model estimation, and enhanced EC.

4.6.3 Projection Information Capacity (PIC)

Sun, 1994, Li and Nachtsheim, 2000, and Mee et al., 2017 defined the Projection Information Capacity (PIC) as augmenting EC with the mean D-efficiency across all models of equal size. Table 30 shows the PIC sequence of the comparative designs for the case of k=7 and n=48, and Table 31 shows the PIC sequence of the comparative designs for the case of k=6 and n=24.

Table 30.: Projection information capacity for three-quarter designs with k=7 and n=48

Design	PIC_1	PIC_2	PIC_3	PIC_4	PIC_5	PIC_6	PIC_7
\mathcal{D}_{1r}	0.9990	0.9943	0.9853	0.9714	0.9518	0.9253	0.8891
\mathcal{D}_{1f_3}	1.0000	0.9946	0.9859	0.9499	0.8331	0.5534	0
\mathcal{D}_{1f_6}	0.9918	0.9837	0.9775	0.9696	0.9579	0.9417	0.9208
$\mathcal{D}_{1f_{12}}$	0.9918	0.9837	0.9782	0.9716	0.9620	0.9478	0.9275

Table 31.: Projection information capacity for three-quarter designs with k=6 and n=24

Design	PIC_1	PIC_2	PIC_3	PIC_4	PIC_5	PIC_6
\mathcal{D}_{2r}	0.9809	0.9028	0.7680	0.5622	0.2978	0
\mathcal{D}_{2f_3}	1.0000	0.9924	0.9803	0.8324	0.2978	0
\mathcal{D}_{2f_6}	0.9905	0.9771	0.9155	0.7327	0.2691	0
$\mathcal{D}_{2f_{12}}$	0.9953	0.9866	0.9660	0.9104	0.8075	0

For case k=7 and n=48, clearly, $\mathcal{D}_{1f_{12}}$ and \mathcal{D}_{1r} both have the highest values for the sequences of PIC, so these designs are the best designs with respect to PIC. The case with k=6 and n=24, all the design have excellent PIC, however, three-quarter of regular design is slightly worse. Again this show the effectiveness of these designs for estimating models.

4.6.4 Generalize Resolution (GR)

Let, j-interaction columns be denoted as the product for j MEs. For a regular design, the sum for this column is either $\pm n$ or 0. If the sum is n, that means this column forms a full aliasing, which means it is difficult to estimate this column. How-

ever, if the sum is 0, that corresponds to orthogonality, which allows for estimating this column independently from other columns. For nonregular designs, this sum may take different values than $\pm n$ or 0, which indicates partial aliasing among the columns. The absolute value for the maximum number of the sum of j-interaction columns is called J-characteristic. Generalized resolution is defined as p = t + (2 - J/n), such that t is the strength of the design, J is the J-characteristic, and n is the run size.

Table 32.: Generalize resolution for three-quarter designs with 7 factors and n=48 runs

Design	GR
\mathcal{D}_{1r}	1.9167
\mathcal{D}_{1f_3}	2.6667
\mathcal{D}_{1f_6}	1.6667
$\mathcal{D}_{1f_{12}}$	1.8333

Table 32 shows the generalized resolution for the comparison designs with k=7 and n=48, and Table 33 shows the generalized resolution for the comparison designs with k=6 and n=24 that were shown earlier. The highest generalized resolution is associated with \mathcal{D}_{1f_3} and \mathcal{D}_{2f_3} respectively. In fact, the high resolution is desirable for a design to be an efficient in estimating the effects independently.

Table 33.: Generalize resolution for three-quarter designs with 6 factors and n=24

Design	GR
\mathcal{D}_{2r}	1.6667
\mathcal{D}_{2f_3}	2.6667
\mathcal{D}_{2f_6}	1.6667
$\mathcal{D}_{2f_{12}}$	1.8333

4.6.5 Generalize aliasing length pattern (GALP)

As we mentioned earlier, Generalized Aliasing Length Pattern (GALP) is the main diagonal of the matrix $(X'X/n)^2$, where X is the model matrix for the MEs and 2FIs model. In this section, we evaluate three-quarter design of regular/4-PFD design based on GALP.

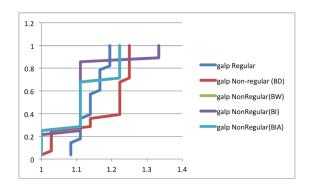


Fig. 27.: GALP distribution for three-quarter designs of k=7 and n=48

Figure 27 shows the GALP distribution for the three-quarter designs of regular/4-PFD designs. It is clear that three-quarter design of regular design \mathcal{D}_{1r} has more distinct values than the other designs. Three-quarter designs of 4-PFD design have the lowest aliasing for the MEs, but the highest aliasing for the 2FIs. This indicates that the three-quarter designs of 4-PFD designs may do well identifying the active

MEs, more than the three-quarter design of regular design. However, they will have more difficulty in identifying the active 2FIs.

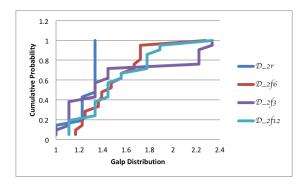


Fig. 28.: GALP distribution for three-quarter designs of k=6 and n=24

Figure 28 shows the GALP distribution for the three-quarter designs of regular/4-PFD designs with k=6 and n=24 that was shown earlier. In this case, three-quarter design of 4-PFD \mathcal{D}_{2f_6} has more distinct value than the three-quarter design of regular design. Also, for this case, it seems that three-quarters of 4-PFD have the lowest aliasing for the MEs, but the highest aliasing for 2FIs. Therefore, these observations again indicate that three-quarters of 4-PFD designs may identify active MEs better than three-quarters of regular designs, but these designs may still have difficulty on identifying active 2FIs.

4.7 Conclusion

In this chapter, we have constructed a new type of nonregular design by omitting a quarter of run size of regular design and 4-PFD. General properties for constructed design were developed using the concepts of parallel flats design and indicator function. We also provided a comparison between three-quarter design of regular/4-PFD based on the standard criteria for ranking designs. It was seen that in some cases, removing a quarter of the run size permits estimation of all MEs and 2FIs with orthogonality to the MEs. Also, it was noted and proved that three-quarter of 4-PFD

belong to the family of parallel flats designs. Almost all the considered criteria show the effectiveness of three-quarter designs of 4-PFD.

Due to the orthogonality of some constructed three-quarters designs, future work includes investigating more properties of three-quarter design and finding the ideal selection of blocking effects to get orthogonal three-quarter design. Also, our research focused deeply on construction three-quarter design of regular design and 4-PFD. What is the difference if we use different than theses design? Consider designs such as 3-PFD, 6-PFD, 8-PFD could be open research problems, and should be considered for future work. This suggests to welcome further research about the efficiency and the features of this type of designs. We hope this project gives more improvement for the area of the construction of nonregular designs and design choices.

CHAPTER 5

UTILIZING THE BLOCK DIAGONAL STRUCTURE OF NONREGULAR DESIGNS FOR DATA ANALYSIS

5.1 Introduction and Motivation

One strategy for improving the data-analysis is to consider the structure of a design. Standard model selection strategies such as stepwise regression (forward selection and backward elimination procedure) and dantzig selector are general tools that do not take any advantages of the structure about the design. In this chapter, we propose a new model selection procedure for block diagonal structure designs. These designs have a special structure, such that for any two effects belong to different blocks are uncorrelated, resulting in the creation of orthogonality between the blocks. We leverage this structure for block diagonal designs to develop an effective, design-based model selection procedure. The simulation results show improvement in the data-analysis by using the new approach for model selection.

