Computer-algebraic methods for the construction of designs of experiments

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Computer-Algebraic Methods for the Construction of Designs of Experiments

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In memory of my father

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CHAPTER 1

Introduction

1.1. A case study

Suppose that you are a *quality engineer* in a software firm. Your responsibility is to use statistical techniques for lowering the cost of design and production while maintaining customer satisfaction. What would you do if confronted with the following challenge? A competitor improves its product while simultaneously reducing the price. Your job is to identify components in your company's software production process which can be changed to reduce the production time and lower the price, while making the product more robust [Madhav, 2004]. You are required to carry out a series of *experiments*, in which a range of parameters, called *factors*, can be varied. The outcome of these experiments will be used to decide which strategy should be followed in the future. To be precise, you will perform experiments and measure some quantitative outcomes, called *responses*, when values of the factors are varied. Each experiment is also called an *experimental run*, or just a *run*. In each run, the factors are set to specific values from a certain finite set of *settings* or *levels*, and the responses are recorded.

Identifying important factors and the number of levels. The board wants to study as many parameters as possible within a limited budget. They have identified 8 factors that could affect the outcome. The factors and their levels are described in Table 1.1, where # stands for the number of levels of each factor. An initial investigation indicates that employees should have at least one year of experience, and that there is a great difference between an employee with three years experience and one with five years. We choose 5 levels for years of experience, which we call factor A. Factor B is the programming language that our software is written in. Of the

			Level				
Factor	Description	#	0	1	2	3	4
A	years of experience	5	1	3	5	7	9
B	programming languages	4	C++	Java	Perl	XML	
C	applications	2	scientific	business			
D	operating systems	2	Windows	Linux			
E	interviewing customers	2	no	yes			
F	weekly bonus policy	2	no	yes			
G	teamwork training	2	no	yes			
H	overwork policy	2	no	yes			

TABLE 1.1. Eight factors, the number of levels and the level meanings

many languages used in the market nowadays, we choose 4 which are appropriate for large applications.

Although there are many different applications of software (factor C), we can classify them into two major categories: scientific applications and business applications (such as finance, accountancy, and tax). For the former, the software developers require a fair knowledge of exact sciences like mathematics or physics, but relatively little knowledge of the particular customers. On the other hand, for the latter, the clients have specific requirements, which we need to know before designing, implementing and testing the software. We use two popular operating systems, Windows and Linux, for factor D. Whether we interview the customers is factor E – as mentioned, we expect this to interact with factor C. The factors F, G, H are self-explanatory, and each clearly has two levels.

Conflicting demands. Selecting the right combinations of levels in these factors is crucial. The total number of possible combinations is $5 \cdot 4 \cdot 2^6 = 1280$. But the experiments are costly and the board has decided that the budget allows for only 100 experiments.

A known model. Let N be the number of experimental runs in the experiment; each run will be assigned to a particular combination of factor levels. Let $M := 5 \cdot 4 \cdot 2^6$ denote the number of possible level combinations of the factors A, B, C, D, E, F, G and H. We restrict ourselves to studying only one response, Y, the number of failures (errors or crashes) occurring in a week. To minimize the average number of failures in new products, we study the *combined influence of the factors* using *linear regression models*. In these models, we make a distinction between *main effects*, *two-factor interactions*, and *higher-order interactions*. The main effect of a factor models the average change in the response when the setting of that factor is changed. A model containing just the main effects takes the form

$$Y = \theta_0 + \sum_{i=1}^{4} \theta_{A_i} a^i + \sum_{j=1}^{3} \theta_{B_j} b^j + \theta_C c + \ldots + \theta_H h + \epsilon, \tag{1.1.1}$$

where ϵ is a random error term, $a = 0, 1, 2, 3, 4$, $b = 0, 1, 2, 3$, and $c, d, e, f, g, h = 0$ or 1, and the parameters θ_* are the *regression coefficients*. In particular, θ_0, the number of failures when all factors are set to the values 0, is called the *intercept* of the model. These coefficients are estimated by taking linear combinations of the responses.

Two-factor interactions, or two-interactions, model changes in the main effects of a factor due to a change in the setting of another factor. To study the activity of all two-interactions simultaneously, we may want to augment Model (1.1.1) by adding

$$\begin{aligned} &\sum_{i=1}^{4}\sum_{j=1}^{3} \theta_{A_iB_j} a^i b^j + \sum_{i=1}^{4} \theta_{A_iC} a^i c + \ldots + \sum_{i=1}^{4} \theta_{A_iH} a^i h + \\ &\sum_{j=1}^{3} \theta_{B_jC} b^j c + \ldots + \sum_{j=1}^{3} \theta_{B_jH} b^j h + \theta_{CD}\, cd + \ldots + \theta_{GH} gh. \end{aligned} \tag{1.1.2}$$

We can also define higher-order interactions but these are usually considered unimportant.

The total number of intercept, main effect and two interaction parameters is

$$1 + \sum_{i=1}^{8}(s_i - 1) + \sum_{\substack{i,j=1\\ i<j}}^{8}(s_i - 1)(s_j - 1).$$

This formula shows that we need 83 parameters up to two-factor interactions to model the combined influences of the factors. In fact, only some of the two-factor interactions turn out to be important, so we need even fewer than 83 parameters. This is in contrast with a model including interactions up to order 8, which needs 1280 parameters.

A suggested fractional factorial design. The *full factorial design* of the eight factors described above is the Cartesian product $\{0, 1, \ldots, 4\} \times \{0, 1, \ldots, 3\} \times \{0, 1\}^6$. Using this design, we are able to estimate all interactions, but performing all 1280 runs exceeds the firm's budget. Instead we use a *fractional factorial design*, that is, a subset of elements in the full factorial design. We want to choose a fractional design that still allows us to estimate the main effects and some of the two-interactions. If we want to measure simultaneously all effects up to 2-interactions of the above 8 factors, an 83 run fractional design would be needed. Constructing an 83 run design is possible, and could be found with trial-and-error algorithms. But it lacks some attractive features such as *balance*, which is discussed below. An algebraic approach can also be used to construct such a design, but it is infeasible for large run size designs; for more details see Section 2.7.

A workable solution is the 80 run experimental design presented in Table 1.2. This allows us to estimate the main effect of each factor and some of their pairwise interactions. The construction of this design is presented in Chapter 6. Note that the responses Y have been computed by simulation, not by conducting actual experiments.

A nice property of the design. A notable property of the array in Table 1.2 is that it has *strength* 3. That is, if we choose any 3 columns in the table and go down we find that every triple of symbols in those columns appears the same number of times. This property is also called 3-balance or 3-orthogonality; and the array (fractional design) itself is called a *strength* 3 *orthogonal array* or a 3-*balanced fractional design*.

By Hedayat et al. [1999, Theorem 11.3], a strength 3 design allows us to measure all the main effects and some of the two-interactions. We could, in fact, investigate all main effects and all two-interactions of the abovementioned eight factors by using an 160 run strength 3 orthogonal array; see Hedayat et al. [1999, Section 11.4] for a detailed explanation. But the board would have to increase the current budget by at least 60 percent if we use an 160 run orthogonal array. If we insist in estimating all main effects and all two-interactions with a 80 run orthogonal array, then we can study the non-binary factors A and B and four binary factors only.

Using the fractional factorial design in Table 1.2, we can study the 2-interactions. In particular, we analyze:

(1) the main effect of the factors A, B and G (these are typically important for large projects, since, for instance, A largely determines wage expenses and B influences the cost of post-sale maintenance);
(2) the interaction between the pairs of factors A and B, B and G, and C and E; and

run	A	B	C	D	E	F	G	H	Y	run	A	B	C	D	E	F	G	H	Y
	5	4	2	2	2	2	2	2			5	4	2	2	2	2	2	2	
1	0	0	0	0	0	0	0	0	25	41	2	2	0	0	1	1	0	0	12
2	0	0	1	0	1	0	1	0	15	42	2	2	1	0	0	0	1	1	6
3	0	0	1	1	0	1	0	1	15	43	2	2	1	1	1	1	1	0	12
4	0	0	0	1	1	1	1	1	15	44	2	2	0	1	0	0	0	1	15
5	0	1	0	0	0	0	0	1	5	45	2	3	0	0	1	0	0	0	12
6	0	1	1	0	1	1	1	0	15	46	2	3	1	0	0	0	1	0	15
7	0	1	1	1	0	1	0	0	10	47	2	3	1	1	1	1	1	1	0
8	0	1	0	1	1	0	1	1	15	48	2	3	0	1	0	1	0	1	21
9	0	2	0	0	0	1	1	1	25	49	3	0	0	0	0	1	1	0	4
10	0	2	1	0	1	1	0	1	30	50	3	0	1	0	1	1	1	1	4
11	0	2	1	1	0	0	1	0	20	51	3	0	1	1	1	0	0	0	4
12	0	2	0	1	1	0	0	0	10	52	3	0	0	1	0	0	0	1	8
13	0	3	0	0	0	1	1	0	15	53	3	1	0	0	1	1	0	0	8
14	0	3	1	0	1	0	0	1	30	54	3	1	1	0	0	0	1	0	8
15	0	3	1	1	0	0	1	1	30	55	3	1	1	1	0	0	1	1	0
16	0	3	0	1	1	1	0	0	10	56	3	1	0	1	1	1	0	1	2
17	1	0	0	0	0	0	0	1	20	57	3	2	0	0	0	0	0	0	4
18	1	0	1	0	1	1	0	0	4	58	3	2	1	0	1	0	0	1	6
19	1	0	1	1	0	1	1	1	4	59	3	2	1	1	1	1	1	0	14
20	1	0	0	1	1	0	1	0	8	60	3	2	0	1	0	1	1	1	6
21	1	1	0	0	1	0	1	0	0	61	3	3	0	0	1	0	1	1	14
22	1	1	1	0	0	1	1	1	16	62	3	3	1	0	0	1	0	1	8
23	1	1	1	1	1	0	0	1	4	63	3	3	1	1	0	1	0	0	4
24	1	1	0	1	0	1	0	0	20	64	3	3	0	1	1	0	1	0	0
25	1	2	0	0	0	1	1	0	24	65	4	0	0	0	1	1	0	1	2
26	1	2	1	0	1	0	1	1	28	66	4	0	1	0	0	0	1	1	4
27	1	2	1	1	0	0	0	0	16	67	4	0	1	1	0	0	1	0	4
28	1	2	0	1	1	1	0	1	24	68	4	0	0	1	1	1	0	0	0
29	1	3	0	0	1	1	0	1	0	69	4	1	0	0	0	0	0	1	2
30	1	3	1	0	0	0	0	0	12	70	4	1	1	0	1	0	0	0	1
31	1	3	1	1	1	1	1	0	12	**71**	4	1	1	1	1	1	1	1	2
32	1	3	0	1	0	0	1	1	8	**72**	4	1	0	1	0	1	1	0	4
33	2	0	0	0	1	0	1	1	12	73	4	2	0	0	1	0	1	0	5
34	2	0	1	0	0	1	0	0	12	74	4	2	1	0	0	1	0	0	6
35	2	0	1	1	1	0	0	1	6	75	4	2	1	1	0	1	0	1	6
36	2	0	0	1	0	1	1	0	3	76	4	2	0	1	1	0	1	1	6
37	2	1	0	0	1	1	1	1	6	77	4	3	0	0	0	1	1	1	3
38	2	1	1	0	0	1	0	1	0	78	4	3	1	0	1	1	1	0	6
39	2	1	1	1	1	0	0	0	15	79	4	3	1	1	1	0	0	1	7
40	2	1	0	1	0	0	1	0	6	80	4	3	0	1	0	0	0	0	8

TABLE 1.2. A mixed orthogonal design with 3 distinct sections

(3) which runs result in the most reliable software product.

Analyzing the experimental outcomes. Given factors W and X, let $Y(W = k)$ denote the mean of the responses for the runs having factor W set to level k and let $Y(W = k, X = l)$ the mean of the responses for all runs with $W = k$ and $X = l$. We could now estimate parameters of (1.1.1) together with augmented parameters (1.1.2) using these means, but it is easier to work with the means themselves. Table

k	0	0	0	0	1	1	1	1	2	2
l	0	1	2	3	0	1	2	3	0	1
$Y(A=k,B=l)$	17	11	21	21	9	10	23	8	8	6
k	2	2	3	3	3	3	4	4	4	4
l	2	3	0	1	2	3	0	1	2	3
$Y(A=k,B=l)$	11	1	5	4	7	6	2	2	5	6

TABLE 1.3. Combined influence of A and B

i	0	0	1	1	2	2	3	3
j	0	1	0	1	0	1	0	1
$Y(B=i,G=j)$	9	6	13	10	7	7	14	11

TABLE 1.4. Combined influence of B and G

i	0	0	1	1
j	0	1	0	1
$Y(C=i,E=j)$	11	8	10	11

TABLE 1.5. Combined influence of C and E

1.3 and Figure 1.1 indicate a strong interaction between A and B; eg,

$$\begin{aligned} Y(A=1,B=2)-Y(A=2,B=2) &= 23-11=12=5+7=5+(8-1)\\ &= 5+(Y(A=1,B=3)-Y(A=2,B=3)). \end{aligned}$$

Since the interaction between A and B is rather strong, we only look at their combined influence. However, we see that the years of experience are crucial for reducing the failures, no matter which language was used, eg, $Y(A=4)=4$. Looking at Tables 1.3 and Figure 1.1, we find that the good responses are given by $A=4$ and $B=1$ (runs $69,70,71,72$ in Table 1.2). On the other hand, Table 1.4 and Figure 1.2 show that there is no strong interaction between the programming language used (B) and the choice of whether to attend teamwork training classes (G). Therefore, the effect of G can be modeled with just its main effects. It models the overall change in the number of failures if G is changed from setting 1 to setting 0. In the example, the overall change is $404-394=10$ failures; so we set $G=1$, which is slightly better $G=0$. Hence, the best responses are given by $A=4$, $B=1$ and $G=1$, that is we choose the runs $71,72$ in Table 1.2. Besides, as we expected, Table 1.5 and Figure 1.3 tell us that there is an interaction between the application chosen (C) and interviewing customers (E). This needs further investigation. The binary factors D,F,H do not strongly affect the outcome, so their levels can be set such that the budget is minimized.

1.2. The scope and structure of this thesis

The goal of this thesis is twofold: to find designs of strength 3, allowing the study of many factors and their interactions; and to select designs which are appropriate for practical problems. We consider all our designs to be qualitative, in the sense that there is no order relationship or a measure of distance among the levels.

In Chapter 2, we review the algebraic and statistical fundamentals for constructing fractional factorial designs with algebraic geometry. We discuss two basic

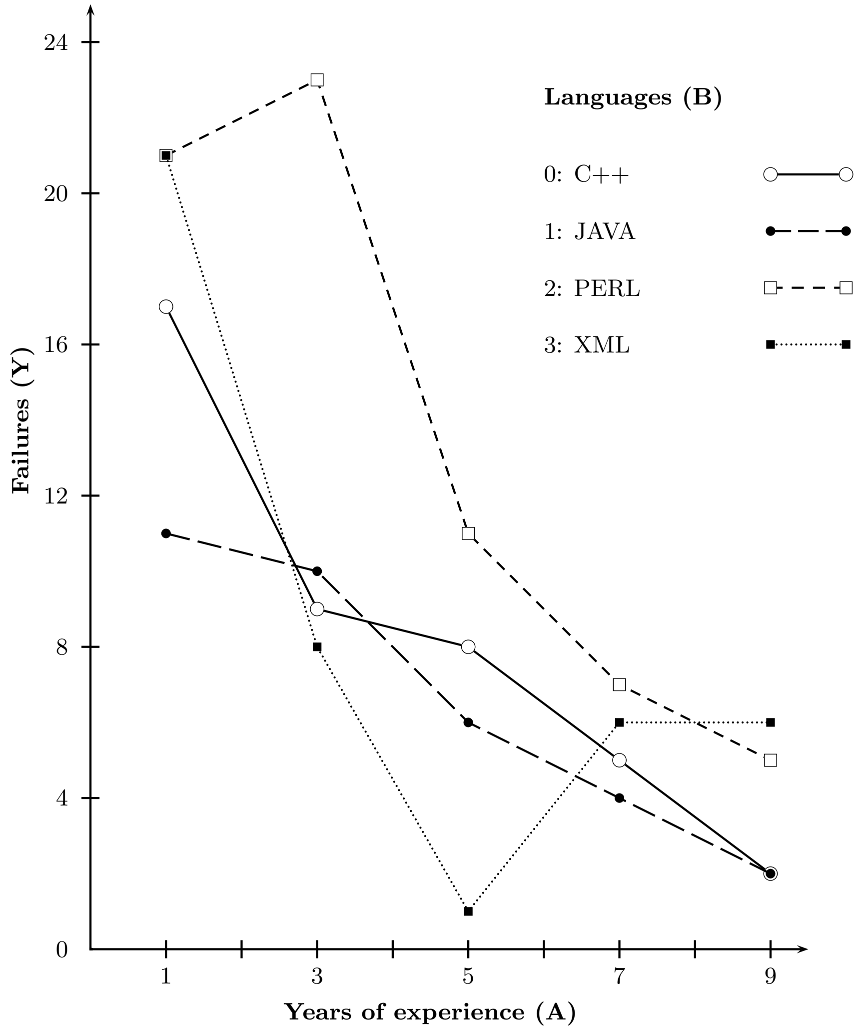

FIGURE 1.1. Years-Languages interaction

problems: finding the estimators of a design and constructing a design with given run size and set of estimators.

Chapter 3 presents some constructions of orthogonal arrays of strength 3. We describe tools for constructing a single array with a given parameter set.

In Chapter 4, we discuss the problem of enumerating all isomorphism classes of orthogonal arrays of strength 3 with given parameters.

We discuss, in Chapter 5, statistical criteria for selecting orthogonal arrays that are suitable for particular applications. Often there are many isomorphism classes of arrays having very distinct statistical features, so we would like to select the best arrays for a particular purpose.

Chapter 6 applies the techniques of Chapters 3 and 4, to enumerate many isomorphism classes of orthogonal arrays of strength 3 with run size at most 100.

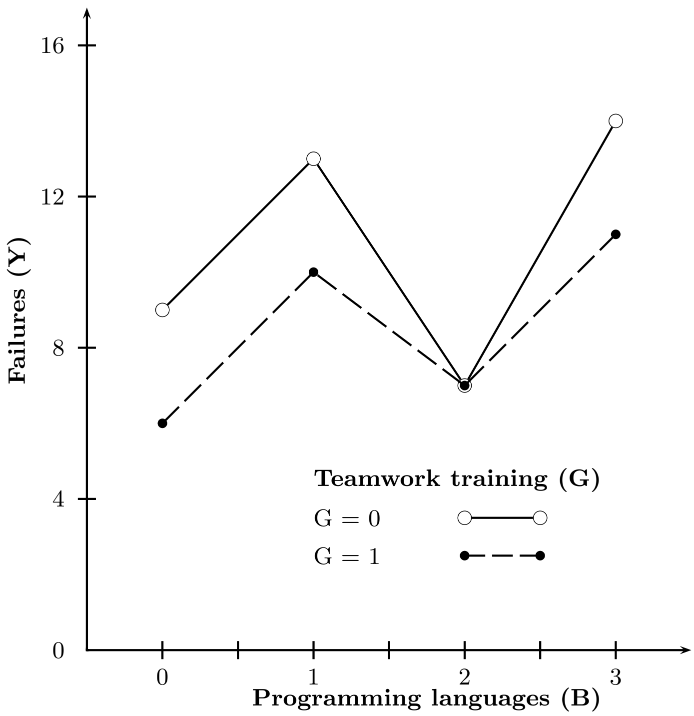

FIGURE 1.2. Languages-Teamwork training interaction

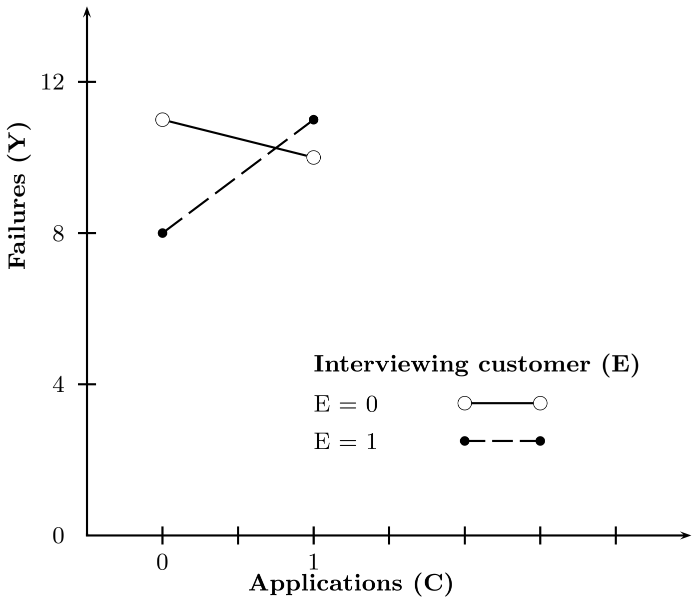

FIGURE 1.3. Applications-interviewing customer interaction

CHAPTER 2

Some basic problems in design of experiments

2.1. Introduction

In this chapter, we present methods for investigating designs using algebraic geometry. We show how to find the estimable interactions of a given design. Conversely, we show how to construct a fractional design with a given set of estimable interactions.

In Section 2.2, we review the Gröbner basis methods which we require. These methods have been described in Pistone et al. [2001]. Finding estimable interactions given a design is reviewed in Section 2.3. Section 2.4 presents a use of multiplication matrices to find a design with given estimable interactions. In Section 2.5, we present a necessary and sufficient condition for obtaining t-balanced designs, for positive integers t. Implementation issues are discussed in 2.6, and finally, Section 2.7 closes this chapter with some remarks. For basic notation, see Appendix B.

2.2. Gröbner bases

In this section, we consider all our factor sets Q_i to be subsets of $\mathbb{Q}$.

An algebraic setting. Let V be a subset of $\overline{\mathbb{Q}}^d$ and let $P = \overline{\mathbb{Q}}[\boldsymbol{x}] = \overline{\mathbb{Q}}[x_1, \ldots, x_d]$. The set of all polynomials $f \in P$ which are zero on all points of V forms an ideal of P. This is called the *vanishing ideal* of V in P and is denoted $\mathrm{I}(V)$. The Hilbert Basis Theorem [Kreuzer and Robbiano, 2000] says that this ideal has a finite generating set. Conversely, for a subset J of P, the *zero set* of J is defined as

$$\mathrm{Z}(J) = \big\{(p_1, \ldots, p_d) \in \overline{\mathbb{Q}}^d : f(p_1, \ldots, p_d) = 0 \text{ for all } f \in J\big\}.$$

For a single polynomial f, we denote $\mathrm{Z}(\{f\})$ by $\mathrm{Z}(f)$. For instance, the zero set $\mathrm{Z}(J)$ of $J = \{x_1 - p_1, \ldots, x_d - p_d\}$ consists of the single point $\boldsymbol{p} = (p_1, \ldots, p_d) \in \overline{\mathbb{Q}}^d$.

Let $D := Q_1 \times \ldots \times Q_d$ be the full factorial design in d factors $Q_1, Q_2, \ldots, Q_d$, and suppose that $Q_i = \{a_{i1}, \ldots, a_{ir_i}\} \subseteq \overline{\mathbb{Q}}$. Write f_i for the polynomial

$$f_i(x_r) = (x_r - a_{i1}) \ldots (x_r - a_{ir_i}) \quad \text{for } i = 1, \ldots, d.$$

The polynomials $f_1, \ldots, f_d$ are called the *canonical polynomials* of D. Then D is the zero set of $\{f_1, \ldots, f_d\}$. So D is also the zero set of the vanishing ideal $\mathrm{I}(D)$ generated by $f_1, \ldots, f_d$. We call $\mathrm{I}(D)$ the *defining ideal* or the *design ideal* of D.

We now show that the design ideal $\mathrm{I}(D)$ is the intersection of the vanishing ideals of the single points in D, ie, $\mathrm{I}(D) = \bigcap_{\boldsymbol{p} \in D} \mathrm{I}(\boldsymbol{p})$. Each single point $\boldsymbol{p} = (p_1, \ldots, p_d)$ corresponds to the variety defined by the ideal $\big((x_1 - p_1), \ldots, (x_d - p_d)\big)$. We know that finite unions of varieties correspond to finite intersections of ideals. The conclusion follows. Algorithms to compute $\mathrm{I}(D)$ can be found in Pistone et al. [2001, Section 3.2].

A *term order* on $\boldsymbol{x}^*$ is a total order, denoted by $<$, such that for all $u, v, w \in \boldsymbol{x}^*$, $u < v$ implies $uw < vw$; and $1 < u$ for every $u \in \boldsymbol{x}^*$, $u \neq 1$. For any term $\boldsymbol{x}^{\boldsymbol{\alpha}}$ in $\boldsymbol{x}^*$, put $\deg(\boldsymbol{x}^{\boldsymbol{\alpha}}) = \alpha_1 + \ldots + \alpha_d$, called the *total degree* of $\boldsymbol{x}^{\boldsymbol{\alpha}}$. Some useful term orders are:

Lexicographical order: $\boldsymbol{x}^{\boldsymbol{\alpha}} < \boldsymbol{x}^{\boldsymbol{\beta}}$ if there exists an $i = 1, \ldots, d$ such that

$$\alpha_1 = \beta_1, \ldots, \alpha_{i-1} = \beta_{i-1}, \alpha_i < \beta_i$$

(ie, the left-most nonzero entry in $\boldsymbol{\alpha} - \boldsymbol{\beta}$ is negative).

Degree reverse lexicographical order: $\boldsymbol{x}^{\boldsymbol{\alpha}} < \boldsymbol{x}^{\boldsymbol{\beta}}$ if $\deg(\boldsymbol{x}^{\boldsymbol{\alpha}}) < \deg(\boldsymbol{x}^{\boldsymbol{\beta}})$, or $\deg(\boldsymbol{x}^{\boldsymbol{\alpha}}) = \deg(\boldsymbol{x}^{\boldsymbol{\beta}})$ and there exists $i = 1, \ldots, d$ such that

$$\alpha_d = \beta_d, \ldots, \alpha_{i+1} = \beta_{i+1}, \alpha_i > \beta_i$$

(ie, the right-most nonzero entry in $\boldsymbol{\alpha} - \boldsymbol{\beta}$ is positive).

The second order is also called graded reverse lexicographical order. For instance, for $d = 5$, in the latter order we have $x_5 < x_4 < x_3 < x_2 < x_1$, and $x_1x_4 < x_2x_3$. Furthermore, if each indeterminate x_i is assigned a positive integer weight, then the degree reverse lexicographical order is now called the *weighted reverse lexicographic order*. This order is used in Section 2.6. For example, in this case, if let $[1, 2, 2, 2, 2]$ be the weight vector for x_1, x_2, x_3, x_4, x_5, then we have $x_1 < x_5 < x_4 < x_3 < x_2$.

A *monomial* is a product of a term and a scalar. The *support of a polynomial* g, denoted $\mathrm{Supp}(g)$, is the set of terms of g with nonzero coefficients. For a polynomial $g \in P$, let $\mathrm{LM}(g)$ be the *leading monomial* with respect to a fixed term order $<$ on $\boldsymbol{x}^*$; that means it is the monomial whose term is maximal in $\mathrm{Supp}(g)$ with respect to $<$. The coefficient of $\mathrm{LM}(g)$, denoted by $\mathrm{LC}(g)$, is called the *leading coefficient* of g; the *leading term* of g is $\mathrm{LT}(g) := \mathrm{LM}(g)/\mathrm{LC}(g)$, [Kreuzer and Robbiano, 2000, Definition 15.2]. Let J be a non-zero ideal of $k[\boldsymbol{x}]$. Denote by $\mathrm{LT}(J)$ the set of leading terms of elements of the ideal J with respect to $<$, and $(\mathrm{LT}(J))$ the *leading term ideal* generated by such leading terms. For example, with the lexicographical term-order,

$$\mathrm{LT}(\mathrm{I}(D)) = \{x_1^{r_1}, \ldots, x_d^{r_d}\}.$$

A finite subset B of the ring $k[\boldsymbol{x}]$ is called a *Gröbner basis* if $\mathrm{LT}(B) = \mathrm{LT}((B))$ [Cohen et al., 1999, Section 3, Chapter 1]. If $J = (B)$, we say that B is a Gröbner basis of J. For any ideal J of $k[\boldsymbol{x}]$, the Buchberger algorithm returns a Gröbner basis of J, [Kreuzer and Robbiano, 2000, Theorem 2.5.5]. For more details on Gröbner base and their computation, see Cohen et al. [1999] or Kreuzer and Robbiano [2000].

Fix a term ordering and let $B = \{g_1, \ldots, g_s\}$ be a Gröbner basis of J. We say that B is a *reduced Gröbner basis* of J if the following conditions are satisfied:

- $\mathrm{LC}(g_i) = 1$, for $i = 1, \ldots, s$.
- $\{\mathrm{LT}(g_1), \ldots, \mathrm{LT}(g_s)\}$ is a minimal system of generators of $\mathrm{LT}(J)$ as a monoid.
- $\mathrm{Supp}(g_i - \mathrm{LT}(g_i)) \cap \mathrm{LT}(M) = \emptyset$ for $i = 1, \ldots, s$.

An ideal can have several Gröbner bases, but only one reduced Gröbner basis [Cohen et al., 1999, Theorem 3.16, page 14]. We need the following lemma about the relationship between the set of leading terms of an ideal over the rationals $\mathbb{Q}$ and over the algebraic closure.

Lemma 1. [Kreuzer and Robbiano, 2000, Lemma 2.4.16] *Let J be an ideal of $\mathbb{Q}[\boldsymbol{x}]$ and $\overline{J} = J\overline{\mathbb{Q}}[\boldsymbol{x}]$, the ideal of $\overline{\mathbb{Q}}[\boldsymbol{x}]$ generated by the elements of J. Then, a Gröbner basis of J is also a Gröbner basis of $\overline{J}$. In particular, we have* $\mathrm{LT}(J) =$

$\mathrm{LT}(\overline{J})$. *Moreover, the reduced Gröbner basis of J is also the reduced Gröbner basis of $\overline{J}$.*

For a ring R, an *R-module* J is a commutative group $(J, +)$ with an operation $R \times J \to J, (r, m) \mapsto rm$ (called scalar multiplication) such that $1m = m$ for $m \in J$, and such that the associative and distributive laws are satisfied. A commutative subgroup $N \subseteq J$ is called an *R-submodule* if we have $R \cdot N \subseteq N$.

THEOREM 2. [Kreuzer and Robbiano, 2000, Theorem 1.5.7] *Let $J \subseteq k[\boldsymbol{x}]^r$ be a $k[\boldsymbol{x}]$-submodule, and let $B = \boldsymbol{x}^* \setminus \mathrm{LT}(J)$. Then the residue classes of the elements of B form a basis of the k-vector space $k[\boldsymbol{x}]^r/J$.*

When $r = 1$, the submodule J is a $k[\boldsymbol{x}]$-ideal, and the residue classes of the elements of B form a basis of the k-vector space $k[\boldsymbol{x}]/M$. Let J be an ideal of $k[\boldsymbol{x}]$. Then J is called *maximal* if the only ideal properly containing J is $k[\boldsymbol{x}]$; and if J is generated by a single element in $k[\boldsymbol{x}]$, it is called a *principal ideal*. Every ideal in the ring $k[x_i]$ is principal [Kreuzer and Robbiano, 2000, page 19].

THEOREM 3. [Kreuzer and Robbiano, 2000, Theorem 2.6.6(a)] *Let J be a maximal ideal of $k[\boldsymbol{x}]$. Then the intersection $J \cap k[x_i]$ is a non-zero ideal for every $i = 1, \ldots, d$.*

COROLLARY 4. *Let k be an algebraically closed field and J a maximal ideal in $k[\boldsymbol{x}]$. Then there exist elements $p_1, \ldots, p_d$ in k such that*

$$J = (x_1 - p_1, \ldots, x_d - p_d).$$

PROOF. The previous theorem supplies non-zero polynomials $f_1, \ldots, f_d \in J$ such that $f_i \in k[x_i]$ for $i = 1, \ldots, d$. Because k is an algebraically closed field, every polynomial f_i factorizes completely into linear factors. Since J is a maximal ideal, it contains one of the linear factors of each f_i, say $x_i - p_i$. So J must contain the ideal $K = (x_1 - p_1, \ldots, x_d - p_d)$. But K is maximal, hence $J = K$. $\square$

Some other concepts are needed before introducing three basic problems in designs of experiments. A *fraction* of a full design D is a subset F consisting of elements of D. Note that in this section we only consider fractions without *replications*, but see Cohen et al. [2001] for an approach dealing with replications. The *defining ideal* of F is the vanishing ideal $\mathrm{I}(F)$. Each equation of the form $f(x_1, \ldots, x_d) = 0$ with $f \in \mathrm{I}(F)$ is called a *confounding equation*. Note that $\mathrm{I}(D) \subseteq \mathrm{I}(F)$ if $F \subseteq D$. Any set of polynomials that, together with the ideal $\mathrm{I}(D)$ of the design D, generates the ideal $\mathrm{I}(F)$, is called a *set of defining equations* of F in D. The *indicator function* I_F of a fractional design F is the function from D to $\{0, 1\}$ such that

$$I_F(A) = \begin{cases} 1 & \text{if } A \in F, \\ 0 & \text{if } A \notin F. \end{cases}$$

For each fraction $F \subseteq D$, $\{I_F\}$ is the set of defining equations of F. In the remaining subsections, we fix $F := [\boldsymbol{p}_1, \ldots, \boldsymbol{p}_N]$ a fraction of D with $N = |F| \leq M$, where $M = r_1 r_2 \ldots r_d$. Observe that $\mathrm{I}(D)$ is the ideal generated by the canonical polynomials $f_1, \ldots, f_d$. Follow Kreuzer and Robbiano [2000, Theorem 2.4.13], there exists a unique reduced Gröbner basis of $\mathrm{I}(F)$, denoted $g_1, \ldots, g_l$. We have

THEOREM 5. [Cox et al., 1998] *Let k be an algebraically closed field, let V be the affine variety with ideal $I \subseteq k[\boldsymbol{x}]$, and let G be a Gröbner basis of I. The following statements are equivalent:*

- *V is finite;*
- *there is $\alpha_i > 0$ and $g \in G$ such that $x_i^{\alpha_i} = LT(g)$, for each $i = 1, \dots, d$;*
- *the k-vector space $k[\boldsymbol{x}]/I$ is finite-dimensional.*

By this theorem, the polynomials g_j can be written in the form

$$g_j(x_1, \dots, x_d) = \boldsymbol{x}^{\boldsymbol{\alpha}_j} - s_j(x_1, \dots, x_d).$$

Define the set

$$\mathrm{Est}(F) = \Big\{ \boldsymbol{x}^{\boldsymbol{\alpha}} : \boldsymbol{x}^{\boldsymbol{\alpha}} \notin \big(\mathrm{LT}(\mathrm{I}(F))\big) \Big\}, \tag{2.2.1}$$

called the *standard basis* of F with respect to the term order $<$. A set $E \subseteq \boldsymbol{x}^*$ is an *order ideal* of monomials if, for each $u \in E$ and $v \in \boldsymbol{x}^*$ such that v divides u, we have $v \in E$. For example, $\{1, x_1, x_2, x_1x_2\}$ is an order ideal. Note that the standard basis $\mathrm{Est}(F)$ of F is an order ideal.

Since each polynomial f in $k[\boldsymbol{x}]$ can be reduced to a minimal form modulo $\mathrm{I}(F)$ by using

$$\boldsymbol{x}^{\alpha_j} \equiv s_j(x_1, \dots, x_d),$$

f can be written as a unique linear combination of elements of $\mathrm{Est}(F)$ modulo $\mathrm{I}(F)$. This polynomial is called the *normal form* of f and denoted $\mathrm{NF}_F(f)$. Denote by $\overline{\mathrm{Est}(F)}$ the set of residue classes of terms in $\mathrm{Est}(F)$ in the space $\mathbb{Q}[\boldsymbol{x}]/\,\mathrm{I}(F)$. As a result, from Theorem 2, $\overline{\mathrm{Est}(F)}$ is a basis of the quotient space $\mathbb{Q}[\boldsymbol{x}]/\,\mathrm{I}(F)$.