The main contribution to screening designs is providing potential factors that have an impact on the response. Two-level fractional factorial designs FFDs are widely used for screening experiments to identify the active factors. The most common choice for screening are regular designs. These designs are constructed by generating additional factors, through using the product of the factors for a full factorial design. The aliasing structure for these designs is simple, such that any two factorial effects are either orthogonal or fully aliased. However, these design are limited in choice of the run size which must be power of 2. On the other hand, nonregular designs are more complected than regular designs, since they have a complex aliasing

structure, due to the appearance of partial aliasing between its effects. However, nonregular designs are considered an alternative choice for regular designs, due to the flexibility of run sizes for these designs, which are multiples of 4.

Researchers were avoiding using Plackett-Burman design because of the complex aliasing between 2FIs. However, Hamada and Wu, 1992 proposed a procedure that uses foldover technique to analyze the complex aliasing for Plackett-Burman design. Hamada and Wu, 1992 illustrated that the major advantages of using a foldover for Plackett-Burman design is that the identification of active MEs is not affected by the presence of active 2FIs. The reason for using a foldover technique in this work is the orthogonality between the set of MEs and the set of 2FIs, that is produced using this technique.

In addition, Miller and Sitter, 2001 proposed an effective sequential approach to analyze Placket-Burman design using foldover technique. This approach consists of two steps: first is to estimate the MEs by using standard methods to select active effects, second, use only the active MEs selected in the first step to create a design matrix, and then use weak-heredity principle to consider the second-order model, and use all subset procedure to select the final model.

Miller and Sitter, 2005 evaluated the structure and performance of a design obtained by folding over non-orthogonal design. They demonstrated that the orthogonality between MEs and 2FIs could have an impact on the design's ability to identify active MEs and 2FIs, which makes the analysis simpler. Also, Miller and Sitter, 2005 provided a simple two-step procedure, which is similar to that provided on Miller and Sitter, 2001. Moreover, Jones et al., 2019 constructed a new type of supersaturated designs, which have the property of group orthogonality. Jones et al., 2019 utilized this property to produce an efficient model selection procedure for these designs.

All the previous works provide strategies, which explicitly utilize the structure of

a design into the analysis. A design with a block diagonal structure has orthogonality between blocks, where any two effects belong to different blocks and are uncorrelated. This property of this type of design is very attractive for estimating the effect separately. Also, it seems very useful for understanding the aliasing structure of a design. Based on that, our purpose for this chapter is utilizing the block diagonal structure for a design to improve the analysis. As mentioned on Edwards and Mee, 2020, one possible strategy for a design analysis is performing a model selection separately for each block. Building on that, we propose a new model selection strategy for block diagonal structure design, which focuses on performing model selection for each block, and we investigate this strategy through a simulation research. Also, our goal is to test the effectiveness of the proposed method by comparing its performance with the performance of the classical standard model selection method.

The remainder of this chapter is organized as follows: in Section 5.2 we provide background on parallel flats designs, block diagonal structure. In Section 5.3, we provide our proposed method of model selection for block diagonal structure designs. Section 5.5, contains the simulation results, and Section 5.6 concludes the chapter.

5.2 Foundation

5.2.1 Parallel Flats Designs

A regular fractional factorial design 2^{k-m} , is known as a single-flat design. An aliasing relation between its effects appears due to reducing the run size for these design. Thus, a single-flat design can be defined by the alias matrix \mathbf{A} , and the coset indicator vector c_i , such that $\mathbf{A}x = \mathbf{c}_i$, where $x = (x_1, ..., x_k)$, \mathbf{A} is $m \times k$ of elements $a_{ij} \in \{1, 0\}$, and m is the rank of \mathbf{A} . Suppose that f single flat designs are all defined by \mathbf{A} , then combining these f single flat designs produce a design called f - PFD.

Thus, f - PFD defined by two matrices \mathbf{A} , and \mathbf{C} such that C is a coset indicator matrix contains coset indicator vectors $\mathbf{c}_1, ..., \mathbf{c}_f$. So, clearly f - PFD has run size equals to $n = f \times 2^{k-m}$.

For example, consider a design where n = 16 and k=6 that is shown in Table 34.

Table 34.: Nonregular design with k=6 and n=16

A	В	С	D	\mathbf{E}	F
-1	-1	-1	-1	1	1
1	-1	-1	-1	1	-1
-1	1	-1	-1	-1	1
1	1	-1	-1	-1	1
-1	-1	1	-1	1	-1
1	-1	1	-1	-1	-1
-1	1	1	-1	1	1
1	1	1	-1	-1	-1
-1	-1	-1	1	-1	-1
1	-1	-1	1	-1	1
-1	1	-1	1	1	-1
1	1	-1	1	1	-1
-1	-1	1	1	-1	1
1	-1	1	1	1	1
-1	1	1	1	-1	-1
1	1	1	1	1	1

This design is determined by (A, C) where **A**, and **C** are

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

This design is 4-PFD, since there are 4 columns in **C** matrix. Each row in the **A** matrix represents a term in the defining relation for a flat. So, each flat is a regular 2^{6-4} satisfying $I = \pm CDF = \pm A = \pm B = \pm E$.

Connor and Young, 1961 were the first ones to introduce the parallel flats designs. General theories and features of parallel flats designs were provided by Srivastava et al., 1984. One of the special properties of parallel flats design with $f \leq n$ is the block diagonal matrix of its information matrix. The information matrix is X'X, which can be written as

$$X'X = \begin{bmatrix} X_1'X_1 & 0 & \dots & 0 \\ 0 & X_2'X_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \dots \\ 0 & 0 & \dots & X_g'X_g \end{bmatrix}$$

where X is the design matrix, and the effects of each submatrix represent an alias set, g is the number of alias sets, and all off-diagonal submatrices are zero matrices. The zero matrices indicate the orthogonality between the diagonal submatrices. Thus, any effects belonging to two different submatrices are orthogonal, meaning these effects can be estimated independently.

5.2.2 Block Diagonal Structure

The block diagonal structure of a design is a special property for the design. The effects for this design are portioned on separate blocks where any two effects belonging to two different block, are uncorrelated. The reason for this structure is that the effects for this design are arranged into alias sets. Common designs that have block diagonal structure are parallel flat designs (PFD), foldover designs, semifoldover designs, and three-quarters of regular/non-regular designs. For example, consider a nonregular design with n=16, and k=5 that shown in Table 35.

Table 35.: 2^{5-1} design

This design is 4-PFD, and it is from Edwards, 2011. This design is determined by **A** and **C**, where

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \end{bmatrix}$$

$$\mathbf{C} = \begin{bmatrix} -1 & -1 & -1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \end{bmatrix}$$

Each flat for this design satisfies $\{I = \pm ADE = \pm ABDE = \pm ACDE = \pm B = \pm C = \pm BC = \pm ABCDE\}$. The principal group is that containing the identity (intercept), the terms in the defining relation, and every possible interaction. So, the principal group for this design is

$$\{I, ADE, ABDE, ACDE, B, C, BC, ABCDE\}.$$

For 2^5 , there are 32 columns for the full factorial model. In the principal group 8 of these columns are listed, so there are 24 columns divided into 3 co-sets of size 8. Multiplying the principal group with A, E, D, respectively, we obtained the following

alias sets:

 $\{A, DE, BDE, CDE, AB, AC, ABC, BCDE\}$ $\{E, AD, ABD, ACD, BE, CE, BCE, ABCD\}$ $\{D, AE, ABE, ACE, BD, CD, BCD, ABCE\}$

If we arranged the identical columns of this design, we would have block diagonal structure. The block diagonal structure for this design is shown in Figure 29.