A *response* f is a rational-valued function defined on F. We denote by $L(F)$ the vector space of all responses defined on F. Hence, $\mathbb{Q}[\boldsymbol{x}]/\,\mathrm{I}(F)$ is an algebraic representation on the space $L(F)$,

$$L(F) \cong \left\{ \sum_{\boldsymbol{x}^{\boldsymbol{\alpha}} \in \mathrm{Est}(F)} \theta_\alpha \, \overline{\boldsymbol{x}^\alpha} : \theta_{\boldsymbol{\alpha}} \text{ is a rational number} \right\}, \tag{2.2.2}$$

where $\overline{\boldsymbol{x}^\alpha}$ is the image of $\boldsymbol{x}^\alpha$ in $\mathbb{Q}[\boldsymbol{x}]/\,\mathrm{I}(F)$. We denote by X_i the ith projection function, mapping a run $\boldsymbol{p} = (p_1, \dots, p_d)$ to p_i. We identify X_i with the ith factor Q_i. *Interaction terms* are defined as functions

$$X_1^{\alpha_1} X_2^{\alpha_2} \dots X_d^{\alpha_d} : F \to \overline{\mathbb{Q}}, \quad \boldsymbol{p} \mapsto \boldsymbol{p}^{\boldsymbol{\alpha}} = p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_d^{\alpha_d}$$
$$\text{where } 0 \le \alpha_i \le r_i - 1, \text{ for } i = 1, \dots, d.$$

We write $\boldsymbol{X}^{\boldsymbol{\alpha}}$ for $X_1^{\alpha_1} X_2^{\alpha_2} \dots X_d^{\alpha_d}$, with $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_d)$. The term $\boldsymbol{X}^{\boldsymbol{\alpha}}$ has *order* l if the d-tuple $\boldsymbol{\alpha}$ has exactly l non-zero components. A term $\boldsymbol{X}^{\boldsymbol{\alpha}}$ of order l $(1 \le l \le d)$ is called an *l-factor effect* [Galetto et al., 2003]. A one-factor effect is just a power of a single factor, called the *main effect* of that factor; while the term 'interaction' is used frequently for at least two factors. Notice that in the non-binary case (ie, at least a factor Q_i has more than 2 levels for some $i = 1, \dots, d$), the order l of a term $\boldsymbol{X}^{\boldsymbol{\alpha}}$ differs from its total degree $\sum_{i=1}^d \alpha_i$. For instance, when $d = 3$, suppose that F has a ternary factor Q_1, and two binary factors Q_2, Q_3. The main effect of Q_1 then is a pair of terms X_1, X_1^2; the main effect of Q_2 and Q_3 are X_2 and X_3 respectively. The 2-factor effect or 2-factor interaction between the first and the second factor includes terms $X_1X_2, X_1^2X_2$.

Regression analysis. We aim to discover how the variables $\boldsymbol{x} = (x_1, \dots, x_d)$ (called independent variables or regressors) affect the response variable Y. A *regression model* is defined by

$$Y(\boldsymbol{x}) = f(\boldsymbol{x}, \boldsymbol{\theta}) + \epsilon(\boldsymbol{x}),$$

in which $f(.,\boldsymbol{\theta}) \in L(F)$, the vector $\boldsymbol{\theta}$ consists of q parameters that determine the model, and $\epsilon(\boldsymbol{x})$ is a random variable for all $\boldsymbol{x} \in F$ called the *error*. For $F = [\boldsymbol{p}_1, \dots, \boldsymbol{p}_N]$, $\epsilon_i := \epsilon(\boldsymbol{p}_i)$ is the error caused when conducting the experimental run $\boldsymbol{p}_i$. To estimate parameters of $\boldsymbol{\theta} := [\theta_1, \dots, \theta_q]$ we assume our model satisfies the Gauss-Markov conditions:

$$\begin{aligned}
\mathrm{E}(\epsilon_i) &= 0 \text{ for all } i,\\
\mathrm{Var}(\epsilon_i) &= c \text{ for all } i,\\
\mathrm{E}(\epsilon_i \epsilon_j) &= 0 \text{ when } i \neq j = 1, \dots, n,
\end{aligned}$$

where c is a rational constant, E is the expectation, and Var is the variance.

Linear (regression) models are models such that $f(\boldsymbol{x}, \boldsymbol{\theta})$ is a linear function of the components of the parameter vector $\boldsymbol{\theta}$, that is

$$Y(\boldsymbol{x}) = \sum_{j=1}^{q} \boldsymbol{\theta}_j . p_j(\boldsymbol{x}) + \epsilon(\boldsymbol{x}), \tag{2.2.3}$$

where p_j are elements of $L(F)$, and ϵ satisfies the Gauss-Markov conditions. Now suppose that we have observations $Y_1, \dots Y_N$ corresponding to runs $\boldsymbol{p}_1, \dots, \boldsymbol{p}_N$. Let $f(\boldsymbol{x}, \boldsymbol{\theta}) = \sum_{\boldsymbol{\alpha}} \boldsymbol{\theta}_{\boldsymbol{\alpha}} . \boldsymbol{X}^{\boldsymbol{\alpha}}$ be a linear model of F such that $\boldsymbol{X}^{\boldsymbol{\alpha}} \in \boldsymbol{x}^*$. Let

$$\begin{aligned}
&S(f) := \mathrm{Supp}(f) = \left\{\boldsymbol{X}^{\boldsymbol{\alpha}_1}, \dots, \boldsymbol{X}^{\boldsymbol{\alpha}_r}\right\},\\
&r := |S(f)|, \quad \text{ and } \quad L := \{\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_r\}.
\end{aligned}$$

The $N \times r$-matrix

$$Z = Z(S(f), F) = \left[Z_{ij}\right] = \left[\boldsymbol{X}^{\boldsymbol{\alpha}_j}(\boldsymbol{p}_i)\right] \tag{2.2.4}$$

whose element Z_{ij} is the evaluation of $\boldsymbol{X}^{\boldsymbol{\alpha}_j}$ at the ith run $\boldsymbol{p}_i = (p_{i1}, p_{i2}, \dots, p_{id})$, is called the *design matrix* of F. The corresponding model is now

$$Y(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in L} \boldsymbol{\theta}_{\boldsymbol{\alpha}} . \boldsymbol{X}^{\boldsymbol{\alpha}}(\boldsymbol{x}) + \epsilon(\boldsymbol{x}), \tag{2.2.5}$$

and so in vector notation:

$$\boldsymbol{Y} = Z\boldsymbol{\theta} + \boldsymbol{\epsilon}, \tag{2.2.6}$$

where $\boldsymbol{Y} = (Y_1, \dots Y_N)$ is the vector of responses. The linear model (2.2.5) is *identifiable* by a fraction F if the functions $\boldsymbol{X}^{\boldsymbol{\alpha}}$ ($\boldsymbol{\alpha} \in L$) are linearly independent elements of $L(F)$. The corresponding terms $\boldsymbol{X}^{\boldsymbol{\alpha}}$ then, are called *estimable terms*. We can also say (2.2.5) is *identifiable* if $\mathrm{rank}(Z) = r$, ie, by taking $f(\boldsymbol{p}_i, \boldsymbol{\theta})$ equal to Y_i at the runs $\boldsymbol{p}_i \in F$, we can uniquely determine its coefficients $\boldsymbol{\theta}_{\boldsymbol{\alpha}}$. Recall from (2.2.1) that

$$\mathrm{Est}(F) = \left\{\boldsymbol{x}^{\boldsymbol{\alpha}} : \boldsymbol{x}^{\boldsymbol{\alpha}} \notin \left(\mathrm{LT}(\mathrm{I}(F))\right)\right\}.$$

We employ the following theorems, summarizing known results, (cf. Cohen et al. [2001, Theorem 6], or Pistone et al. [2000, Theorem 2.5]).

THEOREM 6. *If $S(f)$ is a subset of* $\mathrm{Est}(F)$*, then Model (2.2.5) is identifiable. The set* $\mathrm{Est}(F)$ *has exactly N elements, and* $r \leq |\mathrm{Est}(F)| = |F| = N$.

THEOREM 7. *Let F be a fraction and let $f(\boldsymbol{x}, \boldsymbol{\theta})$ be a linear model supported by F. Let $S(f)$ be the support and Z be the design matrix of F, respectively. Then the following conditions are equivalent*

- *$f(x)$ is identifiable by F.*
- $\operatorname{rank}(Z) = r$,
- *$S(f)$ is a set of linearly independent functions on F.*

These results will be used in Sections 2.3, 2.4, and 2.5, where the following three problems will be discussed:

(1) compute $\operatorname{Est}(F)$ for a given fractional design F;
(2) the *inverse problem* of Problem (1), that is given an order ideal E, construct a fraction F such that $E = \operatorname{Est}(F)$;
(3) given an order ideal E, construct a t-balanced fraction F such that $E = \operatorname{Est}(F)$.

The solution of the first problem will be reviewed in the next subsection. The last two problems require more ingredients to solve, so we postpone the discussion until Subsections 2.4 and 2.5, respectively.

2.3. Determining all estimable terms of a model

Let $F = \{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_N\}$ be a fractional design and Z its design matrix (Definition (2.2.4)). We compute the set $\operatorname{Est}(F)$ with given a term order $<$. Why do we need to know the standard basis $\operatorname{Est}(F)$? Firstly, because the space $L(F)$ of all responses on F is generated by the set $\overline{\operatorname{Est}(F)}$ (see Equation (2.2.2)). Secondly, to find an identifiable linear model f of a fraction F, we should choose the support $S(f)$ of f such that $S(f) \subseteq \operatorname{Est}(F)$ or, better, $S(f) = \operatorname{Est}(F)$, by Theorem 6. In this section, we only consider saturated designs, ie, we let $S(f) = \operatorname{Est}(F)$. In this case, Z is a square matrix. Denote by K an extension of k. We use Theorem 7 and the following to compute all estimable terms of Model 2.2.5.

THEOREM 8. [Pistone et al., 2001, Theorem 26] *Z is non-singular (so Z has full rank). Moreover, if $f : F \to K$ is a response mapping and $\boldsymbol{Y} = \big(f(\boldsymbol{p}_1), \ldots, f(\boldsymbol{p}_N)\big)$ is the vector of responses (observed values), we calculate vector $\boldsymbol{\theta}$ of coefficients of f by $\boldsymbol{\theta} = [\theta_{\boldsymbol{\alpha}}] = Z^{-1} \cdot Y$. And we have*

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{x}^{\boldsymbol{\alpha}} \in \operatorname{Est}(F)} \theta_{\boldsymbol{\alpha}} \cdot \boldsymbol{x}^{\boldsymbol{\alpha}}. \tag{2.3.1}$$

For instance, if $<$ is the degree reverse lexicographical order and the fraction F is an $\mathrm{OA}(24; 3^1 \cdot 2^4; 3)$:

$$\begin{bmatrix} 0&0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&2&2&2&2&2&2&2&2 \\ 0&0&0&0&1&1&1&1&0&0&0&0&1&1&1&1&0&0&0&0&1&1&1&1 \\ 0&0&1&1&0&0&1&1&0&0&1&1&0&0&1&1&0&0&1&1&0&0&1&1 \\ 0&0&1&1&1&1&0&0&0&1&0&1&0&1&0&1&1&1&0&0&0&0&1&1 \\ 0&1&0&1&0&1&0&1&0&0&1&1&0&1&0&0&1&0&1&0&1&0&1&0&1 \end{bmatrix}^T,$$

the estimable terms of F are

$$\begin{aligned} \operatorname{Est}(F) = [&1, x_5, x_4, x_3, x_2, x_1, x_4x_5, x_3x_5, x_2x_5, x_1x_5, x_3x_4, x_2x_4, x_1x_4, x_2x_3, x_1x_3, \\ &x_1x_2, x_1^2, x_3x_4x_5, x_2x_4x_5, x_1x_4x_5, x_2x_3x_5, x_1x_3x_5, x_1x_2x_5, x_1^2x_5]. \end{aligned}$$

2.4. Constructing a fraction with given estimable terms

Let D be a full factorial design, let $C=\{f_1,\dots,f_d\}$ be the set of canonical polynomials of D. The set

$$\mathrm{O}(D)=\{x_1^{\alpha_1}x_2^{\alpha_2}\dots x_d^{\alpha_d}:\alpha_i=0,1,\dots,r_i-1,i=1,\dots,d\}$$

is called the complete set of *estimable terms* of D. Note that $\mathrm{O}(D)$ depends only on the type of D (not on the ordering). For instance, if $D=\{-1,1\}^3$, then

$$\mathrm{O}(D)=\{1,x_1,x_2,x_3,x_1x_2,x_1x_3,x_2x_3,x_1x_2x_3\}.$$

Suppose that $E=\{t_1,\dots,t_\mu\}$ is a fixed order ideal contained in $\mathrm{O}(D)$. We compute a fraction F of D, such that $E=\mathrm{Est}(F)$, that is, $\overline{E}$ is a basis of $R=\mathbb{Q}[\boldsymbol{x}]/\,\mathrm{I}(F)$ as a $\mathbb{Q}$-vector space.

We need the Finiteness Criterion below [Kreuzer and Robbiano, 2000, Proposition 3.7.1] and the concept of border basis to solve this problem. Let J be an ideal of $k[\boldsymbol{x}]$. The set

$$\sqrt{J}=\{r\in k[\boldsymbol{x}]:r^i\ \in J\ \text{ for some } i\geq 0\}$$

is an ideal in $k[\boldsymbol{x}]$, called the *radical* of J. If $J=\sqrt{J}$ then J is called a *radical ideal*.

Lemma 9. *Let k be an algebraically closed field and let J be a proper ideal of $k[\boldsymbol{x}]$. Then $\mathrm{I}(\mathrm{Z}(J))=\sqrt{J}$.*

Proposition 10 (Finiteness Criterion). *Let $K=(f_1,\dots,f_s)$ be a proper ideal of $k[\boldsymbol{x}]$. Then the following conditions are equivalent.*

(a) *$\mathrm{Z}(K)$ is finite.*
(b) *$\overline{K}$ is contained in only finitely maximal ideals of $\overline{k}[\boldsymbol{x}]$.*
(c) *For every $i=1,\dots,d$, there exists an $\alpha_i\geq 0$ such that $x_i^{\alpha_i}\in\mathrm{LT}(K)$.*
(d) *$\boldsymbol{x}^*\setminus\mathrm{LT}(K)$ is finite.*
(e) *$k[\boldsymbol{x}]/K$ is a finite dimensional k-vector space.*
(f) *$K\cap k[x_i]\neq(0)$ for $i=1,\dots,d$.*

We write $P\ =k[\boldsymbol{x}]$ and $\overline{P}=\overline{k}[\boldsymbol{x}]$ and use them interchangeably from now.

Proof. Firstly, we show that $(a)\Longrightarrow(b)$, that is the number of maximal ideals J containing K is finite if $\mathrm{Z}(K)$ is finite. From Corollary 4, every maximal ideal J of $\overline{P}$ is of the form

$$J=(x_1-p_1,\dots,x_d-p_d)$$

with $p_1,\dots,p_d\in\overline{k}$. Consider the substitution homomorphism $\phi:\overline{P}\to\overline{k}$ defined by $x_i\mapsto p_i$ for $i=1,\dots,d$. Since J contains K, each polynomial in K has the pattern $f=\sum_{i=1}^d h_i.(x_i-p_i)$, $h_i\in P$. That is, f lies in the kernel of ϕ, or $(p_1,\dots,p_d)\in\mathrm{Z}(K)$. Since $\mathrm{Z}(K)$ is finite, there are a finite number of possibilities for $(p_1,\dots,p_d)$, and hence for J. We have shown $(a)\Longrightarrow(b)$.

Next, we consider $(b)\Longrightarrow(c)$. Let $J_1,\dots,J_t$ be the maximal ideals of $\overline{P}$ containing K. Due to Corollary 4, there are tuples $(p_{i1},\dots,p_{id})$ such that $J_i=(x_1-p_{i1},\dots,x_d-p_{id})$ for $i=1,\dots,t$. Since $K\subseteq J_i$, every polynomial $f\in K$ can be written as $f=\sum_{j=1}^d h_j.(x_j-p_{ij})$, $h_j\in P$, and so each tuple $(p_{i1},\dots,p_{id})$ is in $\mathrm{Z}(K)$. For $j=1,\dots,d$, put $g_j=\prod_{i=1}^t(x_j-p_{ij})\in\overline{k}[x_j]$; then g_j vanishes on every solution of $\mathrm{Z}(K)$, that is, g_j belongs to vanishing ideal $\mathrm{I}(\mathrm{Z}(K))$. Using Theorem 9, there exists an integer $\alpha_j \geq 0$ such that $g_j^{\alpha_j} \in K$, which implies $x_j^{t.\alpha_j} \in \mathrm{LT}(K.\overline{P})$. From Lemma 1, we have $x_j^{t.\alpha_j} \in \mathrm{LT}(K.P) = \mathrm{LT}(K)$.

$(c) \Longrightarrow (d)$ is true since every term of sufficiently high degree is divisible by one of the terms $x_j^{t.\alpha_j}$, for $j = 1, \ldots, d$.

The implication $(d) \Longrightarrow (e)$ is a consequence of Theorem 2.

Next we consider $(e) \Longrightarrow (f)$. Indeed, if the space P/K has finite dimension over k, the residue classes $1+K, x_i+K, x_i^2+K, \ldots$ are k-linearly dependent, for each $i = 1, \ldots, d$. Hence there are non-zero polynomials $g_i \in K \cap k[x_i]$ for $i = 1, \ldots, d$.

Finally, we prove $(f) \Longrightarrow (a)$. We show that there are finitely many $\boldsymbol{p} = (p_1, \ldots, p_d) \in \mathrm{Z}(K)$. For $i = 1, \ldots, d$, there exists non-zero polynomials $g_i \in K \cap k[x_i]$, so $g_i \in K \cap k[\boldsymbol{x}]$. Since $\boldsymbol{p} \in \mathrm{Z}(K)$, we get $g_i(\boldsymbol{p}) = 0$, that is, the ith component p_i of $\boldsymbol{p}$ must be a solution of the polynomial g_i, for every $i = 1, \ldots, d$. As a result, the number of solutions $\boldsymbol{p}$ is at most $\deg(g_1) \cdots \deg(g_m)$. □

An ideal $I = (f_1, \ldots, f_s)$ is called *zero-dimensional* if it satisfies the equivalent conditions of Proposition 10. Let I be a zero-dimensional proper ideal in $P = k[\boldsymbol{x}]$, let $\pi : k[\boldsymbol{x}] \to k[\boldsymbol{x}]/I$ be the canonical surjection, and let $\mu = \dim_k(k[\boldsymbol{x}]/I) < \infty$. Let $E = \{h_1, \ldots, h_\mu\}$ be a set of polynomials such that $\overline{E} = \{\overline{h}_1, \ldots, \overline{h}_\mu\}$ is a basis for $k[\boldsymbol{x}]/I$ as a k-vector space. We denote by $\mathrm{V}(E)$ the k-vector space of $k[\boldsymbol{x}]$ generated by E. We consider three linear maps

$$\mathrm{NF}_{E,I} : k[\boldsymbol{x}] \to \mathrm{V}(E), \quad \nu : \mathrm{V}(E) \to k^\mu, \quad \text{and } \mathrm{NFV}_{E,I} : k[\boldsymbol{x}] \to k^\mu$$

defined by

$$\mathrm{NF}_{E,I}(f) = \sum_{i=1}^{\mu} a_i h_i, \quad \nu\Big(\sum_{i=1}^{\mu} a_i h_i\Big) = \sum_{i=1}^{\mu} a_i e_i, \quad \text{and } \mathrm{NFV}_{E,I} = \nu \circ \mathrm{NF}_{E,I},$$

where $e_1, \ldots, e_\mu$ are the standard basis vectors of k^μ and the a_i are defined by $\pi(f) = \sum_{i=1}^{\mu} a_i \overline{h_i}$. The polynomial $\mathrm{NF}_{E,I}(f)$ is called the *normal form* of f with respect to E and I; the vector $\mathrm{NFV}_{E,I}(f)$ is called the *normal form vector* of f with respect to E and I.

Multiplication matrices and the border basis. The concepts and results in this section are from Caboara and Robbiano [2001]. These authors define the concept of *border basis* G of an ideal E and relate it to the matrices associated with the left multiplication by x_i, for $i = 1, \ldots, d$. They then prove that the ideal I generated by G is zero dimensional (ie, the zero set $\mathrm{Z}(I)$ is finite or $\dim_k(k[\boldsymbol{x}]/I) < \infty$), if the left multiplication matrices are pairwise commuting. Then $\mathrm{Z}(I)$ is the set of runs of a fraction F such that $\mathrm{Est}(F) = E$. These notions will be used in Theorem 14. Denote by $\mathrm{Mat}_\mu(k)$ the ring of square matrices of degree μ with entries in k. We view k^μ as a space of column vectors.

Proposition 11. *Let $\phi : P \to k^\mu$ be a surjective k-linear map such that $I = \mathrm{Ker}(\phi)$ is a proper ideal in P and let $\omega = \phi(1)$, viewed as column vector.*

- *(a) The ideal I is zero dimensional. Moreover, if we pick $E = \{h_1, \ldots, h_\mu\}$ such that $\phi(h_i) = e_i$ for $i = 1, \ldots, \mu$, then $\phi = \mathrm{NFV}_{E,I}$.*
- *(b) There exists a unique n-tuple of pairwise commuting matrices $M_1, \ldots, M_d$ in $\mathrm{Mat}_\mu(k)$ such that $\phi(x_i f) = M_i\, \phi(f)$ for all $f \in P$ and $i = 1, \ldots, d$.*
- *(c) $\phi(f) = f(M_1, \ldots, M_d)\, \omega$ for all $f \in P$.*

Proof. (a) Since the space P/I is finite dimensional I is zero dimensional. If we let $f \in P$, we get $\overline{f} \in P/I$, so $f = \sum_{i=1}^{\mu} a_i h_i + g$, where $g \in I$. Hence,

$$\phi(f) = \sum_{i=1}^{\mu} a_i \phi(h_i) + \phi(g) = \sum_{i=1}^{\mu} a_i \phi(h_i) = \sum_{i=1}^{\mu} a_i e_i.$$

So $\phi = \mathrm{NFV}_{E,I}$ by definition.

(b) We construct the matrices M_i in $\mathrm{Mat}_\mu(k)$. Since $\phi : P \to k^\mu$ is surjective, there exist polynomials $h_1, \ldots, h_\mu \in P$ such that $\phi(h_k) = e_k$, for $k = 1, \ldots, \mu$. We define M_i to be the $\mu \times \mu$ matrix whose columns are the vectors $\phi(x_i h_1), \ldots, \phi(x_i h_\mu)$. We need to prove that the M_i are well-defined and unique by selecting other polynomials $l_1, \ldots, l_\mu \in P$ such that $\phi(l_k) = e_k$, and then checking that $\phi(x_i h_k) = \phi(x_i l_k)$ for all i and k. This is clear because $\phi(h_k - l_k) = 0$ so $h_k - l_k \in I$ and $x_i\,(h_k - l_k) \in I$. Next we check that $\phi(x_i f) = M_i\,\phi(f)$ for $f \in P$. Using the sum decomposition of f given in (a), since

$$\phi(f) = \sum_{k=1}^{\mu} a_k e_k,$$

we have $f - \sum_{k=1}^{\mu} a_k h_k \in I$, and so $x_i f - \sum_{k=1}^{\mu} a_k x_i h_k \in I$. Hence,

$$\phi(x_i f) = \phi\left(\sum_{k=1}^{\mu} a_k x_i h_k\right) = \sum_{k=1}^{\mu} a_k \phi(x_i h_k) = \sum_{k=1}^{\mu} a_k M_i e_k = M_i\,\phi(f)$$

since $M_i e_k$ is the k-th column of M_i. Finally we prove that the matrices M_i are pairwise commuting. Since $M_j e_k = \phi(x_j h_k)$, we get

$$M_i M_j e_k = \phi(x_i x_j h_k) = \phi(x_j x_i h_k) = M_j M_i e_k,$$

and so $M_i M_j = M_j M_i$.

(c) Since ϕ is linear, we only need to prove the formula for $f = \boldsymbol{X}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} \ldots x_d^{\alpha_d}$. If $f(x) = 1$ the formula is correct since $\phi(1) = \omega$. We continue by induction on the total degree $\sum_i \alpha_i$. Without loss of generality we can assume that $\alpha_1 > 0$. Put $g = x_1^{\alpha_1 - 1} \ldots x_d^{\alpha_d}$. By the inductive assumption and Part (b) we have

$$\begin{aligned}\phi(f) &= \phi(x_1 g) = M_1 \phi(g) = M_1 g(M_1, \ldots, M_d)\omega \\ &= M_1 M_1^{a_1 - 1} M_2^{a_2} \cdots M_d^{a_d} \omega = f(M_1, \ldots, M_d)\omega.\end{aligned}$$

The proof is complete. □

The matrices $M_1, \ldots, M_d$ are called the *multiplication matrices* of ϕ.

Theorem 12 (Converse of Proposition 11). *Let $\omega \in k^\mu$ be a non-zero vector and let $M_1, \ldots, M_d$ be pairwise commuting matrices in $\mathrm{Mat}_\mu(k)$. Then,*

(1) there is a unique k-linear map $\phi : P \to k^\mu$ such that
  - (a) *$\phi(1) = \omega$, and*
  - (b) *$\phi(x_i f) = M_i\,\phi(f)$, for all $f \in P$ and $i = 1, \ldots, d$;*

(2) the kernel of ϕ is a zero-dimensional ideal;

(3) if ϕ is surjective and $I = \mathrm{Ker}(\phi)$, then for every $E = \{h_1, \ldots, h_\mu\}$ such that $\phi(h_i) = e_i$ we have $\phi = \mathrm{NFV}_{E,I}$. In this case, the matrices $M_1, \ldots, M_d$ are the multiplication matrices of $\mathrm{NFV}_{E,I}$.

PROOF. In Caboara and Robbiano [2001, Theorem 2.9], proofs of the first and the third items were given. We prove the second item. First, we show that $\mathrm{Ker}(\phi)$ is an ideal. Let $f \in \mathrm{Ker}(\phi)$ and $g \in P$. By linearity, we can assume that g is a term, and using Item (1)(b), we can assume that g is an indeterminate, say x_i. Then $\phi(x_i f) = M_i \cdot \phi(f) = 0$. Hence $x_i f \in \mathrm{Ker}(\phi)$. Of course $f + g \in \mathrm{Ker}(\phi)$ if $f, g \in \mathrm{Ker}(\phi)$ since ϕ is k-linear. Hence $\mathrm{Ker}(\phi)$ is an ideal. It is a proper ideal since $\phi(1) = \omega \neq 0$. It is zero-dimensional because the space $P/\mathrm{Ker}(\phi)$ is a finite dimensional k-vector space. □

Suppose that $E = \{t_1, \ldots, t_\mu\}$ is an order ideal. Define

$$E^+ = \{x_i\, t : t \in E,\ i = 1, \ldots, d, \text{ and } x_i t \notin E\}.$$

This set is finite since E is finite and the number of indeterminates is finite.

PROPOSITION 13. *Let I be a proper ideal in P, let $E = \{t_1, \ldots, t_\mu\}$ be an order ideal such that $\overline{E} = \{\overline{t_1}, \ldots, \overline{t_\mu}\}$ is a basis of P/I as k-vector space, and let $E^+ = \{b_1, \ldots, b_v\}$. Then there exists unique $a_{jl} \in k \quad (l = 1, \ldots, \mu)$ with*

$$g_j = b_j - \sum_{l=1}^{\mu} a_{jl} t_l \in I, \text{ for each } j = 1, \ldots, v. \tag{2.4.1}$$

Moreover, the ideal I is generated by $g_1, \ldots, g_v$.

PROOF. We have $P = \mathrm{V}(E) \oplus I$, so every polynomial f in P can be written uniquely as $f = h + g$ where $h \in \mathrm{V}(E)$ and $g \in I$. We can write

$$b_j = \sum_{l=1}^{\mu} a_{jl} t_l + g_j, \tag{2.4.2}$$

where $a_{jl} \in \mathbb{Q}$ and $g_j \in I$. The constants a_{jl} are unique because $\{\overline{t_1}, \ldots, \overline{t_\mu}\}$ is a basis of P/I.

Let J be the ideal generated by $\{g_1, \ldots, g_v\}$. We show that $I = J$. Since

$$g_j = b_j - \sum_{l=1}^{\mu} a_{jl} t_l \in I$$

we have $J \subseteq I$. We only need that $I \subseteq J$, or equivalently that $P = \mathrm{V}(E) + J$. We prove this for $f \in \mathrm{V}(E) \oplus I$ by induction on $\deg(f) = d$. If $d = 0$, then $1 \in E \subseteq \mathrm{V}(E)$, so $f \in \mathrm{V}(E)$. Let f be a term of total degree $d > 0$. Then there exists an indeterminate x_i and a term t of degree $d - 1$ such that $f = x_i.t$. The term t must have the decomposition $t = \sum_{l=1}^{\mu} a_{jl} t_l + g$, with $g \in J$. As a result

$$f = x_i.t = \sum_{l=1}^{\mu} a_{jl} x_i\, t_l + x_i\, g.$$

If every $x_i\, t_l \in E$, the proof is finished. If there exist some $x_i\, t_l \notin E$, that is $x_i\, t_l = b_j \in E^+$, then $x_i \cdot t_l = b_j \in \mathrm{V}(E) + J$, by (2.4.2). The proof is complete. □

A pair (g, t) is a *marked polynomial* if g is a non-zero polynomial and t is in $\mathrm{Supp}(g)$. We also say that g is marked at t. Let $G = [g_1, \ldots, g_v]$ be a sequence of non-zero polynomials and let $T = [t_1, \ldots, t_v]$ be a sequence of terms. If (g_1, t_1), …, (g_v, t_v) are marked polynomials, we say G is marked by T. Denote by $G = [g_1, \ldots, g_v]$ a sequence of polynomials marked by the corresponding elements of E^+

in the order given by $<$. Then the pair (G, E^+) is called the *border basis* of I with respect to E.

Constructing matrices associated with the border basis (G, E^+). Let $E = \{t_1, \ldots, t_\mu\}$ be an order ideal and let $E^+ = \{b_1, \ldots, b_v\}$. From (2.4.1), $G = \{g_1, \ldots, g_v\}$ consists of polynomials marked by the corresponding elements of E^+ such that $\mathrm{Supp}(g_k - b_k) \subseteq E$ for $k = 1, \ldots, v$. We construct matrices $M_1, \ldots, M_d \in \mathrm{Mat}_\mu(k)$ as follows:

- If $x_i t_j = t_l \in E$, then the j-th column of M_i is e_l
- If $x_i t_j \in E^+$ then there exists a $k \in \{ 1, \ldots, v\}$ such that $x_i t_j = b_k$. Then the j-column of M_i contains the coefficients of $t_1, \ldots, t_\mu$ in the representation of the polynomial $b_k - g_k$ as a linear combination of the elements in E.

The matrices $M_1, \ldots, M_d$ constructed above are called the *matrices associated to* (G, E^+).

THEOREM 14. [Caboara and Robbiano, 2001] *Let $E = \{t_1, \ldots, t_\mu\}$ be an order ideal and let $E^+ = \{b_1, \ldots, b_v\}$. Furthermore, let $G = [g_1, \ldots, g_v]$ be polynomials marked by the corresponding elements of E^+ such that* $\mathrm{Supp}(g_k - b_k) \subseteq E$ *for $k = 1, \ldots, v$. Let I be an ideal generated by G. Then (G, E^+) is the border basis of I with respect to E if and only if the associated matrices $M_1, \ldots, M_d$ are pairwise commuting. In this case*

(1) The ideal I is zero dimensional and $\dim_k(P/I) = \mu$.
(2) The tuple $\overline{E}$ is a basis of P/I as a k-vector space,
(3) The matrices $M_1, \ldots, M_d$ are the multiplication matrices of $\mathrm{NFV}_{E,I}$.

PROOF. $\Longrightarrow$): Let $M_1, \ldots, M_d$ be the matrices associated with (G, E^+). If the pair (G, E^+) is the border basis of I with respect to E, then $\overline{E}$ is a basis of P/I. Then (1) and (2) follow immediately. In addition, from the definition of normal form, we can define $\mathrm{NFV}_{E,I} : P \to k^v$ with $\mathrm{NFV}_{E,I}(1) = e_1$. Applying Proposition 11, we get a unique d-tuple of multiplication matrices $N_1, \ldots, N_d$ of $\mathrm{NFV}_{E,I}$ that are pairwise commuting such that

$$\mathrm{NFV}_{E,I}(x_i f) = N_i \cdot \mathrm{NFV}_{E,I}(f)$$

for all $f \in P$ and $i = 1, \ldots, d$. From the definition of N_i, the j-th column of N_i is

$$N_i \cdot e_j = N_i \cdot \mathrm{NFV}_{E,I}(t_j) = \mathrm{NFV}_{E,I}(x_i t_j).$$

Meanwhile, $\mathrm{NFV}_{E,I}(x_i t_j)$ is the j-th column of matrix M_i, that is $N_i = M_i$. Hence $M_1, \ldots, M_d$ commute pairwise and (3) is true.

$\Longleftarrow$): Since E is an order ideal, we have $1 \in E$ and we can assume that $t_1 = 1$. From the definition of a border basis we need to show that the set $\overline{E} = \{\overline{t_1}, \ldots, \overline{t_\mu}\}$ is a basis of P/I as a k-vector space. Set $\omega = e_1$; since the matrices $M_1, \ldots, M_d$ are pairwise commuting, by Theorem 12, there exists a k-linear map $\phi : P \to k^\mu$ such that

$$\phi(1) = \phi(t_1) = \omega \text{ and } \phi(x_i f) = M_i\, \phi(f)$$

for all $f \in P$, $i = 1, \ldots, d$. We need to show that ϕ is surjective (in order to use the third statement in Theorem 12), or to show that $\phi(t_l) = e_l$ for $l = 1, \ldots, \mu$.

The claim is true when $l = 1$ by construction. So let $t_l \neq 1$, that is $\deg(t_l) > 0$, and use induction on degree. We may write $t_l = x_k\, t_j$ for some indeterminate x_k and some term $t_j \in E$, since E is an order ideal. Then $\phi(t_l) = \phi(x_k\, t_j) =$

$M_k\phi(t_j) = M_k e_j$ (using the inductive assumption). But $M_k e_j$ is in fact the j-th column of M_k. But this is e_l thanks to the definition of M_k. Therefore $\phi(t_l) = e_l$, so $\overline{E}$ is a basis of P/I, where $I = (G)$. From Proposition 13, (G, E^+) is the border basis of I with respect to E. □

If $E = \{t_1, \ldots, t_\mu\}$ is given, then E^+ can be computed. We know that $1 \in E$ and we can assume $t_1 = 1$. Considering $\overline{E}$ as a basis, we can compute the space P/I. From this, we extract $I = (f_1, \ldots, f_l)$. Then the fraction F which we want is the zero set of I (in other words, F is the algebraic variety determined by the ideal I). That means a solution of the inverse problem (Problem (2)) is obtained. Proposition 13 shows that, given E, the ideal I such that $\overline{E}$ is a basis of P/I corresponds to the border basis $G = \{g_1, \ldots, g_v\}$ marked by $\{b_1, \ldots, b_v\}$. To find G, we need the following lemma [Caboara and Robbiano, 2001, Lemma 4.5].

Lemma 15. *Let D be a full factorial design, let $\mathrm{I}(D) = (f_1, \ldots, f_d)$ be the defining ideal in P of D. Let I be a proper ideal of $\overline{k}[\boldsymbol{x}]$ containing $\mathrm{I}(D)$. We have: I is a radical ideal and it defines a fraction F of D. Moreover I can be generated by polynomials in $k[\boldsymbol{x}]$ and every border basis of I is contained in $k[\boldsymbol{x}]$.*

Recall that D is a full factorial design and C is the set of canonical polynomials, The following algorithm [Caboara and Robbiano, 2001, Theorem 4.6], together with Proposition 10 and the above lemma, determines the border basis G of an order ideal E.