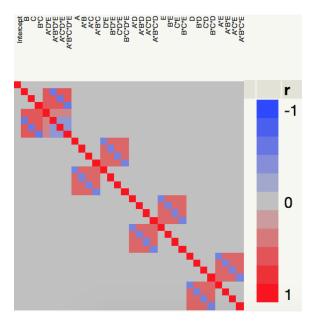


Fig. 29.: Block diagonal structure for desgin in Table 35

The block diagonal structure is appealing for understanding the aliasing relation to a regular/nonregular design. Consider a 1-PFD, which is a regular design, 2^{6-2} with n=16, and k=6, such that E=ABC and F=ABD. The defining relation for 2^{6-2} is I=ABCE=ABDF=CDEF. The effects for the full factorial model for this design are partitioned into 16 aliasing sets, each of size 4. Figure 2 shows the separation of the effects into 16 blocks, for the full factorial model to the design 2^{6-2} . It is noticeable from Figure 30 that the effects within each block are fully confounding.

In fact, the complete aliasing between the factorial effects is undesirable, due to the difficulty distinguishing between the estimated effects.

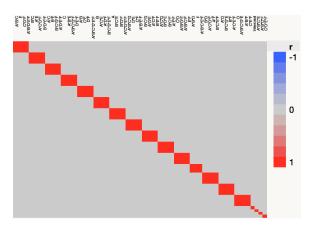


Fig. 30.: Block diagonal structure for regular design 2^{6-2}

As shown earlier, we can see in Figure 30 that the effects for non-regular design separate into separate alias sets, but not all effects within alias set are completely confounded. In this case, partial aliasing appears between some factorial effects within each alias set. So, the block diagonal structure for a design helps to better understand the aliasing relation between the effects for a design, which can have an impact on design choice and data analysis.

5.3 Proposed Method

In this section, we describe our model selection procedure, which is motivated by the works of Jones et al., 2019, Miller and Sitter, 2005, and Jones and Nachtsheim, 2017. They advocated for separating the analysis based on the structure of the design. Miller and Sitter, 2005 used foldover technique to separate the analysis of MEs from the analysis of 2FIs, since, as we mentioned earlier foldover technique creates an orthogonality between MEs and 2FIs. Jones and Nachtsheim, 2017 exploited the properties of Definitive Screening Designs for the same purpose of Miller and Sitter,

2005. Miller and Sitter, 2005, and Jones and Nachtsheim, 2017 showed that the sample space for the response can be separated into sub-sample spaces spanned by the MEs and its orthogonal complement.

The factorial effects for a design of block diagonal structure split into orthogonal blocks, such that any two effects belonging to two different blocks are uncorrelated. Since the blocks are orthogonal, we could test the significant effects of each block separately as in the works of Jones et al., 2019, and Miller and Sitter, 2005, Jones and Nachtsheim, 2017. Let \mathcal{D} denote a design with block diagonal structure, and $G_1, G_2, G_3, ..., G_g$ each denote a block of effects. As usual, we focus on MEs and 2FIs, and assume that third and higher-order effects are negligible, so a model with MEs and 2FIs has the formula

$$y_i = \beta_0 + \sum_{j=1}^k \beta_j x_{ij} + \sum_{j=1}^{k-1} \sum_{t=j+1}^k \beta_{jk} x_{ij} x_{it} + \epsilon$$

for i = 1, ..., n, j = 1, ..., k, and t = 1, ..., k - 1, where the parameters $\beta_0, ..., \beta_{kk}$ are unknown, and ϵ is a random error such that $\epsilon \sim N(0, I)$. Let \mathcal{D}_1 denote the columns of the first block G_1 , \mathcal{D}_2 denote the columns of the second block G_2 , and \mathcal{D}_3 denote the columns of the third block G_3 , and \mathcal{D}_g denote the columns of g block G_g .

The model may be written in matrix form as:

$$Y = \mu + \mathcal{D}_1 \beta_{\mathcal{D}1} + \mathcal{D}_2 \beta_{\mathcal{D}2} + \mathcal{D}_3 \beta_{\mathcal{D}3} + \dots + \mathcal{D}_g \beta_{\mathcal{D}g} + \epsilon$$

where Y is an $n \times 1$ response vector, μ is an $n \times 1$ constant vector, \mathcal{D}_1 is $n \times d_1$, $\beta_{\mathcal{D}1}$ is $d_1 \times 1$, \mathcal{D}_2 is $n \times d_2$, $\beta_{\mathcal{D}2}$ is $d_2 \times 1$, ..., \mathcal{D}_g is $d_g \times 1$, $\beta_{\mathcal{D}g}$ is $d_g \times 1$ where $d_1, d_2, ..., d_g$ is the number of columns for \mathcal{D}_1 , \mathcal{D}_2 ,..., \mathcal{D}_g respectively, and ϵ is the error vector which is $n \times 1$, and it assumed to be normal distribution such that $\epsilon \sim N(0, I\sigma^2)$.

Let $P_r = \mathcal{D}_r(\mathcal{D}'_r\mathcal{D}_r)^-\mathcal{D}'_r$ denote an orthogonal projection for the columns space

of \mathcal{D}_r , r=1,2,...,g. Since the blocks of effects are orthogonal, we generate a separate response vector for each block by obtaining the projections of the columns in a block. In this case, we are separating the space of the response into several sub-spaces $P_1 * Y, P_2 * Y, ..., P_r * Y, ...$, and $P_g * Y$ each correspond to a block. Since each block of effects has its own response vector, in this case, the presence of active effects in other blocks will not cause inflation to the residual for the fitted model for a block. So, our proposed method process as follows. First, for each block we consider a standard general model selection to select the active effects. In this context, we aim to test the performance of two model selection procedures, such as forward selection and dantzig selector.

Second, we pool together all the active effects from all blocks in one matrix denoted by \mathcal{D}_f . Third, we fit a final model, by using \mathcal{D}_f and Y response vector. So, the effects in the final model are the union of the active effects that are found in each block. Then, we conduct the power and type 1 error. The power defined as the average proportion of correctly identified active effects, while type 1 error is the average proportion of identified inactive effects. We called this procedure Block Forward, and Block Dantzig, based on the procedure that used to select the active effects form each block. We denoted these procedures by SBT Forward and SBT Dantzig, respectively.

Next, we evaluate the proposed method in comparison with standard model selection techniques such as forward selection and dantzig selector. With standard model selection techniques, the effects in the final model are selected without using any information with regards to the structure of the design. For both dantzig and forward, we use AIC as a criterion to pick the final model.

5.4 Simulation Study

In this section, we report simulations for comparing selected 5-factor designs with n=12 runs, 6-factor designs with n=16 runs, and 7-factor design with n=12, 16, 20, 40, and 48 runs. We consider a comparison for the simulation result in two parts; first, we compare the performance of analysis methods for the power and type 1 error. Then, we compare the performance of the design for the power and type 1 error based on the number of flats (number of flats =n / number of blocks).

5.4.1 Protocol of Simulation Study

We compared four analysis methods in the simulation study, namely Block Forward (SBT Forward), Block Dantzig (SBT Dantzig), forward, and dantzig. For forward and dantzig procedure, we follow Mee et al., 2017. For each design under study, our simulation is carried out as follows. In each of 1000 iterations:

- 1. We consider the columns of a design matrix, m columns are randomly assigned as the active MEs. The number of active MEs, m is conducted from 2 to 5 for the simulation.
- 2. Under the assumption of weak effects heredity, and based on the selection of the active MEs, g 2FIs are randomly assigned as the active 2FIs. The number of active 2FIs g, is conducted from 1 to 7 for the simulation.
- 3. The coefficients, β , for the active effects are obtained by randomly sampling (with replacement) from $\{0.5, 1, 1.5, 2, 2.5, 2, 3.5\}$. For each coefficient a sign (+ or -) is randomly applied.
- 4. The response vector, Y, is generated as $Y = X * \beta + e$, where X is the matrix which corresponds to the active effects and $e \sim N(0, 1)$.