Algorithm 1 Compute fractional design with given order ideal

Input: D and an order ideal $E = \{t_1, \ldots, t_\mu\} \subseteq \mathrm{O}(D)$.
Output: A fraction F such that $\overline{E}$ is a basis of the ring $\mathbb{Q}[\boldsymbol{x}]/\mathrm{I}(F) = P/\mathrm{I}(F)$ as a $\mathbb{Q}$-vector space.

function Compute-border-basis-G(D, E)

(1) Split the set E^+ into two subsets E_1^+, E_2^+, where

$$E_1^+ = E^+ \cap \{x_1^{r_1}, \ldots, x_d^{r_d}\} \quad \text{and} \quad E_2^+ = E^+ \setminus E_1^+$$

(2) Decompose C into two subsets

$$C_1 = \{f_i : x_i^{r_i} \in E^+\} \quad \text{and} \quad C_2 = C \setminus C_1,$$

where f_i is marked by $x_i^{r_i}$ for every $f_i \in C_1$

(3i) Let $\nu = |E_2^+|$, and for every terms $b_j \in E_2^+$ let $g_j = b_j - \sum_{l=1}^{\mu} a_{jl} t_l$
▷ $g_j \in \mathbb{Q}[\mathrm{A}][x_1, .., x_d]$, where $A := \{a_{jl} : j = 1, \ldots, \nu,\ l = 1, \ldots, \mu\}$

(3ii) Let $G_2 := \{g_j : j = 1, \ldots, \nu\}$ and let $G = C_1 \cup G_2$
▷ note that $|G_2| = |E_2|$, $|C_1| = |E_1|$, so $|G| = |E| = \mu$

(4) Construct $M_1, \ldots, M_d \in \mathrm{Mat}_\mu(\mathbb{Q})$, the matrices associated to (G, E^+)

(5) Impose that $M_1, \ldots, M_d$ are pairwise commuting

(6) Let $\omega = (1, 0, \ldots, 0)^T$ and impose that the equations

$$f_i(M_1, \ldots, M_d) \cdot \omega = (0, 0, \ldots, 0)^T \text{ hold for every } f_i \in C_2$$

(7) Let $\mathrm{I}(E)$ be the set of all polynomials arising from (5) and (6), and
▷ $\mathrm{I}(E) \subset \mathbb{Q}[A]$

(8) Compute the zeros $\mathrm{Z}(\mathrm{I}(E))$; substitute a_{jl} back to G, then the runs of F are $\mathrm{Z}((G))$.

end function

The ideal $\mathrm{I}(E)$ is a zero-dimensional ideal in $\mathbb{Q}[A]$ and each solution in $\mathrm{Z}(\mathrm{I}(E))$ corresponds to an ideal $I = (G)$. Each ideal I determines uniquely a fraction F such that $\mathrm{Est}(F) = E$. Therefore, the problem of making a fraction with given estimable terms is solved.

2.5. Construction of strength t fractions

Recall that a fraction F is said to be t-balanced if, for each choice of t coordinates (columns) from F, each combination of coordinate values from those columns occurs equally often. The following result combines the Gröbner basis method with multiplication matrices to make balanced fractions. This method is due to Arjeh Cohen.

The characteristic polynomial of a left multiplication matrix. Let F be a fraction with d factors $x_1, \ldots, x_d$, considered as a finite subset of k^d. Let $M = \boldsymbol{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_d^{\alpha_d}$ be a term of the ring $P = k[\boldsymbol{x}]$. With respect to the standard basis, let L_M be the matrix determining the left multiplication of M on the space $L(F)$ of all k-valued functions on F. Then L_M represents a linear transformation of that space.

THEOREM 16. *Suppose that F has no repeated runs. The characteristic polynomial of L_M is*

$$\prod_{\boldsymbol{p}=(p_1,\ldots,p_d)\in F} (X - p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_d^{\alpha_d}).$$

PROOF. We denote by N the number of runs of F. Let $\boldsymbol{p} = (p_1, \ldots, p_d)$ be a run in F. The vanishing ideal of $\boldsymbol{p}$ is

$$\mathrm{I}(\boldsymbol{p}) = (x_1 - p_1, \ldots, x_d - p_d). \tag{2.5.1}$$

The vanishing ideal of the fraction F is

$$\mathrm{I}(F) = \bigcap_{\boldsymbol{p}\in F} \mathrm{I}(\boldsymbol{p}). \tag{2.5.2}$$

Applying the Chinese Remainder Theorem for ideals in the ring P, since F has no repeated runs, we decompose the algebra $P/\,\mathrm{I}(F)$ as:

$$P/\,\mathrm{I}(F) = \bigoplus_{\boldsymbol{p}\in F} P/\,\mathrm{I}(\boldsymbol{p}). \tag{2.5.3}$$

A standard result [Pistone et al., 2001, Theorem 14] tells us that each $P/\,\mathrm{I}(\boldsymbol{p})$ is isomorphic to $k[\boldsymbol{p}] = k$ (see Pistone et al. [2001, Definition 19] for the definition of $k[\boldsymbol{p}]$). Hence, $P/\,\mathrm{I}(F)$ is isomorphic to the algebra k^n. From Equation (2.5.1), we have $x_i^{\alpha_i} = p_i^{\alpha_i}$ in $P/\,\mathrm{I}(\boldsymbol{p})$, for all $i = 1, \ldots, d$. Hence, for each $v \in P/\,\mathrm{I}(\boldsymbol{p})$ and $i = 1, \ldots, d$,

$$(x_i^{\alpha_i} - p_i^{\alpha_i})\, v = 0,$$

so

$$L_{x_i}^{\alpha_i}(v) = L_{x_i{}^{\alpha_i}}(v) = x_i^{\alpha_i}.v = p_i^{\alpha_i} v.$$

Hence v is an eigenvector of $L_{x_i}^{\alpha_i} = (L_{x_i})^{\alpha_i}$ with eigenvalue $p_i^{\alpha_i}$. If we choose a term $M = x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_d^{\alpha_d}$, then the left multiplication matrix by M is given by

$$L_M = L_{x_1{}^{\alpha_1} \ldots x_d^{\alpha_d}} = L_{x_1}^{\alpha_1} \ldots L_{x_d}^{\alpha_d},$$

and

$$L_M(v) = p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_d^{\alpha_d} v.$$

Therefore, v is an eigenvector of L_M with eigenvalue $p_1^{\alpha_1}p_2^{\alpha_2}\cdots p_d^{\alpha_d}$. In other words, the N subalgebras $P/\,\mathrm{I}(\boldsymbol{p})$ are eigenspaces for L_M, with corresponding eigenvalues $p_1^{\alpha_1}p_2^{\alpha_2}\cdots p_d^{\alpha_d}$. The theorem is now proved. □

A necessary condition for the existence of balanced fractions. From the above theorem, the trace of L_M is

$$\sum_{\boldsymbol{p}\in F} p_1^{\alpha_1}p_2^{\alpha_2}\cdots p_d^{\alpha_d}.$$

We use this result to seek balanced fractions F. If F is a 1-balanced fraction, then the size of F must be a multiple of the number of levels of each of the factors which form F. If F is a 2-balanced fraction, then the size of F must be a multiple of the products of each pair of levels, and so on.

COROLLARY 17. *Let F be a t-balanced fraction of a design D in k^d. Assume that factor x_i has levels $0, 1, \ldots, s_i - 1$.*

(a) *If $t \geq 1$ and $\alpha_i \in \{0, 1, \ldots, s_i - 1\}$, then $L_{x_i{}^{\alpha_i}}$ has trace*

$$\frac{N}{s_i}\sum_{l=0}^{s_i-1} l^{\alpha_i}.$$

In particular, L_{x_i} has trace $|F|(s_i - 1)/2$.

(b) *If $t \geq 2$, $\alpha_i \in \{0, 1, \ldots, s_i - 1\}$ and $\alpha_j \in \{0, 1, \ldots, s_j - 1\}$, then $L_{x_i{}^{\alpha_i}x_j{}^{\alpha_j}}$ has trace*

$$\frac{N}{s_i s_j}\sum_{l=0}^{s_i-1} l^{\alpha_i}\sum_{m=0}^{s_j-1} m^{\alpha_j}.$$

PROOF. For each factor i, the number $\lambda_i = |F|/s_i$ must be a positive integer. The fraction F can be decomposed into λ_i blocks $F_1, \ldots, F_{\lambda_i}$ each with s_i runs such that their ith coordinates are $0, 1, \ldots s_i - 1$. Hence

$$\sum_{\boldsymbol{p}\in F_l} p_i^{\alpha_i} = \sum_{l=0}^{s_i-1} l^{\alpha_i}, \text{ for every } l = 1, \ldots, \lambda_i,$$

and (a) is proved. By considering the designs combined by each pair of two factors i, j as a full design, applying a similar argument, we get (b). □

2.6. Implementation issues

This section studies the power of the Gröbner basis method and multiplication matrices for finding estimable terms given a design, and for the inverse problem of making fractional designs and t-balanced designs with given estimable terms. We implemented the algorithms of the previous sections in the computer algebra package Singular, version 3.0.0 [SINGULAR research group, 2005]. We wish to determine how large a design the Gröbner basis machinery can handle. We write *dp* for the degree reverse lexicographical order, where $x_1 > x_2 > \ldots > x_d$ (Definition 2.2); and *wp* for the weighted degree reverse lexicographical order. If we use *wp*, then we need a weight vector. For instance, with the weight vector $[1, 2, 2, 2, 2]$, and $d = 5$, we have $x_2 > x_3 > x_4 > x_5 > x_1$. We will see later that there is a close relationship between the variable's weight and the corresponding factor's significance.

Finding estimable terms given a design. We compute the defining ideal of a strength 3 fraction to find its estimable terms. Given a term ordering and a strength 3 fraction F, we compute $\mathrm{Est}(F)$, defined by (2.2.1), from which we extract the number of terms representing main effects (ME) and the number of 2-interactions. We record whether we obtain all main effects (y) or not (n). Results are shown in the 3rd, 4th, and 5th columns of Table 2.1. The last column presents computing time, and the second one shows the term ordering used. The 1st column gives the parameters of the form $[N; s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}]$, where N is the run size, $s_1 > s_2 > \cdots > s_m$ are the levels of the factors, and $a_1, a_2, \ldots, a_m$ their multiplicities.

Table 2.1: Computing estimable terms given a fractional design

Parameters	Ordering	# ME	#2-ints.	All MEs?	Time (sec)
$[16; 4 \cdot 2^3]$	dp	5	7	n	0
$[16; 4 \cdot 2^3]$	wp, $[1, 2, 2, 2]$	6	9	y	0
$[40; 5 \cdot 2^6]$	dp	8	21	n	3
$[40; 5 \cdot 2^6]$	wp,$[1, 2, 2, 2, 2, 2, 2]$	10	27	y	21
$[48; 3 \cdot 2^9]$	dp	11	36	y	10
$[48; 3 \cdot 2^9]$	wp,$[1, 2, 2, 2, 3, 3, 3, 3, 3, 3]$	11	35	y	5
$[54; 3^5 \cdot 2]$	dp	11	27	y	20
$[54; 3^5 \cdot 2]$	wp, $[2, 2, 2, 2, 2, 1]$	11	27	y	22
$[54; 3^5 \cdot 2]$	wp, $[1, 1, 1, 1, 1, 3]$	11	30	y	35
$[64; 4^4 \cdot 2^6]$	dp	14	41	n	50
$[64; 4^4 \cdot 2^6]$	wp,$[1, 1, 2, 2, 2, 2, 2, 3, 3, 3]$	16	42	n	13471
$[64; 4^4 \cdot 2^6]$	wp,$[1, 1, 1, 1, 2, 2, 2, 2, 2, 2]$	18	41	y	103072
$[72; 3^2 \cdot 2^8]$	dp	12	33	y	15
$[72; 3^2 \cdot 2^8]$	wp,$[1, 1, 2, 2, 2, 2, 2, 2, 2, 2]$	12	38	y	157
$[72; 3^2 \cdot 2^8]$	wp,$[2, 2, 1, 1, 1, 1, 1, 1, 1, 1]$	11	30	n	7
$[80; 5 \cdot 4 \cdot 2^6]$	dp	10	32	n	115
$[80; 5 \cdot 4 \cdot 2^6]$	wp,$[1, 2, 3, 3, 3, 3, 3, 3]$	13	49	y	6110
$[81; 9 \cdot 3^4]$	dp	11	36	n	609
$[81; 9 \cdot 3^4]$	wp,$[1, 2, 2, 2, 2]$	14	43	n	66617
$[88; 11 \cdot 2^6]$	dp	10	31	n	15
$[88; 11 \cdot 2^6]$	wp,$[1, 3, 3, 3, 3, 3, 3]$	14	41	n	705
$[96; 8 \cdot 3 \cdot 2^4]$	dp	9	31	n	6
$[96; 8 \cdot 3 \cdot 2^4]$	wp,$[1, 2, 3, 3, 3, 3]$	13	44	y	2192
$[96; 6 \cdot 4^2 \cdot 2^6]$	dp	12	39	n	1978
$[96; 6 \cdot 4^2 \cdot 2^6]$	wp,$[1, 2, 2, 3, 3, 3, 3, 3, 3]$	17	60	y	20172
$[96; 4^2 \cdot 3 \cdot 2^7]$	dp	13	47	n	4740
$[96; 4^2 \cdot 3 \cdot 2^7]$	wp,$[1, 1, 2, 3, 3, 3, 3, 3, 3, 3]$	15	62	y	18900

A few things to notice from this experiment are: 1) if we use *dp*, we often do not obtain all components of the main effect of the largest-level factor; 2) choosing the ordering *wp* with small weights for factors having a large number of levels gives the highest number of main effects and two-interactions; 3) to get all 2-interactions of a specific factor with the other factors, we should use *wp* and assign weight 1 to this factor, and assign larger weights to the others.

For example, with input $\mathrm{OA}(16; 4 \cdot 2^3; 3)$, using *dp* we get estimable terms

$$1, x_4, x_3, x_2, x_1, x_1^2, x_3x_4, x_2x_4, x_1x_4, x_2x_3, x_1x_3, x_1x_2, x_1^2x_4;$$

and using *wp* with the weight vector $[1, 4, 4, 4]$, we obtain the following terms:

$$1, x_1, x_1^2, x_1^3, x_4, x_3, x_2, x_1x_4, x_1x_3, x_1x_2, x_1^2x_4, x_1^2x_3, x_1^2x_2, x_1^3x_4, x_1^3x_3, x_1^3x_2.$$

Finding a balanced design given estimable terms. In this section, we compute and compare the constructions of five relatively small fractional designs, when given an order ideal $\mathrm{Est}(F_i)$ and a term ordering. This requires Algorithm 2.4 and Corollary 17. The largest run size of a strength 3 OA that we have been able to construct is 16. Each order ideal consists of all main effects and some 2-interactions. We use *dp* for the first two (pure) fractional designs, and *wp* for the remaining designs. This is because the last two designs are mixed, and we want to estimate all two-interactions involving a unique factor in each design. By assigning the smallest weight to this unique factor (having the largest number of levels) we push terms involving this factor to the start of the set of estimable terms $\mathrm{Est}(F)$, and the other 2-interactions (not involving this factor) are pushed out of $\mathrm{Est}(F)$. We construct:

A strength 2 design. Using *dp*, input $\mathrm{Est}(F_1) = [1, x_3, x_2, x_1]$.

A strength 3 pure (symmetric) design. Using *dp*, and with input

$$\mathrm{Est}(F_2) = [1, x_4, x_3, x_2, x_1, x_3x_4, x_2x_4, x_1x_4].$$

A strength 2 mixed design. Using *wp*, with the weight vector $[1, 2, 2, 2, 2]$, and with

$$\mathrm{Est}(F_3) = [1, x_1, x_5, x_4, x_3, x_2, x_1^2, x_1^3].$$

A strength 3 mixed design. Using *wp*, with the weight vector $[1, 2, 2, 2]$, and input

$$\begin{aligned}\mathrm{Est}(F_4) = [&1, x_1, x_4, x_3, x_2, x_1^2, x_1x_4, x_1x_3, x_1x_2, x_1^3,\\ &x_3x_4, x_2x_4, x_2x_3, x_1^2x_4, x_1^2x_3, x_1^2x_2].\end{aligned}$$

Since x_1 is the unique non-binary factor in the last two designs, we want to know all its interactions with the binary ones, together with all main effects, and with as many other two-interactions as possible.

In Table 2.2, the first column specifies the parameters of a design, given in the pattern [run size; design type; strength]; the second column indicates which term order we use in the Gröbner basis computation. The 3rd column shows the number of new variables in the list $A = \{a_{jl}\}$, found from Step (3); and the next column gives the pair of number of terms in the border basis E^+ and in E_2^+, found from Step (1) of Algorithm 1, Section 2.4. The 5th column shows the total number of polynomials (in terms of variables a_{jl}) of the system, *Gb* say. The number of non-factorizable polynomials #Red(Gb), say, obtained by reducing *Gb* recursively is in the 6th column, and in the final column we show the number of solutions, ie, $|\,\mathrm{Z}(Gb)|$.

Table 2.2: Computing fractional designs given a set of estimable terms

Design type	Ordering	$\#A$	$[\#E^+, \#E_2^+]$	$\#Gb$	#Red(Gb)	$\#\,\mathrm{Z}(Gb)$
$[4; 2^3; 2]$	dp	12	[6, 3]	45	0	1
$[8; 2^4; 3]$	dp	96	[16,12]	338	0	1
$[8; 4 \cdot 2^4; 2]$	wp, $[1, 2, 2, 2, 2]$	144	[23,18]	593	502	1
$[16; 4 \cdot 2^3; 3]$	wp, $[1, 2, 2, 2]$	352	[26,22]	1140	824	1
$[24; 3 \cdot 2^4; 3]$	wp, $[1, 2, 2, 2, 2]$	1104	[51,46]	NA	NA	NA

The computation was carried out on a 2.8 GHz PC with 2 GB memory. For each case, we list a solution. If the defining ideal is not too large, we list the ideal also. If the PC runs out of memory, we write NA.

$$F_1 = \mathrm{OA}(4; 2^3; 2) = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

$$F_2 = \mathrm{OA}(8; 2^4; 3) = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}^T$$

with the defining ideal $\mathrm{I}(F_2)$

$$\begin{aligned} & x_4^2 - x_4, x_3^2 - x_3, x_2^2 - x_2, x_1^2 - x_1, \\ & 2x_2x_3 - 2x_1x_4 + x_1 - x_2 - x_3 + x_4, \\ & 2x_1x_3 - 2x_2x_4 - x_1 + x_2 - x_3 + x_4, \\ & 2x_1x_2 - 2x_3x_4 - x_1 - x_2 + x_3 + x_4. \end{aligned}$$

$$F_3 = \mathrm{OA}(8; 4 \cdot 2^4; 2) = \begin{bmatrix} 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}^T$$

$$F_4 = \mathrm{OA}(16; 4{\cdot}2^3; 3) = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \end{bmatrix}^T$$

As can be seen from Table 2.2, the number of reduced polynomials increases strongly with run sizes. For this reason, a trial with a 24 run design ran out of memory. We conclude the method is computationally too intensive to construct larger designs.

2.7. Conclusion

In summary, we see that the methods of Gröbner basis and multiplication matrices are good for making small fractional designs and balanced fractional designs. The computation is not very efficient when the input size increases, and it soon becomes infeasible. The largest example that can be constructed with this tool is $\mathrm{OA}(16; 4 \cdot 2^3; 3)$. So, for $N \geq 24$, we need to find more efficient ways to construct fractional designs and t-balanced fractional designs. That will be the theme of the next two chapters.

CHAPTER 3

Constructing strength 3 orthogonal arrays

3.1. Introduction

This chapter presents methods for making strength 3 orthogonal arrays (OAs). We recall a basic fact concerning the minimal run size of a given type of OA in Section 3.2. The basic constructions are discussed in Section 3.3. In Section 3.4, we use the *Fano plane* to make a particular type of OA. In Section 3.5, we present an arithmetic approach in which we realize a new column as a linear functional of the known columns. An interpretation of strength 3 OAs as Latin squares will be employed in Section 3.6. Finding disjoint sub-arrays by computing orbits will be discussed in Section 3.7. Notice that these constructions only give some extensions, they do not find all extensions of a given array. The methods for finding all non-isomorphic extensions will be discussed in Chapter 4.

3.2. Background

Recall that a mixed orthogonal array with m distinct levels is denoted by $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; t)$ where the r_i can be identical for distinct indices; or by $\mathrm{OA}(N; s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}; t)$ when the s_i are distinct, cf. Appendix B. We need the following well-known result, called the *generalized Rao bound* for mixed orthogonal arrays (see Rao [1947], also Hedayat et al. [1999, Theorem 9.4]).

THEOREM 18. *Let $d \geq t \geq 1$ and assume an $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; t)$ exists.*

- *If t is even, then*

$$N \geq \sum_{j=0}^{t/2} \sum_{\substack{|K|=j \\ K \subseteq \{1,\ldots,d\}}} \prod_{i \in K} (r_i - 1).$$

- *If t is odd, then a lower bound for N is found by applying the above bound to the derived design $\mathrm{OA}(N/r_1; r_2 \cdot r_2 \cdots r_d; t-1)$, where r_1 is the largest among the r_j. That is*

$$N \geq r_1 \sum_{j=0}^{(t-1)/2} \sum_{\substack{|K|=j \\ K \subseteq \{2,\ldots,d\}}} \prod_{i \in K} (r_i - 1).$$

In particular, when $t = 2$, the run size N is bounded below by

$$N \geq 1 + \sum_{i=1}^{d} (r_i - 1).$$

Another bound is given by *Delsarte*. The values of the *Delsarte bound* are determined for mixed $\mathrm{OA}(N; 3^b \cdot 2^a; t)$ [Hedayat et al., 1999, Table 9.7, page 203].

From now on we take as our level sets $Q_i := \mathbb{Z}_{r_i}$, for $i = 1, 2, \ldots d$ and for $\mathbb{Z}_{r_i} = \{0, 1, 2, \ldots, r_i - 1\}$, the ring of integers modulo r_i.

3.3. Basic constructions

Trivial designs. A trivial design is a multiple of a full factorial design, (cf. Appendix B). It has strength 3 provided $d \geq 3$. If $\prod_{i=1}^{d} r_i$ divides N, a trivial design exists.

Split. Given an $\mathrm{OA}(N; uv \cdot r_1 \cdot r_2 \cdots r_d; t)$, an $\mathrm{OA}(N; u \cdot v \cdot r_1 \cdot r_2 \cdots r_d; t)$ can be made by replacing the symbols in $\mathbb{Z}_{uv}$ by those of $\mathbb{Z}_u \times \mathbb{Z}_v$. In particular, a 4-level column can be split into two 2-level columns, and a 6-level column can be split into a 2-level and a 3-level column.

Concatenation. Consider orthogonal arrays F_1 and F_2 with the same design type (cf. Appendix B). The concatenated array $\left[\frac{F_1}{F_2}\right]$ (found by putting them on top of each other, without changing symbols in any columns) is an OA with the same type. If F_1 and F_2 both have strength t, then the concatenated array also has strength t. That is, given an $\mathrm{OA}(N'; r_1 \cdot r_2 \cdots r_d; t)$ and an $\mathrm{OA}(N''; r_1 \cdot r_2 \cdots r_d; t)$, we can construct an $\mathrm{OA}(N' + N''; r_1 \cdot r_2 \cdots r_d; t)$.

Hadamard construction. A *Hadamard matrix* H_n of order n is a $n \times n$ matrix with entries in $\{-1, 1\}$ whose rows are *mutually orthogonal* with respect to the standard inner product in $\mathbb{R}^n$. More formally, let $V := \{-1, 1\}^n$, then

$$H_n := [v_1, v_2, \ldots, v_n] \in V^n \text{ such that } v_i \cdot v_j = 0 \text{ if } i \neq j; \text{ and } v_i \cdot v_j = n \text{ if } i = j.$$

It is well known that if a Hadamard matrix H_n exists then $n = 1, 2$, or n is divisible by 4. Conversely, there is the famous Hadamard conjecture, saying that there exists an H_n for every n divisible by 4. This conjecture has not been proved or disproved yet. The case H_{428} was found recently [Kharaghani and Tayfeh-Rezaie, 2004] leaving the smallest unknown order as 668.

Construction of Hadamard matrices of order n, where $n \leq 664$. Sloane [2005] supplies a list of Hadamard matrices with order at most 256 and the one with order 428. We have provided an online service to compute a Hadamard matrix H_n, for each positive multiple n of 4 which is at most 428. We employ 16 methods, reviewed in Table 3.1 below. Except for cases where the tensor method or the Paley methods, return the answer, we list in the fourth column orders where the method works. The third gives the constraints, and the second column of the table either shows employed tools or lists the requirements of the derived parameter q. Above 428, we implemented a construction of H_{596} using Spence's method (cf. Spence [1977b,a, 1975a]), a construction of H_{604} using Yamada's method [Yamada, 1989], and a construction of H_{612} using Turyn's method [Turyn, 1972].

The remaining cases up to 668 are $n = 452, 476, 508, 532, 652$; and we have not implemented yet the next three cases. A construction of H_{452} can be found in [Goethals and Seidel, 1967]; a H_{508} was constructed using Williamson array based supplementary different sets, for more details see Seberry [1999] and Đoković [1993a]; and a H_{652} was constructed in Đoković [1992a]. The list is now shrunk down to $n = 476, 532$.

Table 3.1: Methods for computing Hadamard matrices

Construction	Description	Constraint	Orders
Baumert-Hall	Baumert Hall units		156 [Baumert and Hall, 1965a]
Đoković	Williamson-type mat.	$n = 4q$	$28, 52, 92, 116, 124,$
			$172, 204, 244, 252$
Ehlich	need a skew H_{m+1}	$n = (m-1)^2$	324
	$m-2$ is a prime power		
Golay	T-sequences, T-matrices	$n = 4q$	260 [Kounias et al., 1991]
	require $q - 1 = 2^k$		
Kharaghani	T-sequences		428
Miyamoto	C-matrices	$n = 4q$	452, 508, 604
	q is a prime power		
	need a H_{q-1}		
Paley 1	require a skew $H_{(q+3)/2)}$,	$n = q + 1$	
	q is a prime power		
	and $q \bmod 4 = 3$		
Paley 2	symmetric conference mat.	$n = 2q + 2$	
	q is a prime power		
	and $q \bmod = 1$		
Sawade	Goethals-Seidel array	$n = 4v$	268 [Sawade, 1985]
Spence 1	use relative difference sets	$n = 4q$	$356, 404, 436, 596, 772, 964$
	q is an old prime power		[Elliott and Butson, 1966]
Spence 2	planar difference sets	$n = 4v$	292 [Spence, 1975b]
	q and v are prime powers	$v = q^2 + q + 1$	
tensor	$A \otimes B$ is a Hadamard	$(n \bmod 8) = 0$	
	if A, B are Hadamard mat.	or $n = 4$	
Turyn1	T-sequences	$n = 4q$	236 [Turyn, 1974]
	and Baumert Hall units		
Turyn2	q is a prime power, $q \bmod = 1$	$n = 6(q+1)$	$372, 612, 732, 756$
Turyn-Hedayat	Turyn-Hedayat array	$n = 4q$	188
Yamada	q is a prime power	$n = 4(q+2)$	412 Yamada [1986]
	$q \bmod 8 = 5$,		
	need a skew $H_{(q+3)/2}$		

Use of Hadamard matrices to construct strength 3 orthogonal arrays A Hadamard matrix of order n can be transformed to an $\mathrm{OA}(n; 2^{n-1}; 2)$. This is called a *Placket-Burmann-type design*. Furthermore, we have

LEMMA 19. [Hedayat et al., 1999, Theorem 7.5] *If H is a Hadamard matrix of order n written with $1, -1$-entries, then $\begin{bmatrix} H \\ -H \end{bmatrix}$ is an orthogonal array $\mathrm{OA}(2n; 2^n; 3)$; where $-H$ is the OA of strength 2 obtained by reversing signs. Conversely, every $\mathrm{OA}(2n; 2^n; 3)$ is (equivalent to one) found this way.*

Multiplication Given an array $f := \mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; t)$, we can construct an $\mathrm{OA}(sN; sr_1 \cdot r_2 \cdots r_d; t)$ for any positive integer s by concatenating s copies of f, changing the symbols in the first column so that they are distinct, and keeping identical the other columns.

Note that multiplying essentially is concatenating, but we use only one component array to build up a larger array and we change symbols in one column. For instance, arrays $\mathrm{OA}(sN; s \cdot 2^a; 3)$ can be obtained, from s copies of an $\mathrm{OA}(N; 2^a; 3) = \mathrm{OA}(N; 1 \cdot 2^a; 3)$, where $a \leq N/2$. An $\mathrm{OA}(24; 3 \cdot 2^4; 3)$ is found in this way; arrays $\mathrm{OA}(8s; 2s \cdot 2^3; 3)$ are found from $\mathrm{OA}(8; 2^4; 3) = \mathrm{OA}(8; 2 \cdot 2^3; 3)$: we obtain $\mathrm{OA}(16; 4 \cdot 2^3; 3)$ from two $\mathrm{OA}(8; 2 \cdot 2^3; 3)$; and we get $\mathrm{OA}(24; 6 \cdot 2^3; 3)$ from three $\mathrm{OA}(8; 2 \cdot 2^3; 3)$.

Juxtaposition. Juxtaposing is a combination of concatenating and multiplying. Let F_1, F_2 be orthogonal arrays with the strength t, and with the same number of columns. If the F_i have identical symbol sets on every column but the first, their juxtaposition array is built by putting them on top of each another, with disjoint symbol sets in the first column and identical symbol sets in the remaining columns. Formally, given an $\mathrm{OA}(N'; s' \cdot r_2 \cdots r_d; t)$ and an $\mathrm{OA}(N''; s'' \cdot r_2 \cdots r_d; t)$ we can construct an $\mathrm{OA}(N' + N''; s' + s'' \cdot r_2 \cdots r_d; t)$ by juxtaposing. In this way one obtains, for instance, an $\mathrm{OA}(56; 7 \cdot 2^a; 3)$ from an $\mathrm{OA}(40; 5 \cdot 2^a; 3)$ and an $\mathrm{OA}(16; 2^{a+1}; 3)$ for $a \leq 6$.

This construction can be generalized naturally for a finite set of orthogonal arrays.

Quasi-multiplication. Quasi-multiplying is a mixture of the multiplying and juxtaposing. We construct $\mathrm{OA}(N; s_1^2 \cdot 2^a; 3)$ where $N = s_1^2 2^3$ and 2 divides s_1. Let $n := N/s_1$ and suppose that an array $f = \mathrm{OA}(n, s_1 \cdot 2^a, 2)$ exists. We make $(s_1 - 1)$ arrays $\mathrm{OA}(n, s_1 \cdot 2^a, 2)$ by cyclically taking modulo s_1 for the s_1-column, and modulo 2 for the 2-columns, ie,:

$$f_i = [(A + i) \mod s_1 \,|\, \ (B + i) \mod 2\,], \qquad \text{for } 1 \leq i \leq s_1 - 1,$$

where A is the s_1-column and B is the second part consisting the binary columns. Then the array

$$F := \left[\begin{array}{c|c} \mathbf{0} & f \\ \mathbf{1} & f_1 \\ \cdots & \\ \boldsymbol{j} & f_j \\ \cdots & \\ \boldsymbol{s_1 - 2} & f_{s_1-2} \\ \boldsymbol{s_1 - 1} & f_{s_1-1} \end{array}\right]$$

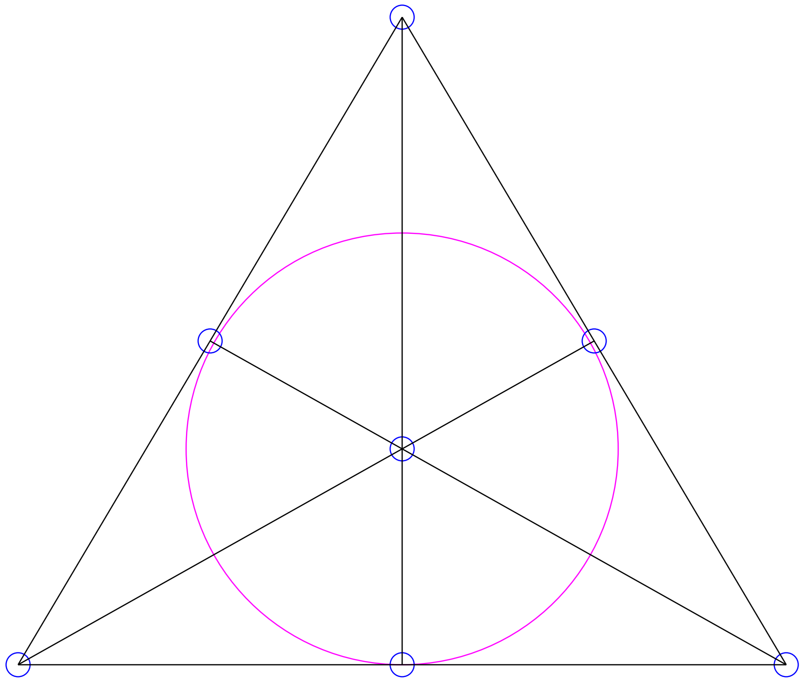

FIGURE 3.1. Fano plane

is an $\mathrm{OA}(N; s_1^2 \cdot 2^a; 3)$, where $\boldsymbol{j}$ is a length n constant vector with entries $j \in \{0, 1, \ldots, s_1 - 1\}$. For example, $\mathrm{OA}(64; 4^2 \cdot 2^{12}; 3)$ exists since $\mathrm{OA}(16; 4 \cdot 2^{12}; 2)$ exists (the latter is found using the method of contractive replacement [Hedayat et al., 1999, Section 9.3]). We find $\mathrm{OA}(96; 4^2 \cdot 2^{20}; 3)$ using $\mathrm{OA}(24; 4 \cdot 2^{20}; 2)$ that exists thank to the method of different schemes[Wu et al., 1992]; and $\mathrm{OA}(144; 6^2 \cdot 2^{13}; 3)$ exists since $\mathrm{OA}(24; 6 \cdot 2^{13}; 2)$ exists. For more details see Section 6.3.

Linear codes. A $[n, k, d]_q$ code is a *linear code* of word length n, dimension k, and minimum distance d. The code words of the dual code (that has dimension $n - k$) form an $\mathrm{OA}(N; q^n; d - 1)$ with $N = q^{n-k}$ [Hedayat et al., 1999, Theorem 4.6]. In particular, the $[6, 3, 4]_4$ hexacode gives an $\mathrm{OA}(64; 4^6; 3)$.

3.4. X construction

This construction is originally from Brouwer et al. [2005]. Recall that a finite projective plane of order n, denoted $PG(n, 2)$, is defined as a set of $n^2 + n + 1$ points with the properties that: i) Any two points determine a line, ii) any two lines determine a point, iii) every point has lines on it, and iv) every line contains points. The Fano plane, Figure 3.1, is the order 2 finite projective plane $PG(2, 2)$.

Applying the Rao bound to the derived designs of an array $\mathrm{OA}(N; s \cdot 2^a; 3)$ with run size $N = 8s$, we find $a \leq 7$. For even s, we have already found these with Construction (M), but for odd s there is no system with $a = 7$. Indeed, all s derived designs are essentially Fano planes, and have 7 triples of columns where half of the combinations of triples occur twice and half of the combinations occur not at all.

We need a matching, where each time 000 occurs twice in one Fano plane, it occurs not at all in some other Fano plane. But $7s$ is odd, and no such matching exists.

On the other hand, such designs exist with $a = 6$ when s is at least 5. Indeed, juxtaposing an array $\mathrm{OA}(8s; s \cdot 2^6; 3)$ and an $\mathrm{OA}(16; 2^7; 3)$ we get one with the run size $N = 8(s + 2)$, the design type $(s + 2) \cdot 2^6$, so it suffices to do the case $s = 5, N = 40$. We need five designs on 8 rows and six columns. Make them by fixing the first column and cyclically permuting the remaining five, starting from the binary matrix:

$$M = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \end{bmatrix}$$

and let M_i $(0 \leq i \leq 4)$ be the matrix obtained from M by fixing the first column and cyclically permuting the remaining five i times. Let N_i be the matrix obtained from M_i by adding a constant column of all i's. An $\mathrm{OA}(40; 5 \cdot 2^6; 3)$ is made by concatenating the N_i.