5. Apply each of the four model selection approaches, SBT Forward, SBT Dantzig, forward, and dantzig, to each design under study.

At the end of 1000 iterations, the power of the overall effects is recorded which is defined as the average proportion of correctly identified effects (MEs and 2FIs). Also, power of the MEs, which is the average proportion of correctly identified MEs, and the power of 2FIs, which is the average proportion of correctly identified 2FIs, are recorded. Moreover, we calculate the type 1 error for overall, MEs, and 2FIs effects.

5.4.2 Simulation Result

5.4.2.1 k=5, n=12

We display the results of our simulation for 5-factor designs with n=12 runs in Figure 31 and 32. We denoted these designs as 12.5.3f and 12.5.6f, which refer to a design with n=12 runs, k=5, and f=3, or 6 respectively. For these figures, each sub figure consists of four rows and four columns. Each row represent, the result for the simulation to a number of active MEs which differ from 2 to 5, while each column represents an analysis method, which is as follows; dantzig selector, SBT Dantzig, forward selection, and SBT Forward. The colored plotted lines show overall power, MEs power, 2FIs power, overall type 1 error, MEs type 1 error, and 2FIs type 1 error for up to seven active 2FIs two for the different designs, 12.5.3f and 12.5.6f.

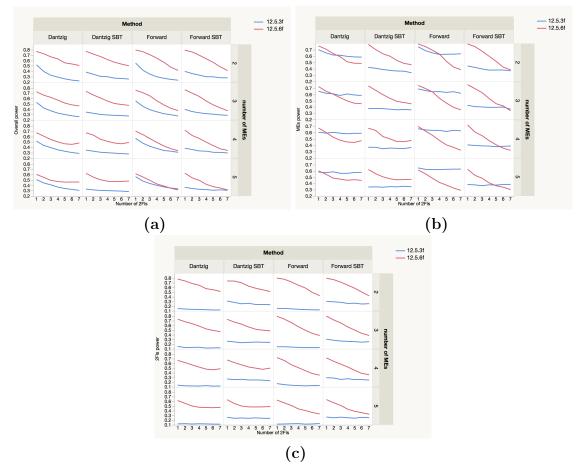


Fig. 31.: Simulation result for n=12, k=5. X-axes for the plots represent the number of active 2FIs. Y-axes:(a) Overall effects power; (b) MEs power; (c) 2FIs power. Blue line:12.5.3f; Red line:12.5.6f

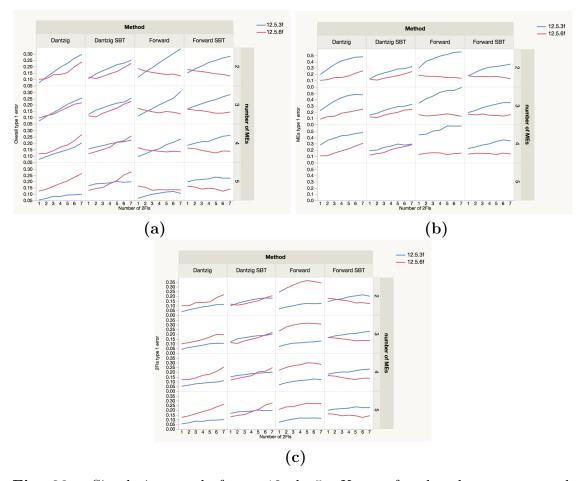


Fig. 32.: Simulation result for n=12, k=5. X-axes for the plots represent the number of active two-factor interactions. Y-axes:(a) Overall type 1 error; (b) MEs type 1 error; (c) 2FIs type 1 error. Blue line:12.5.3f; Red line:12.5.6f

Our comparison of analysis methods focuses on forward comparison with Forward SBT and dantzig comparison with Dantzig SBT. As well, we are curious about which procedure (forward, dantzig) has good performance for the proposed method. Figures 31 and 32 show that for the 12.5.6f design using Forward SBT, the power (overall, MEs, 2FIs) is slightly improved, and type 1 errors (especially 2FIs type 1 errors) have changed significantly. Also, by comparing Dantzig SBT with Dantzig, using Dantzig SBT, we can observe a slight improvement in (overall, ME, 2FI) power, while for (overall, ME, 2FI) type 1 errors have hardly decreased. Thus, it is recommended to

use both Dantzig SBT and Forward SBT methods.

Now, let's compare the analysis method (forward, Dantzig) and the proposed method (SBT Forward, SBT Dantzig) for 12.5.3f, respectively. Unlike design 12.5.6f, the overall and MEs power of design 12.5.3f using Forward SBT and Danzig SBT are reduced, and we see an increase in 2FIs power. From Figure 32 (a, b, c) we can see that the overall type 1 error using Forward SBT and Dantzig SBT is not fixed, it is decreases for 2, 3 and 4 MEs, and increases for 5 active MEs. MEs type 1 error is decreased by using Forward SBT and Dantzig SBT. However, 2FIs type 1 error is increased by using Forward SBT and Dantzig SBT. Thus, the performance for our proposed method for 3 flats design was unexpected.

From Figures 31 and 32, we can see that in almost all analysis methods, the performance of 12.5.6f is better than 12.5.3f, especially the overall power and 2FIs power. Also, by using the two analysis methods of Forward SBT and Dantzig SBT, 12.5.6f produces less type 1 errors (overall, MEs, 2FIs) than 12.5.3f. However, when using forward and Dantzig, 12.5.6f will give an unfixed (overall, MEs, 2FIs) type 1 error. Therefore, the performance of 12.5.6f is better than 12.5.3f especially with respect to the power. Thus, design 12.5.6f is more highly recommended than design 12.5.3f for active effects detection.

5.4.2.2 k=6, n=16

The results of the simulation for 6-factor designs with n=16 runs are displayed in Figures 33 and 34. We denoted these designs as 16.6.4f and 16.6.8f, which refers to a design with n=16 runs, k=6 and f=4, or 8 respectively. As the case of 5-factor, we consider the comparison based on forward comparison with Forward SBT, and dantzig comparison with Dantzig SBT. Design 16.6.8f, by comparing the analysis method Forward SBT with forward, Forward SBT has no dramatic change with respect to

overall, MEs, and 2FIs power, and the same was noticed when comparing the Dantzig SBT comparison with Dantzig. However, as in the case of 12.5.6f design, we see significant change in 2FIs type 1 errors, for both analysis methods Forward SBT and Dantzig SBT. Similarly, for design 16.6.4f, we have no improvement in overall, MEs, 2FIs power, although we have seen a reduction in 2FIs type 1 errors, especially for the forward SBT analysis method. Therefore, it is recommended to use the proposed method (especially Forward SBT) particularly for detective active 2FIs.

For 2FI detection, we recommended design 16.6.8f, and both Dantzig SBT and Forward SBT, since with these methods design 16.6.8f gives higher 2FIs power than 16.6.4f, while both of these designs give similar 2FIs type 1 error.

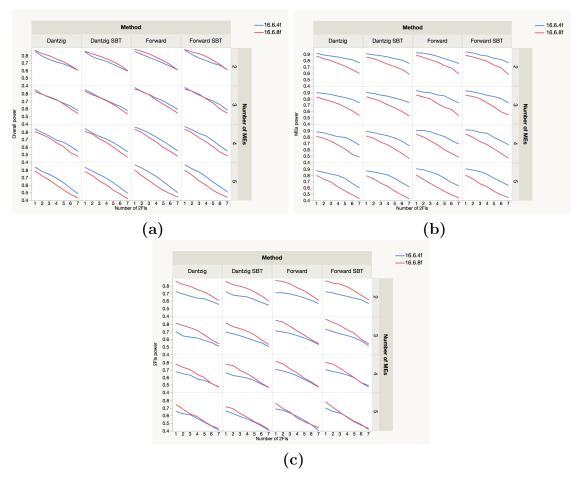


Fig. 33.: Simulation result for n=16, k=6. X-axes for the plots represent the number of active2FIss. Y-axes:(a) Overall effects power; (b) MEs power; (c) 2FIs power. Blue line:16.6.4f; Red line:16.6.8f

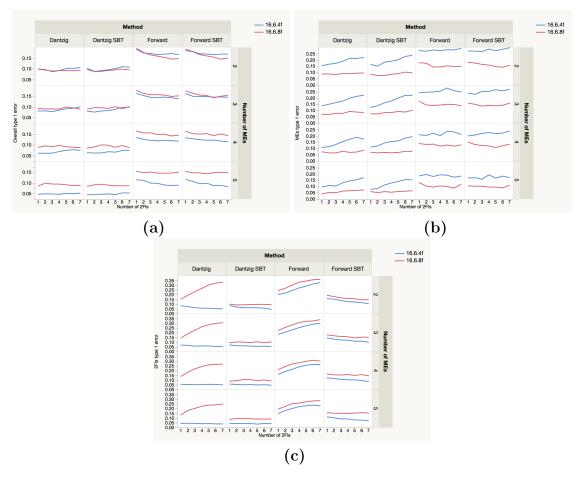


Fig. 34.: Simulation result for n=16, k=6. X-axes for the plots represent the number of active 2FIs. Y-axes:(a) Overall type 1 error; (b) MEs type 1 error; (c) 2FIs type 1 error. Blue line:16.6.4f; Red line:16.6.8f

5.4.2.3 k=6, n=24

The simulation study for the designs with 6-factor and 24 runs are displayed in Figures 35 and 36. We denoted these designs as 24.6.3f, 24.6.6f and 24.6.12f, which refer to a design with n=24 runs, k=6 and f=3, 6, and 12 respectively. As in the a previous case, we have seen improvements in the analysis of the 2FIs type 1 errors of the proposed method, especially in the case of Forward SBT. There is slight improvement in the overall, MEs, and 2FIs power for both design 24.6.6f, and 24.6.12f. There is also decreasing in overall, MEs, and 2FIs type 1 error using the

method Dantzig SBT and Forward SBT. Again, our proposed method for 3 flats design is not recommended since the power, MEs, and 2FIs power are decreasing. For MEs active detection, design 24.6.3f is recommended with the forward analysis method, and for 2FIs active detection, design 24.6.6f is recommended with the proposed method Forward SBT.

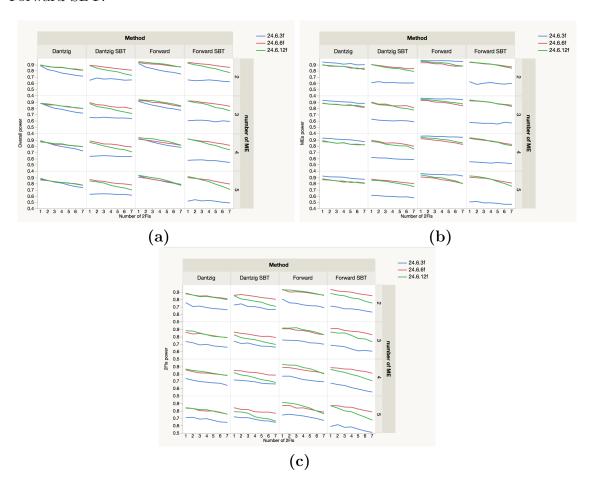


Fig. 35.: Simulation result for n=16, k=6. X-axes for the plots represent the number of active2FIs. Y-axes: Overall power; (b) MEs power; (c) 2FIs power. Blue line:24.7.3f; Red line:24.7.6f; Green line 24.7.12f

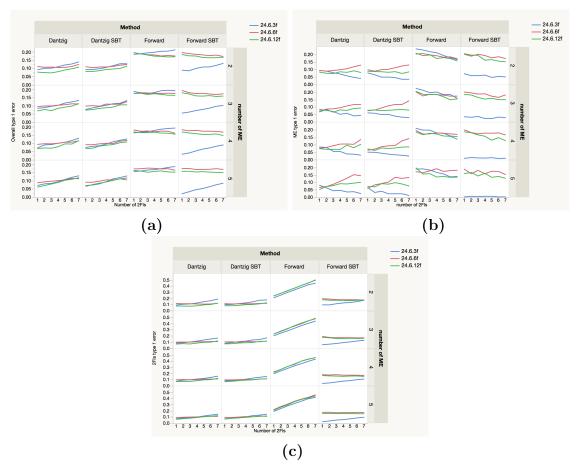


Fig. 36.: Simulation result for n=24, k=6. X-axes for the plots represent the number of active 2FIs. Y-axes:(a) Overall type 1 error; (b) MEs type 1 error; (c) 2FIs type 1 error. Blue line:24.6.3f; Red line:24.6.6f; Green line 24.6.12f

5.4.2.4 k=7, n=20

For this subsection, we have just one design, 20.7.10f, which has n=20, k=7 and f=10. The results for the simulation for 20.7.10f are displayed in Figures 37 and 38. Thus, here, we consider only the comparison between the analysis methods. There is no obvious difference, between the performance for dantzig and Dantzig SBT, for the power and type 1 error. However, when we compare between forward and Forward SBT, again, with Forward SBT, there is a slight improvement in (overall, MEs, 2FIs) power, and there is reduction for type 1 error, especially 2FIs. So, again, the analysis

method Forward SBT is recommended.

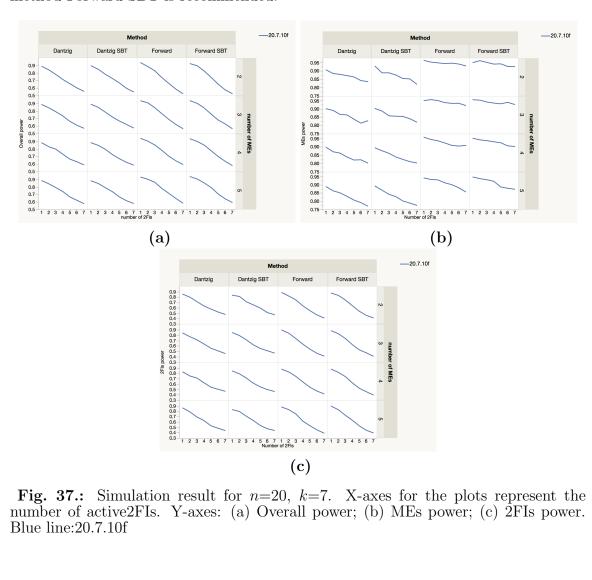


Fig. 37.: Simulation result for n=20, k=7. X-axes for the plots represent the number of active2FIs. Y-axes: (a) Overall power; (b) MEs power; (c) 2FIs power. Blue line:20.7.10f

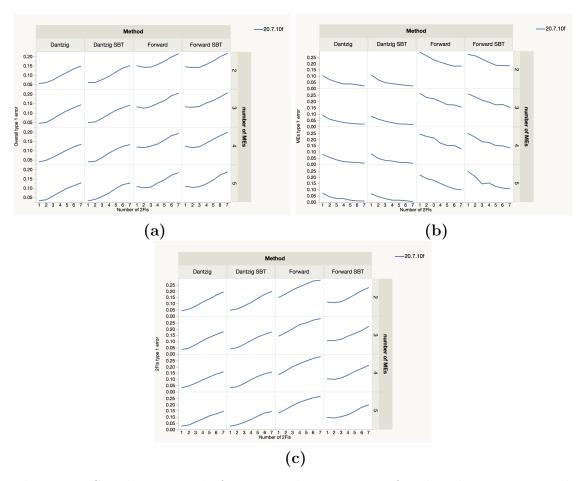


Fig. 38.: Simulation result for n=20, k=7. X-axes for the plots represent the number of active2FIs. Y-axes: (a) Overall type 1 error; (b)MEs type 1 error; (c)2FIs type 1 error.Blue line:20.7.10f