3.5. Arithmetic construction

Introduction. The method described in this section constructs extensions of a full factorial design. Suppose that $d \geq 3$, $r_1 \geq r_2 \geq \ldots \geq r_d$, and s are natural numbers at least 2, and at least one r_i is a multiple of s. Write $D := \prod_{i=1}^{d} Q_i$ for the full design and let S_i be the ith column of D. Let $[D|X_1|X_2|\ldots|X_l] = \mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d \cdot s^l; 3)$ be a putative orthogonal array that is extended from D by l factors $X_1, X_2, \ldots, X_l$ and that has the run size $N = r_1 r_2 \ldots r_d$. The notation $(a, b) \in [S_i, S_j]$ means $(a, b) \in Q_i \times Q_j$, and $[S_i, S_j, S_k]$ stands for the sub-array $\mathrm{OA}(N; r_i \cdot r_j \cdot r_k; 3)$.

First we consider $l = 1$ and let $X := X_1$. Denote by $\boldsymbol{u} := (u_1, u_2, \ldots, u_d)$ an arbitrary run of the design D. Since the columns $S_1, S_2, \cdots, S_d$ form the full design D of N runs, X is determined uniquely by a function

$$f_X : D \to \mathbb{Z}_s, \quad \boldsymbol{u} \mapsto f_X(\boldsymbol{u}).$$

We call f_X the *defining function* of the column X. The problem of finding the maximum number l of columns X_i such that an array $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d \cdot s^l; 3)$ exists is reduced to: determine all distinct functions f_{X_i} such that X_i is orthogonal to any pair of columns of D, ie, the extended array $[D|X_i]$ exists; and then find conditions such that column X_i is orthogonal to the array $[D|X_1|\ldots|X_{i-1}]$, for $i = 2, \ldots, l$, $l > 1$. The following method is generalized from the Construction (X6) in Brouwer et al. [2005].

The construction. For a column X, let $f = f_X$ be the defining function. We characterize f such that $[D|X]$ is a strength 3 orthogonal array with $d+1$ columns.

Conditions on f. Put $K := \{1, 2, \ldots, d\}$. For $i, j \in K$, let

$$Q_{i,j} := \prod_{l \in K \setminus \{i,j\}} Q_l, \quad n_{ij} := \frac{N}{r_i r_j}, \quad q_{ij} := \frac{n_{ij}}{s}; \tag{3.5.1}$$

and, for each $(a, b) \in [S_i, S_j]$, let

$$Q_{ij}(a, b) := \{\boldsymbol{u} = (u_1, u_2, \ldots, u_d) \in D : u_i = a \text{ and } u_j = b\}$$

Define f_{ij}^{ab} to be the restriction of f to $Q_{ij}(a, b)$, considered as a function of the $d - 2$ variables

$$\boldsymbol{y}_{ij} := (u_1, \ldots, u_{i-1}, u_{i+1}, \ldots, u_{j-1}, u_{j+1}, \ldots u_d).$$

LEMMA 20. *If f_{ij}^{ab} is a q_{ij}-to-one mapping for all $i, j \in K$, $a \in \mathbb{Z}_{r_i}$, $b \in \mathbb{Z}_{r_j}$, then $[D|X]$ is a strength 3 orthogonal array.*

PROOF. If the three columns chosen from $[D|X]$ are all S_i, then they are obviously orthogonal. Otherwise, a triple $(a, b, c) \in [S_i, S_j, X]$ occurs with frequency

$$|\,(f_{ij}^{ab})^{-1}(c)| \;=\; q_{ij}.$$

Since this number is independent of a, b, c the conclusion follows. □

A specific f. Knowing the requirement for the existence of f, we now construct a specific function f. Put $n := \operatorname{lcm}(r_1, r_2, \ldots, r_d)$. Since s is a divisor of r_i for some $i \in K$, s is a divisor of n. Define a uniform partition $A_0, A_1, \ldots, A_{s-1}$ of $\mathbb{Z}_n$ by

$$A_p := \left\{ z \in \mathbb{Z}_n : \left\lfloor \frac{zs}{n} \right\rfloor = p \right\},$$

for $p = 0, \ldots, s - 1$. That is

$$\begin{aligned} A_0 &:= \left\{0, 1, \ldots, \frac{n}{s} - 1\right\}, \\ A_1 &:= \left\{\frac{n}{s}, \frac{n}{s} + 1, \ldots, 2\frac{n}{s} - 1\right\}, \\ &\cdots \\ A_{s-1} &:= \left\{n - \frac{n}{s}, \ldots, n - 1\right\}. \end{aligned} \tag{3.5.2}$$

In the special case of $s = 2$, write $A = A_0$, $B = A_1 = \mathbb{Z}_n \setminus A$. We define the *partition function* by

$$g : \mathbb{Z}_n \to \mathbb{Z}_s, \qquad g(z) := p \quad \text{when} \quad z \in A_p. \tag{3.5.3}$$

We remark that D can be identified with $\mathbb{Z}_N$. For $h : D \to \mathbb{Z}_n$, define

$$\begin{aligned} h_{ij}^{ab} &: Q_{ij}(a, b) \to \mathbb{Z}_n, \\ h_{ij}^{ab}(\boldsymbol{y}_{ij}) &:= h(u_1, \ldots, u_{i-1}, a, u_{i+1}, \ldots, u_{j-1}, b, u_{j+1}, \ldots u_d), \end{aligned} \tag{3.5.4}$$

for $i, j \in K$ and $(a, b) \in [S_i, S_j]$. Let h have the property that the number of $\boldsymbol{y}_{ij} \in Q_{ij}(a, b)$ with $h_{ij}^{ab}(\boldsymbol{y}_{ij}) \in A_p$ is the same for all p. This property is referred to as the *uniform scattering condition*.

The scattering coefficient of a pair of columns. The scattering coefficient of the level pair $(a, b) \in [S_i, S_j]$ and A_p is defined as

$$s_{ij}^{ab}(A_p) := |\{\boldsymbol{y} \in Q_{ij}(a, b) : h_{ij}^{ab}(\boldsymbol{y}) \in A_p\}|.$$

If the uniform scattering property is satisfied then $s_{ij}^{ab}(A_p)$ is independent of the choice of $(a, b) \in [S_i, S_j]$ and $p \in \{0, 1, \ldots s-1\}$. We write s_{ij} for that constant, and call it the *scattering coefficient of the columns* $[S_i, S_j]$ in $\mathbb{Z}_n$.

EXAMPLE 3.1. Consider an array $\mathrm{OA}(96; 3 \cdot 4 \cdot 4 \cdot 2 \cdot 2^l; 3)$, ie, $d = 4$, $s_1 = 3$, $s_2 = s_3 = 4$, $s_4 = 2$ and $s = 2$. Then $N = 96$, $D = \mathbb{Z}_3 \times \mathbb{Z}_4 \times \mathbb{Z}_4 \times \mathbb{Z}_2$, $n := \mathrm{lcm}(s_1, s_2, s_3, s_4) = 12$, $A = \{0, 1, 2, 3, 4, 5\}$, $B = \{6, 7, 8, 9, 10, 11\}$. Let $i = 1, j = 4$, then $Q_{14} = \mathbb{Z}_4 \times \mathbb{Z}_4 = \{(0,0), (0,1), \ldots, (3,3)\}$, $n_{14} = 96/(3 \cdot 2) = 16$, $q_{14} = 16/2 = 8$. If we define $h(\boldsymbol{u}) = 3u_1 + 3u_2 + 2u_3 + 6u_4 \pmod{12}$, then $h_{14}^{00} = 3u_2 + 2u_3 \pmod{12}$, and the values of h_{14}^{00} with multiplicities are

$$h_{14}^{00} = \{0^2, 1, 2, 3^2, 4, 5, 6^2, 7, 8, 9^2, 10, 11\}.$$

Hence $s_{14}^{00}(A) = 8 = s_{14}^{00}(B)$, ie, the scattering coefficient of the pair $(0, 0) \in [S_1, S_4]$ is 8. It can be checked that the scattering coefficient s_{14} of the columns $[S_1, S_4]$ in $\mathbb{Z}_{12}$ is 8 as well.

The defining function $f : D \to \mathbb{Z}_s$ of a column X can then be realized as a composition $f = g \circ h$, as follows:

LEMMA 21. *If $h : D \to \mathbb{Z}_n$ satisfies the scattering condition, $g : \mathbb{Z}_n \to \mathbb{Z}_s$ is the partition function, and $f = g \circ h$, then $[D|X]$ is a strength 3 orthogonal array.*

PROOF. Since $|h_{ij}^{ab}(Q_{i,j})| = n_{ij}$ by (3.5.1); then $s_{ij}^{ab}(A_p) = q_{ij}$ elements for $p = 0, \ldots, s-1$. That means the scattering coefficient s_{ij} of the columns $[S_i, S_j]$ in $\mathbb{Z}_n$ is q_{ij}. Because $f := g \circ h$, from (3.5.3), f_{ij}^{ab} is a q_{ij}-to-one mapping. Now we see that the hypothesis of Lemma 20 is satisfied. □

Hence, if one can find a function h satisfying the uniform scattering condition, then an s-level X can be defined such that the orthogonal array $[D|X]$ exists.

A particular class of functions h. Note that if $d = 3$ and $n_{ij} = s$, then $q_{ij} = 1$. That is $h_{i,j}$ is a one-to-one mapping from Q_l to $\mathbb{Z}_n$, for $l \in K \setminus \{i, j\}$. This means that S_l corresponds one-to-one with the column X. Prompted by this special case, and referring to decomposition (3.5.2) for $d \geq 3$, a natural candidate of function $h : D \to \mathbb{Z}_n$ is a linear functional in d variables

$$h(\boldsymbol{u}) = c_1 u_1 + c_2 u_2 + \ldots + c_d u_d \pmod{n}, \quad \text{where } c_i \in \mathbb{Z}_n^\times \text{ for } i = 1, \ldots d. \tag{3.5.5}$$

In this case, finding h is reduced to finding a vector $\boldsymbol{c} = (c_1, c_2, \ldots, c_d) \in \mathbb{Z}_n^k$.

EXAMPLE 3.2. Consider an array $\mathrm{OA}(64; 4^4 \cdot 2^6; 3)$. Here $d = 3$, $s_1 = s_2 = s_3 = 4$, $s = 2$, $n = \mathrm{lcm}(4, 4, 4) = 4$, $D = \mathbb{Z}_4 \times \mathbb{Z}_4 \times \mathbb{Z}_4 \equiv \mathbb{Z}_{64}$, $A := \{0, 1\}$ and $B := \mathbb{Z}_4 \setminus A = \{2, 3\}$. Let $h : D \to \mathbb{Z}_n$ be defined by

$$h(\boldsymbol{u}) = u_1 + 2u_2 + 3u_3 \mod 4.$$

For $i = 1, j = 2$, $Q_{12} = \mathbb{Z}_4$, $n_{12} = \frac{64}{16} = 4$, $q_{12} = \frac{4}{2} = 2$. Then

$$h_{12}^{00}(\mathbb{Z}_4) = \{0, 3, 2, 1\} = A \cup B;$$
$$h_{12}^{32}(\mathbb{Z}_4) = \{3, 2, 1, 0\} = A \cup B.$$

The same decomposition of $h_{12}^{ab}(\mathbb{Z}_4)$ can be found for the other level pairs (a, b) in S_1, S_2. The scattering coefficient of the columns S_1, S_2 in $\mathbb{Z}_{12}$ is $s_{12} = 1 + 1 = q_{12}$.

Also $Q_{13} = \mathbb{Z}_4$, $n_{13} = \frac{64}{16} = 4$, $q_{13} = \frac{4}{2} = 2$. For $(a, b) = (0, 0), (1, 3), (2, 1)$, we get

$$\begin{aligned} h_{13}^{00}(\mathbb{Z}_4) &= \{0, 2, 0, 2\} = [0^2, 1^0, 2^2, 3^0], \\ h_{13}^{13}(\mathbb{Z}_4) &= \{2, 0, 2, 0\} = [0^2, 1^0, 2^2, 3^0], \\ h_{13}^{21}(\mathbb{Z}_4) &= \{1, 3, 1, 3\} = [0^0, 1^2, 2^0, 3^2] \ldots \end{aligned}$$

The scattering coefficient of the columns S_1, S_3 in $\mathbb{Z}_{12}$ is $s_{13} = 0 + 2 = q_{13} \ldots$ In this example, the condition of Lemma 21 is fulfilled, therefore a binary column S exists, and it is orthogonal to $D = \mathrm{OA}(64; 4^3; 3)$.

See Section 6.3 for more applications of this method.

3.6. Latin squares method

We describe a geometric method to construct orthogonal arrays $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^a; 3)$ for $a \le 5$ and $\mathrm{OA}(80; 5 \cdot 4 \cdot 2^a; 3)$ for $a \le 6$ in this section. Recall that if f is an orthogonal array, $[f|S]$ stands for an orthogonal array made by appending a column S to f, and having the same strength as f. Recall from Section 3.3 that, $\left[\frac{F}{F_1}\right]$ denotes the concatenation of two orthogonal arrays F and F_1. The *Hamming distance* between two vectors of the same length is the number of unequal coordinates.

Construction of $D_a = \mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^a; 3)$ *for* $a \le 5$. We suppose

$$D_a = [Z|X|Y|S_1|\cdots|S_a]$$

where Z is the 6-factor, X and Y are the 4-factors, and S_i $(1 \le i \le a)$ are the binary factors. The notation (x, y, s_1) means coordinates of a run in columns XYS_1. We fix $f = \mathrm{OA}(16; 4^2; 2)$ to be the trivial design. If D_a exists, decomposing it at the column Z gives us 6 derived designs of the form $\mathrm{OA}(16; 4^2 \cdot 2^a; 2)$.

Appending a single column to f. The full design $f = \mathrm{OA}(16; 4^2; 2)$ is the set $\{0, 1, 2, 3\}^2$, ie, each row of f corresponds to an element $(i, j) \in (\mathbb{Z}_4)^2$. We identify f with the positions in a 4×4 matrix J. So the rows of J correspond to the levels of X and the columns of J correspond to the levels of Y. Now let S be a binary column to be appended to f to form a strength 2 array $\mathrm{OA}(16; 4^2 \cdot 2; 2)$. This is equivalent to assigning a symbol 0 to exactly 2 entries in each column and each row of J; and assigning a symbol 1 to the remaining entries. Such a matrix indeed represents a strength 2 array since, for each $(x, y) \in XY$, there are exactly two pairs $(x, 0)$ (resp. $(x, 1)$) in XS and exactly two pairs $(y, 0)$ (resp. $(y, 1)$) in YS. The $(0, 1)$-matrices of this form are also called *grids*. For example, consider the grid

$$g = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}. \tag{3.6.1}$$

The corresponding orthogonal array of 16 runs is found by concatenating rows to form a length-16 vector V, and appending it to f. In this example:

$$[X|Y|V] = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}^T.$$

$$a_1 = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}, \quad a_2 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \quad a_3 = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix},$$

$$a_4 = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix}, \quad a_5 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}, \quad a_6 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix},$$

$$a_7 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \quad a_8 = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \quad a_9 = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}.$$

FIGURE 3.2. Grids of class A

REMARK 3.1. We identify the grid g with the corresponding length-16 vector V and identify $[f|g]$ with the corresponding array $[f|V] = [X|Y|V] = \mathrm{OA}(16; 4^2 \cdot 2; 2)$.

For any grid g, its *complement grid*, denoted g^c, is defined by

$$(g^c)_{ij} := (g_{ij} + 1) \mod 2.$$

Similarly we define the complement of a vector in $\{0,1\}^4$.

An *isomorphism class of grids* is a minimal set of grids closed under permuting rows and permuting columns. By computing the orbit space of grids under the action of the full group of row and column permutations as in Section 4.2, we find that there are only 2 isomorphism classes of grids. These classes can be characterized by Hamming distances. Let class A consist of grids such that the Hamming distances between the columns are 0 or 4, and let class B consist of grids such that the Hamming distances between the columns are 2 or 4. The grid given by (3.6.1) is a representative of A and b_1 below is a representative of B. Every $g \in A$ has exactly one of the vectors

$$u := [0110]^T, v := [0101]^T, w := [0011]^T$$

as a column. Indeed, to make sure that the Hamming distances between the columns are 0 and 4, each grid in A must be built by a pair of complement columns like $[u|u^c|u|u^c]$. Each vector occurs in $\binom{4}{2} = 6$ grids, and when this vector is fixed there are 3 choices for the index of the column in which the vector is being repeated. So we get 18 grids for this class. In Figure 3.2 we list nine grids a_1 to a_9; now $A = \{a_1, \ldots, a_9, a_1^c, \ldots, a_9^c\}$.

The second class, B, consists of grids with the Hamming distances between columns of 2 or 4. Each grid in B has exactly two of the vectors u, v, w as columns; and there are 24 grids corresponding to each such pair. Therefore, B has $\binom{3}{2} \cdot 24 = 72$ distinct isomorphic grids. A representative with the pair $\{v, w\}$ is

$$b_1 = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix} \tag{3.6.2}$$

In summary, we find 90 grids with which we can make length-16 binary vectors in $\mathrm{OA}(16; 4^2 \cdot 2; 2)$.

Appending a pair of columns to f. Let $G := A \cup B$, and let $g, h \in G$. The *superimposed grid* of g, h, denoted $g * h$, is the 4×4-matrix with entries in $\{0, 1, 2, 3\}$ where $(g * h)_{ij}$ has binary expansion g_{ij}, h_{ij}. Note that this operation is not symmetric.

By Remark 3.1, for the first binary factor we can choose a grid $g_1 \in G$ to form an array $[X|Y|V_1] = \mathrm{OA}(16; 4^2 \cdot 2; 2)$. Any candidate for the second length-16 column V_2 must be orthogonal to V_1. That means when choosing another grid, g_2 say, and building the superimposed grid $g_1 * g_2$, each pair 00, 01, 10 and 11 has to appear exactly 4 times in the array $[X|Y|V_1|V_2] := \mathrm{OA}(16; 4^2 \cdot 2 \cdot 2; 2)$. Equivalently, each symbol 0, 1, 2, 3 must appear 4 times in $g_1 * g_2$. For example,

$$a_1 * a_2 = \begin{bmatrix} 1 & 3 & 2 & 0 \\ 3 & 1 & 0 & 2 \\ 2 & 0 & 1 & 3 \\ 0 & 2 & 3 & 1 \end{bmatrix}$$

satisfies this condition, so we get an array $[X|Y|V_1|V_2] = \mathrm{OA}(16; 4^2 \cdot 2 \cdot 2; 2)$:

$$[X|Y|V_1|V_2] = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \end{bmatrix}^T.$$

REMARK 3.2. We identify the superimposed grid $g_1 * g_2$ with the corresponding pair of length-16 vectors V_1, V_2; and identify $[f|g_1|g_2]$ with the corresponding array $[X|Y|V_1|V_2] = \mathrm{OA}(16; 4^2 \cdot 2 \cdot 2; 2)$.