5.4.2.5 k=7, n=40

Here we consider foldover the design in the previous subsection which gives a design 40.7.10f that has n=40, k=7 and f=10. The result for of the simulation is shown in Figures 39 and 40. Again, in this case, there is no comparison for design with regard to number of flat. We only consider comparison between the analysis methods. Also, here we see the same pattern as in the case of 20.7.10f. There is no obvious difference between the performance for the dantzig and Dantzig SBT on the power and type 1 error. However, there is a slight improvement for (overall,

MEs, 2FIs) power, when we compare between forward and Forward SBT. As well, Forward SBT provides less 2FIs type 1 error. So, also, with 40.7.10f, Forward SBT is recommended.

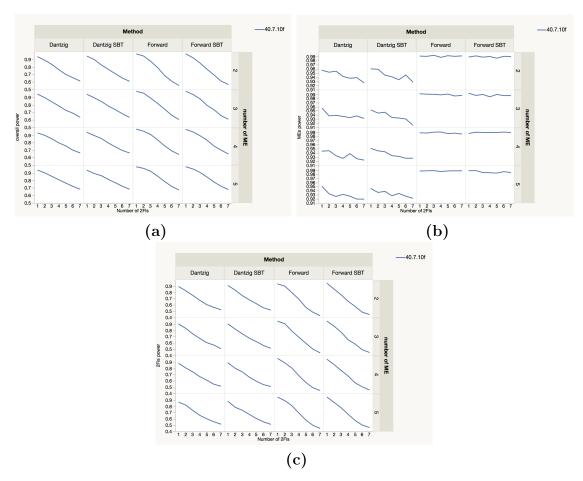


Fig. 39.: Simulation result for n=40, k=7. X-axes for the plots represent the number of active 2FIs. Y-axes:(a) Overall power; (b) MEs power; (c) 2FIs power. Black plotted line:40.7.10f

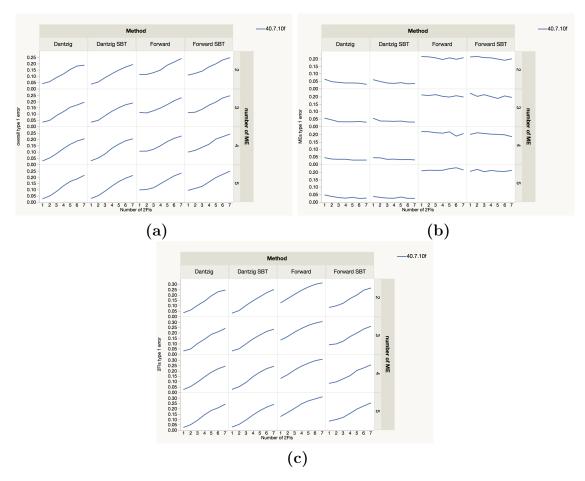


Fig. 40.: Simulation result for n=40, k=7. X-axes for the plots represent the number of active 2FIs. Y-axes:(a) Overall type 1 error; (b) MEs type 1 error; (c) 2FIs type 1 error. Black plotted line:40.7.10f

5.4.2.6 k=7, n=48

The results for the simulation for designs with n=48 and k=7 are displayed in Figures 41 and 42. We denoted these designs as 48.7.3f, 48.7.6f, and 48.7.12f. The figures are organized in the same way as those in the previous subsections. Our comments for the results are as follows. There is no difference for the performance of 48.7.3f, 48.7.6f, and 48.7.12f on the power and type 1 error, by using dantzig and forward. Also, 48.7.6f and 48.7.12f have the same performance for overall, MEs, 2FIs power and type 1 error by using Dantzig SBT and Forward SBT. However, 48.7.3f

has less overall, MEs, 2FIs power and type 1 error than 48.7.6f, and 48.7.12f, by using Dantzig SBT and Forward SBT. In this case, both 48.7.6f and 48.7.12f are better than 48.7.3f regarding power and type 1 error for all analysis methods, except that 48.7.3f is the best for overall, MEs, 2FIs type 1 error using Forward SBT. Based on the plots in Figures 13 and 14, again, we see improvement on the analysis, when we compare forward and Forward SBT for 48.7.3f, 48.7.6f, and 48.7.12f. This improvement is observed with 2FIs type 1 error, where this error is decreased using Forward SBT. For active MEs detection and 2FIs, both design 48.7.6f and 48.7.12 are recommended.

Therefore, in general, we can see the same results in all subsections. The proposed method, especially the Forward SBT, is recommended for active 2FIs detection because it produces less 2FIs type 1 errors, but the proposed method is not recommended for 3 flats.

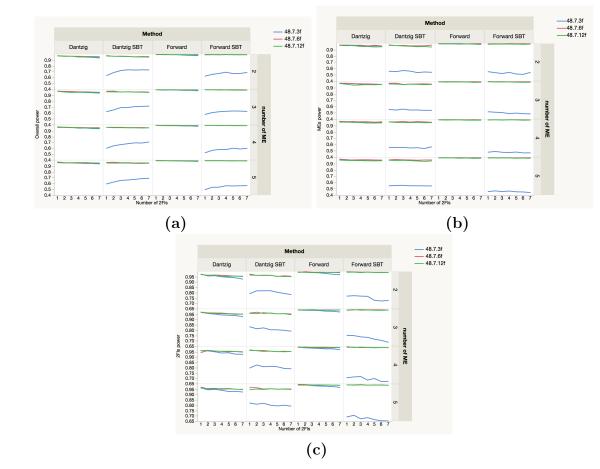


Fig. 41.: Simulation result for n=48, k=7. X-axes for the plots represent the number of active 2FIs. Y-axes: Overall power; (b) MEs power; (c) 2FIs power. Blue line:48.7.3f; Red line:48.7.6f; Green line 48.7.12f

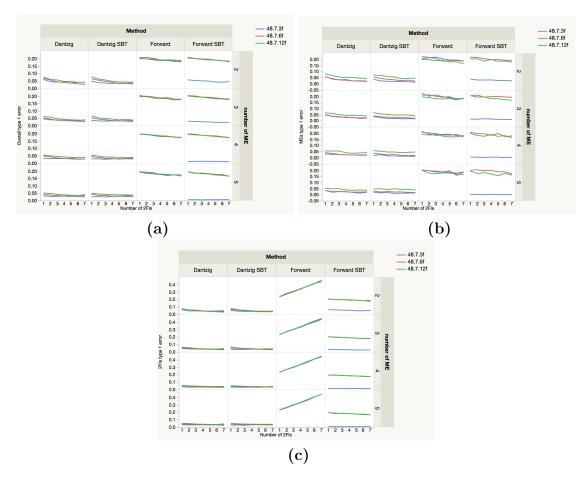


Fig. 42.: Simulation result for n=48, k=7. X-axes for the plots represent the number of active2FIs. Y-axes: (a) Overall type 1 error; (b) MEs type 1 error; (c) 2FIs type 1 error. Blue line:48.7.3f; Red line:48.7.6f; Green line 48.7.12f

5.5 Fitting model

In sections 5.3, we describe the designs and compare the results of the simulation study based on different numbers of flats and the performance for the four model selection procedures. Here in this subsection, we describe the analysis of the simulation results for varying factors, that include number of MEs, number of 2FIs, run size, factors, flats, and analysis methods, by fitting MEs and 2FIs order model using the standard forward stepwise procedure, based on minumum AICc. Figures 43, and 44 show the table of effects test for the MEs and 2FIs model for overall power, MEs

power, 2FIs power, overall type 1 error, MEs type 1 error, and 2FIs type 1 error. Figures 43 and 44 shows that all MEs, and almost all 2FIs, are statistically significant. That means they are have an impact on the overall, MEs, 2FIs power and overall, MEs, and 2FIs type 1 error.

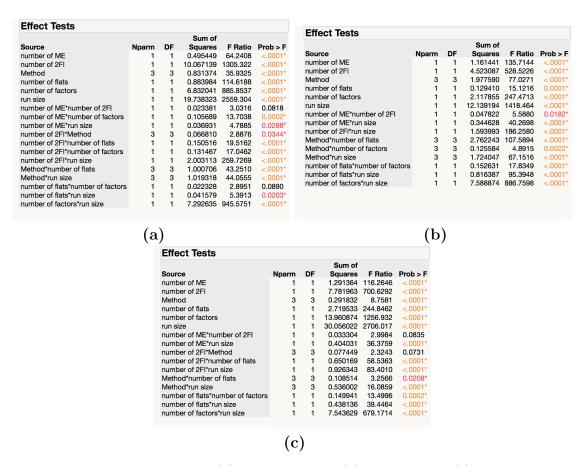


Fig. 43.: Effect tests to: (a) overall power; (b) MEs power; (c) 2FIs power

Effect Tests						Effe	ect Tests						
			Sum of								Sum of		
Source	Nparm	DF	Squares		Prob > F	Sour			Nparn		Squares		Prob >
number of ME	1	1	0.1544855		<.0001*		ber of ME				0.1560970	44.7043	<.0001
number of 2FI	1	1	0.1126966	98.1119	<.0001*	Meth				3 3	4.3214898		<.0001
Method	3	3	2.3410565		<.0001*	num	ber of flats			1 1	0.1036992	29.6982	<.0001
number of flats	1	1	0.0800346	69.6768	<.0001*	num	ber of factors			1 1	0.6212179		<.0001
run size	1	1	0.2833311		<.0001*	run s					1.4702189		<.0001
number of ME*Method	3	3	0.0197866	5.7420	0.0007*	num	ber of ME*Me	ethod	:	3 3	0.0248551	2.3727	0.0685
number of ME*number of flats	1	1	0.0230049	20.0277	<.0001*	num	ber of ME*nu	mber of flat	s	1 1	0.0145965	4.1802	0.0410
number of ME*run size	1	1	0.0037974	3.3060	0.0692	num	ber of ME*nu	mber of fac	tors	1 1	0.0511803	14.6574	0.0001
number of 2FI*Method	3	3	0.0801846	23.2691	<.0001*	num	ber of ME*rur	n size		1 1	0.0545717	15.6286	<.0001
number of 2FI*number of flats	1	1	0.0200251	17.4336	<.0001*	num	ber of 2FI*Me	thod	:	3 3	0.1194363	11.4017	<.0001
number of 2FI*number of factors	1	1	0.0217725	18.9548	<.0001*	num	ber of 2FI*nu	mber of flat	s ·	1 1	0.0211785	6.0653	0.0139
number of 2FI*run size	1	1	0.0231368	20.1425	<.0001*	num	ber of 2FI*rur	ı size		1 1	0.0330965	9.4784	0.0021
Method*number of flats	3	3	0.1218194	35.3513	<.0001*	Meth	od*number o	of flats		3 3	0.3286326	31.3721	<.0001
Method*number of factors	3	3	0.0085990	2.4954	0.0582	Meth	nod*number o	of factors		3 3	0.0627858	5.9937	0.0005
Method*run size	3	3	0.2680241	77,7792	<.0001*	Meth	od*run size		:	3 3	0.3385041	32.3145	<.0001
number of flats*run size	1	1	0.0347616	30.2629	<.0001*	num	ber of flats*ru	ın size		1 1	0.4209228	120.5471	<.000
number of factors*run size	1	1	0.0796230	69.3185	<.0001*		ber of factors			1 1	0.7885502		<.000
		Soul	ect Tests		Nparm	DF	Sum of Squares	F Ratio	Prob > F				
			ber of ME		1	1	0.1560970	44.7043	<.0001*				
		Meth	nod		3	3	4.3214898	412.5405	<.0001*				
		num	ber of flats		1	1	0.1036992	29.6982	<.0001*				
			ber of factors		1	1	0.6212179		<.0001*				
		run s	size		1	1	1.4702189	421.0526	<.0001*				
		num	ber of ME*Me	ethod	3	3	0.0248551	2.3727	0.0685				
		num	ber of ME*nu	mber of flat	s 1	1	0.0145965	4.1802	0.0410*				
		num	ber of ME*nu	mber of fac	tors 1	1	0.0511803	14.6574	0.0001*				
		num	ber of ME*run	size	1	1	0.0545717	15.6286	<.0001*				
		num	ber of 2FI*Me	thod	3	3	0.1194363	11.4017	<.0001*				
		num	ber of 2FI*nur	mber of flat	s 1	1	0.0211785	6.0653	0.0139*				
		num	ber of 2FI*run	size	1	1	0.0330965	9.4784	0.0021*				
		Meth	od*number o	of flats	3	3	0.3286326	31.3721	<.0001*				
		Meth	od*number o	f factors	3	3	0.0627858	5.9937	0.0005*				
		Meth	od*run size		3	3	0.3385041	32.3145	<.0001*				
		num	ber of flats*ru	n size	1	1	0.4209228	120.5471	<.0001*				
			ber of factors		1	1	0.7885502		<.0001*				

Fig. 44.: Effect Tests to: (a) overall type 1 error; (b)MEs type 1 error; (c)2FIs type 1 error

In order to understand this effect more clearly, we use other graphs as the predicted values of the model to show the overall, MEs, 2FIs power and overall, MEs, and 2FIs type 1 errors, as shown in Figure 45. This is achieved by using the profile plots with the statistical software JMP. In general, the results are as expected in some concepts, however, it is unexpected in others. Figure 45(a) shows one setting for the factors that gives high value for overall power. We can see in Figure 45(a) that by using the proposed method for both forward selection and dantzig selector, the overall power is reduced, which is unexpected. It can be clearly seen from Figure 45(a) that when the number of run size increases, the overall power will also increase. In addition, as the number of MEs and the number of 2FIs increase, the overall power

also increases. Similarly, the number of flats also affects the overall power. The prediction profile in Figure 45(a) shows that increasing the number of flats will result in an increase in overall power.

Figure 43(b) shows that all factors, including the number of flats, the number of factors, the number of MEs, the number of 2FIs, the analysis method, and the run size, have a statistically significant effect on the MEs power. Also, the 2FIs of these factors have an impact on the MEs power. Figure 45(b) shows a setting of these factors, which provides a high value for the power of MEs. It is obvious that as the number of MEs and 2FIs increases, the power of MEs also increases. Figure 45(b) shows that there is a strong relationship between the number of flats and the method used. With a high number of flats, which is 12 flats, the new proposed methods (Forward SBT, Dantzig SBT) give higher MEs power than the usual forward and dantzig. While with a small number of flats like 3 flats, the proposed methods give few MEs power. Also, there is a statistically significant interaction between the number of flats and the run size that has an impact on the MEs power.

As the overall power and MEs power, the 2FIs power is affected by all the MEs (the number of flats, the number of factors, the number of MEs, the number of 2FIs, the method of analysis, and the run size) and several two-factor interaction, which are clearly obvious in the predicted profile plots in Figure 45(c) and the table of effects test in Figure 43(c).

The result for overall type 1 error is similar to the result for the overall power. All the MEs and some of the 2FIs have impact on type 1 error. There are an infinite number of settings for the factors that give the minimum value to overall type 1 error. One of these settings is in Figure 45(d). It is clear from Figure 45(d) that as the number of MEs and 2FIs is increasing, the overall type 1 error is decreasing. Also, the overall type 1 error is affected by the method of model selection that is used.

From the predicted profile plots in Figure 45(d), it shows that the proposed method, especially Forward SBT, has lowest type 1 error. Also, this result is repeated for MEs type 1 error and 2FIs type 1 error. Again, the proposed method is recommended, especially for active 2FIs detection.

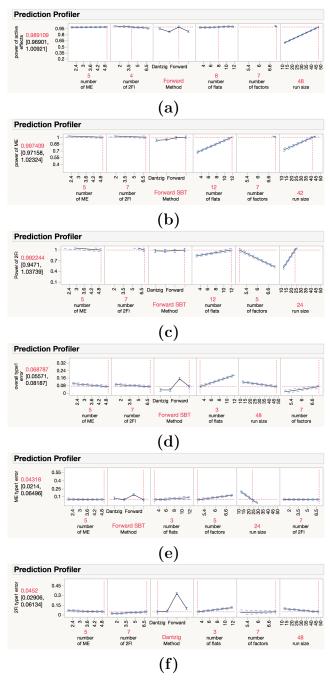


Fig. 45.: Prediction Profiler: (a) overall power; (b) MEs power; (c) 2FIs power; (d) overall type 1 error; (e) MEs type 1 error; (f)2FIs type 1 error

5.6 Discussion

In this chapter we develop a new model selection approach for block diagonal structure designs. We provide a new method to analyze these types of designs, making explicit use of the structure of the design. We are utilizing the special property for the block diagonal structure designs, which is the concept of blocks of factors that are orthogonal. Our approach focused on separating the response vector into several responses, each response corresponds to a block. In conclusion, this new approach has a benefit for the analysis, especially for 2FIs type 1 error. From our experience working with these types of designs (block diagonal structure designs) we can provide some recommendations:

- 1. The proposed methods are not recommended for 3 flats designs. By using the proposed methods, the simulation results for 3 flats design give less power than the standard model selection procedures. We consider the reason for this to be that a high correlation between the effects with 3 flats may cause decreasing on the power.
- 2. We also consider a method where one selects the active effects from each block, by using the standard method (forward, and Dantzig), then conduct the power and type 1 error by taking the union of these active effects. This method gives superior power, however, the type 1 error for this procedure is inflated so that this procedure cannot be recommended.
- 3. We considered the group lasso method as procedure for selecting the active blocks. Then, using the standard method (forward and Dantzig) for selecting significant effects from each selected active blocks. Next, consider the union of these significant effects, then conduct the power and type 1 error based on

this union of effects. Although the result shows less type 1 error by using this method, it gives much less power when we compare it with results for usual forward and Dantzig, which was unexpected.

5.7 Appendix

-	1	2.5.3	f		12.5.6f
Γ-1	-1	-1	-1	-1 ₇	$\Gamma - 1$ -1 -1 1 -1
-1	-1	-1	-1	-1	$\begin{vmatrix} -1 & -1 & -1 & -1 & 1 \end{vmatrix}$
-1	-1	-1	1	1	$\begin{bmatrix} -1 & 1 & -1 & 1 & -1 \end{bmatrix}$
-1	-1	-1	1	1	$\begin{bmatrix} -1 & 1 & -1 & -1 & 1 \end{bmatrix}$
-1	1	1	-1	-1	$\begin{vmatrix} -1 & -1 & 1 & 1 & 1 \end{vmatrix}$
-1	1	1	-1	-1	$\begin{bmatrix} -1 & -1 & 1 & -1 & -1 \end{bmatrix}$
-1	1	1	1	1	$\begin{bmatrix} -1 & 1 & 1 & 1 & -1 \end{bmatrix}$
-1	1	1	1	1	$\begin{bmatrix} -1 & 1 & 1 & -1 & 1 \end{bmatrix}$
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L 1	-1	1	1	-1	$\begin{bmatrix} 1 & 1 & -1 & -1 & 1 \end{bmatrix}$

		16.6	3.4f					16.6	3.8f		
r-1	-1	-1	-1	1	-11	r-1	-1	-1	-1	1	11
1 1	-1	-1	-1	-1	1	1	-1	-1	-1	1	-1
-1	1	-1	-1	-1	1	-1	1	-1	-1	-1	1
1 1	1	-1	-1	1	1	1	1	-1	-1	-1	1
-1	-1	1	-1	1	1	-1	-1	1	-1	1	-1
1	-1	1	-1	-1	-1	1	-1	1	-1	-1	-1
-1	1	1	-1	-1	-1	-1	1	1	-1	1	1
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CHAPTER 6

CONCLUSION AND FINAL COMMENTS

Data analysis is an important area in the field of experimental design. It aims on discovering new information, enhancing or contradicting existing assumptions, and finding new applications that are helpful for prediction. This dissertation aimed to identify effective strategies for improving data analysis. Based on simulation studies that comprehensively focus on detecting the active effects, it can be concluded that the structure of the screening design is an important factor to consider when analyzing data. The result indicates that the orthogonality between the factors and the considered model is one of the features of a design that has an impact on the analysis.

One of the important structural properties of the screening design is the dependency between its columns. This dependency might cause difficulties in discriminating between models. So, MDS is one of the biggest concerns regarding screening designs. However, several researchers used the concept of MDSs for understanding and improving the data analysis, especially for the model discrimination. Therefore, in this dissertation, we focused on utilizing the MDSs for screening designs on the data analysis. In Chapter 3, we provided a new classification for the MDSs and test the effectiveness of this classification in active effects detection through a simulation study. We found there is a benefit for using our classification on the power, as we expected. In fact, our approach for the classification was focusing on the impact of the number of factors in a MDS. However, there are infinite ways to classify the MDSs that have not been explored yet. There are still different ways to consider and extend this work. For example, MDSs may have an impact on other statistical

concepts, not just power. For instance, false discovery rate, estimation capability, projection estimation capability, generalized alias length, etc. Thus, further research on finding other ways to classify MDSs is considered an open research area needing more improvement and discovery.

While omitting a quarter of run size has been soundly investigated for regular design, less research has been devoted to this technique of construction design for non-regular designs. In Chapter 4, we provided a new strategy for the construction of a new type of non-regular design, which is three quarters design of non-regular design. This strategy focused on dividing the 4-PFD into 4 equal sets by using blocking, and then dropping one block to get three quarters designs. We found a relation between the orthogonality of the effects and blocking the design. Also, there is a relation between belonging of the blocking effects to aliasing sets and the number of flats for the resulting design. Our research focused deeply on construction three-quarter design of 1-PFD and 4-PFD. What is the difference if we use different than theses design? Consider designs such as 3-PFD, 6-PFD, 8-PFD could be open research problems, and should be considered for future work. What is the optimal choice for the effects that are used for blocking, which provides an orthogonal three quarters design? So, these questions are open research problems, and should be considered for future works.

In Chapter 5, we provided a new approach for model selection. Our approach has an impact on improving the data analysis, as we expected. It gave a decreasing type 1 error, especially for 2FIs by using the forward selection as a model selection procedure. While we do not notice a dramatic increase on the power by our approach. Consistently, the rate of the power gives insight into searching further about the reason for that and how to improve it. Our method focused on using two model selection procedures, forward selection and danzing selector, is there another analysis method

available in the literature, that might help to improve our proposed method ?

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