The grids $g * h, g * h^c$, $g^c * h$ and $g^c * h^c$ are called the *derived grids* of g and h. We put

$$\mathrm{Der}(g, h) := \{g * h, g^c * h, g * h^c, g^c * h^c\}.$$

Latin squares are $n \times n$ matrices whose entries are the symbols $0, 1, \ldots, n-1$ such that each symbol occurs exactly once in every row and every column.

LEMMA 22. *$g * h$ is a Latin square if and only if the other derived grids are.*

PROOF. Consider any symbol i $(0 \le i \le 3)$ in the grid $g * h$. This symbol turns into the symbol $(i + 2) \bmod 4$ in $g^c * h$, and into the symbol $(3 - i) \bmod 4$ in $g^c * h^c$. In addition, $g * h^c$ is the complement of $g^c * h$, in the sense that $g * h^c \ni 0 = 00 \iff 11 = 3 \in g^c * h$, and $g * h^c \ni 1 = 01 \iff 10 = 2 \in g^c * h$. Hence, the number of symbol 0 (1, 2 and 3) in each row and each column of $g * h^c$, $g^c * h$ and $g^c * h^c$ is exactly 1 if and only if it is for $g * h$. The conclusion follows. □

Now we confine ourselves to using A only. Table 3.2 describes whether the superimposed grids in A are Latin squares or not. Note that for each fixed grid $g \in A$, there are exactly 4 grids $h \in A$ such that $g * h$ is a Latin square, and there are 4 grids $h \in A$ such that $g * h$ is not a Latin square. For instance, grids $h \in \{a_5, a_6, a_8, a_9\}$ do not form Latin squares when superimposing with a_1. Take $h = a_5$; then their derived grids are given in Figure 3.3.

Constructing $D_1 = \mathrm{OA}(96; 6 \cdot 4^2 \cdot 2; 3)$ by concatenating six $\mathrm{OA}(16; 4^2 \cdot 2; 2)$. If $D_1 = [Z|X|Y|S]$ then each $(x, y, 0)$ and each $(x, y, 1)$ must appear exactly 3 times for $0 \le x, y \le 3$.

Let $F_1 := [f|g]$ be an $\mathrm{OA}(16; 4^2 \cdot 2; 2)$ and denote $F_1^c := [f|g^c]$ for $g \in A$. Each triple $(x, y, 0)$ and $(x, y, 1)$ appears exactly once in the concatenation array $\left[\frac{F_1}{F_1^c}\right]$.

Grids	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9
a_1		yes	yes	yes			yes		
a_2	yes		yes			yes			yes
a_3	yes	yes			yes			yes	
a_4	yes					yes	yes	yes	
a_5			yes				yes	yes	yes
a_6		yes		yes				yes	yes
a_7	yes			yes	yes				yes
a_8			yes	yes	yes	yes			
a_9		yes			yes	yes	yes		

TABLE 3.2. The pairs whose superimposed grids form Latin squares

$$a_1 * a_5 = \begin{bmatrix} 1 & 2 & 2 & 1 \\ 3 & 0 & 0 & 3 \\ 2 & 1 & 1 & 2 \\ 0 & 3 & 3 & 0 \end{bmatrix}, \qquad a_1^c * a_5 = \begin{bmatrix} 3 & 0 & 0 & 3 \\ 1 & 2 & 2 & 1 \\ 0 & 3 & 3 & 0 \\ 2 & 1 & 1 & 2 \end{bmatrix},$$

$$a_1 * a_5^c = \begin{bmatrix} 0 & 3 & 3 & 0 \\ 2 & 1 & 1 & 2 \\ 3 & 0 & 0 & 3 \\ 1 & 2 & 2 & 1 \end{bmatrix}, \qquad a_1^c * a_5^c = \begin{bmatrix} 2 & 1 & 1 & 2 \\ 0 & 3 & 3 & 0 \\ 1 & 2 & 2 & 1 \\ 3 & 0 & 0 & 3 \end{bmatrix}.$$

FIGURE 3.3. Derived grids $\mathrm{Der}(a_1, a_5)$

REMARK 3.3. Evidently, if we use one of the three alternatives below:

(i) a pair (F_1, F_1^c) three times, ie, the column S in the array D_1 has the form $[g, g^c, g, g^c, g, g^c]$ (after reordering the grids); or
(ii) two distinct complement pairs (one is replicated twice), ie, S is of the form $[g, g^c, g, g^c, h, h^c]$; in which $h \neq g, g^c$;
(iii) three distinct complement pairs, ie, $[g, g^c, h, h^c, k, k^c]$ in which $h \neq g, g^c$ and $k \neq g, g^c, h, h^c$

to build the binary column of D_1, then D_1 is an array as required.

For example, the superimposed grid

$$a_2 * a_2^c = \begin{bmatrix} 2 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 \\ 1 & 2 & 1 & 2 \\ 1 & 1 & 2 & 2 \end{bmatrix}$$

indicates that each triple $(x, y, 0)$ and $(x, y, 1)$ occurs exactly once in 32 runs of $\begin{bmatrix} f|a_2 \\ f|a_2^c \end{bmatrix}$ for all $0 \leq x, y \leq 3$. A good column S could then be $[a_2, a_2^c, a_3, a_3^c, a_4, a_4^c]^T$.

From this point, let J be the all-one square matrix of order 4. We have the converse of the statement in Remark 3.3:

LEMMA 23. *Let $g_0, \ldots, g_5 \in A$. Then*

$$D_1 = \begin{bmatrix} \mathbf{0}^T & \mathbf{1}^T & \mathbf{2}^T & \mathbf{3}^T & \mathbf{4}^T & \mathbf{5}^T \\ f^T & f^T & f^T & f^T & f^T & f^T \\ g_0^T & g_1^T & g_2^T & g_3^T & g_4^T & g_5^T \end{bmatrix}^T$$

is an $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2; 3)$ *if and only if* $g_0, \ldots, g_5$ *form three complementary pairs, ie, they can be reordered so that* $g_3 = g_0^c$*,* $g_4 = g_1^c$ *and* $g_5 = g_2^c$*.*

PROOF. Write $D_1 = [Z|X|Y|S]$. Clearly the triples (Z, X, S), (Z, Y, S) and (Z, X, Y) are orthogonal. We prove that (X, Y, S) are orthogonal in three steps.

If six grids in S do not make any complementary pair, that is

$$S = [g_1, h_1, g_2, h_2, g_3, h_3]$$

such that there is no complement pair $u, u^c \in S$ for any $u \in \{g_i, h_i, g_i^c, h_i^c\} \subseteq A$; then D_1 can not have strength 3. In this case, no pair from the six grids results in a superimposed grid solely consisting of the symbols 1 and 2.

Now suppose that there is only one complementary superimposed grid (ie, two grids g, h have no complement pairs) in S, that is

$$S = [g, h, g_1, h_1, a, a^c]$$

where there is no complement pair $u, u^c \in S$ for any $u \in \{g, h, g_1, h_1\}$, and $a, g, g_1, h, h_1 \in A$. Since a, a^c contributes one triple $(x, y, 0)$ (and $(x, y, 1)$) for any pair $xy \in XY$, if the four grids $\{g, h, g_1, h_1\}$ contribute less than or more than two triplets $(x, y, 0)$, (or less than or more than two triplets $(x, y, 1)$) for some co-ordinates xy, then we have a contradiction. We consider three cases: two identical pairs, one identical pair and no identical pairs at all. Note that

- for every $g \in G$, $g * g$ only contains the symbols 0 and 3;
- since all grids in G are distinct, we have

$$g * g + h * h = 3J \iff h = g^c.$$

First of all, the superimposed grid $g * g$ consists only of symbols 0 and 3 for every $g \in G$, since g is a 0,1-grid. Secondly, when $h = g^c$, evidently we have

$$g * g + h * h = g * g + g^c * g^c = 3J,$$

since

$$g * g \ni 0 \equiv 00 \iff 11 \equiv 3 \in g^c * g^c,$$

and

$$g * g \ni 3 \equiv 11 \iff 00 \equiv 0 \in g^c * g^c.$$

To see the 'only if' part (the necessity condition), suppose that $g*g+h*h = 3J$ and $h \neq g^c$, then there exist $0 \leq x, y \leq 3$ such that $g[x, y] = h[x, y] = 0$ (in grids), and $(g * g)[x, y] = 0$ (in the superimposed grid). That means $(h * h)[x, y] = 0$, contradiction.

If there are two distinct identical pairs, g, g and h, h where $h \neq g, g^c \in G$, the sums $g * g + h * h$ always differ from the constant matrix $3J$, contradiction. Indeed, if there exist $0 \leq x, y \leq 3$ such that $(g*g)[x, y], (h*h)[x, y] = 0$ or 3 and $(g*g)[x, y] + (h * h)[x, y] \in \{0, 6\}$ then $|\{xy0\}| = 1 + 4 > 3$ or $|\{xy1\}| = 1 + 4 > 3$ in the whole fraction, contradiction. Similarly, if there is only one identical pair, then $g_1 \neq h_1$. The superimposed grid $g * g$ only consists of 0 and 3, meanwhile $g_1 * h_1$ has all symbols $0, 1, 2, 3$; they do not match with each other. (Indeed, if so, there exist $0 \leq, x, y \leq 3$ such that $(g * g)[x, y] = 0$ (or 3) and $(g_1 * h_1)[x, y] = 1$ (or 2), so the triple $(x, y, 0)$ (or $(x, y, 1)$) occurs 4 times in the whole fraction). After all, if all of the grids $\{g, h, g_1, h_1\}$ are distinct and if they do not make complementary pairs, the pairs $g * h$ and $g_1 * h_1$ consist of the symbols $0, 1, 2, 3$. We want that their sum equals $3J$. By computer search, there is no match between the four.

Lastly, suppose there are two complementary superimposed grids (ie, only one grid g has no complementary pair) in column S,

$$S = [g, h, a, a^c, b, b^c],$$

with $a, b, g, h \in A$ and $h \neq g^c$. Looking at the superimposed grids comprised by grids in S, we see that $(a, a^c), (b, b^c)$ contribute to D_1 two triplets $(x, y, 0)$ and $(x, y, 1)$ for any pair $xy \in XY$. If $h = g$ then the superimposed grid $g * g$ consists only of the symbols 0 and 3; if $h \neq g$ then the grid $g * h$ always has an entry 0 or 3 (symbol 0 stands for the pair 00, and symbol 3 stands for the pair 11). That means on the whole, $|\{xy0\}| \geq 4$ or $|\{xy1\}| \geq 4$, contradiction. $\square$

Constructing an $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2 \cdot 2; 3)$ *by concatenating six* $\mathrm{OA}(16; 4^2 \cdot 2 \cdot 2; 2)$. Let $D_2 = \mathrm{OA}(96; 6 \cdot 4^2 \cdot 2 \cdot 2; 3) = [Z|X|Y|S_1|S_2]$. Using the above lemma to form columns S_1, S_2, we obtain orthogonalities between S_1 and S_2 with XY independent, but we do not assure that column X (and Y) are orthogonal to the pair S_1S_2 in D_2. We now find (geometrical) requirements for the orthogonalities between columns X, S_1, S_2 and between Y, S_1, S_2.

Let $F_2 := \mathrm{OA}(16; 4^2 \cdot 2^2; 2) = [f|g_1|g_2]$ be the array with two appended columns which are determined by grids g_1, g_2. Now F_2 to be embedded in the 3-dimensional space ZXY must be composed of two grids $[f|g_1]$ and $[f|g_2]$ that satisfy Lemma 23. Then D_2 has strength 3 if and only if the sub-arrays (X, S_1, S_2) and (Y, S_1, S_2) have strength 3. In other words, for each $0 \leq i, j \leq 3$, the intersections of D_2 with planes $X = i$ and $Y = j$ must have exactly 6 points $00, 01, 10, 11$ (that means the number of symbols 0,1,2 and 3 in each column and each row from 6 superimposed grids is 6).

If we can choose grids forming columns S_1, S_2 such that the six superimposed grids are Latin squares, then we are done. For example, from Table 3.2, we might choose $S_1 = [a_1, a_1, a_1, a_1^c, a_1^c, a_1^c]$, and $S_2 = [a_2, a_2^c, a_3, a_3^c, a_4, a_4^c]$. How about the converse statement? What happens if some parts of S_1, S_2 do not intersect to give a Latin square? We now determined the patterns of the two S_1, S_2. To prove the next proposition, we need the lemma below.

Lemma 24. *The number of symbol i $(0 \leq i \leq 3)$ in each column and in each row of derived grids* $\mathrm{Der}(g * h)$ *is always* 4*, for any pair $g \neq h \in A$.*

This is obvious by an argument similar to Lemma 22.

Proposition 25. *Let $S_1 = [g_0, \dots, g_5]$ and $S_2 = [h_0, \dots, h_5]$ with $g_i, h_i \in A$. The triples (X, S_1, S_2) and (Y, S_1, S_2) are orthogonal if and only if one of the following conditions is satisfied:*

(1) all six superimposed grids $g_i * h_i$ $(i = 0, \dots 5)$ are Latin squares; or

(2) four superimposed grids are Latin squares, and two remaining superimposed grids are of the form

$$[a * b, a^c * b] \quad \text{or} \quad [a * b, a * b^c]$$

where $a, b \in A$; or

(3) only two superimposed grids are Latin squares, and the remaining four superimposed grids are

(i) $\mathrm{Der}(a, b)$ *for some $a, b \in A$;*

(ii) *$a * b, a * b^c, d * e, d * e^c$, for $a, b, d, e \in G$, $a \neq b, b^c$; and $d \neq e, e^c$; or*

(iii) *grids that sum to $6J$.*

PROOF. The 'if' part is clear for the first case. The second case follows from the fact that if a superimposed grid $a * b$ is not a Latin square then it has precisely two rows, say y_1, y_2, (or two columns, not both) in which the symbol 0 (or 1,2,3) occurs twice. Then $a^c * b^c$ has symbol 0 in those rows as well. As a result $|\{y_1 00\}| = |\{y_2 00\}| = 8$. If we use grid $a^c * b$ (or $a * b^c$), then the symbol 0 occurs twice in complement rows of $\{y_1, y_2\}$ in the grid $[f|a^c|b]$ (or $[f|a|b^c]$). That is, Y is orthogonal to the pair $S_1 S_2$. If so, in $a * b$, the symbol 0 still distributes uniformly over 4 columns. So column X is orthogonal to the pair of columns $S_1 S_2$.

Case ($3i$) is clear by Lemma 24. For instance

$$S_1 = [a_3, a_3^c, a_3, a_3^c, a_9, a_9^c], \quad \text{and} \quad S_2 = [a_7, a_7, a_7^c, a_7^c, a_6, a_6^c]$$

are good pairs, because $a_6 * a_9$ and $a_6^c * a_9^c$ are Latin squares. If Case ($3ii$) occurs, using the same argument as in the second case, two superimposed grids $a * b$ and $a * b^c$ supply two 0 (and two 1, 2, 3) in each row and column of grids. The conclusion follows. Since there are only three ways of writing the number 6 as a sum of four numbers 0,1,2,3: $6 = 0 + 0 + 3 + 3 = 1 + 2 + 0 + 3 = 1 + 2 + 1 + 2$; if Case ($3iii$) happens, then the symbol 0 (1,2,3) appears exactly 4 times in four non-Latin square grids. The orthogonality of (X, S_1, S_2) and (Y, S_1, S_2) follows ($\diamond$).

The 'only if' part is proved follows. Let n_{12} be the number of Latin squares comprised of components of the columns S_1, S_2. Suppose that $n_{12} \leq 5$. By the above reasoning $n_{12} \neq 5$. If $n_{12} = 4$ then we get (2). If $n_{12} = 3$, that is we have three Latin squares, the remaining superimposed grids, say $g_3 * h_3$, $g_4 * h_4$ and $g_5 * h_5$ are not. Since $g_3 * h_3$ is not a Latin square, it either has precisely two rows, say y_1, y_2, or has two columns in which symbol 0 (or 1,2,3) occurs twice. Then in grid $g_4 * h_4$ (or $g_5 * h_5$) we must see two 0s at rows y_3, y_4; otherwise the symbol 0 already occurs $3+2+2 = 7$ times in row y_1 or row y_2, contradiction. Therefore, (using only five superimposed grids) symbol 0 already occurs $3 + 2 = 5$ times at every row and column, and the last superimposed grid $g_5 * h_5$ (or $g_4 * h_4$) contributes two more 0s to some row (or column), contradiction.

Now we consider $n_{12} = 2$. By similar reasoning as above, we get two 0s in every row and every column from two Latin square grids. Suppose that the remaining four grids $g_2 * h_2, g_3 * h_3, g_4 * h_4$ and $g_5 * h_5$ are not Latin squares. If $g_3 * h_3 = g_2 * h_2^c$ or $g_3 * h_3 = g_2^c * h_2$, we get 4 symbols 0 in every row and in every column. It follows that $g_4 * h_4$ and $g_5 * h_5$ must be one of the forms in case (2). We have obtained Case ($3ii$). If these four grids do not have pattern ($3i$) or ($3ii$), they must be of the pattern ($3iii$), by using ($\diamond$). □

From Table 3.2, we see that the derived grids of the triple a_1, a_2, a_3 form Latin squares, and so do those of the triple a_4, a_6, a_8, and a_5, a_7, a_9. These are all possibilities composed from 9 grids. Furthermore, none of these triples is extendable.

Find conditions for appending the third binary column S_3. Let

$$D_3 = \mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^3; 3) = [Z|X|Y|S_1|S_2|S_3]$$

be a putative array formed by 6 arrays $[f|g_1|g_2|g_3]$ where g_1, g_2, g_3 are selected as above. We embed grids into the 5-dimensional space $XYS_1S_2S_3$. Then D_3 has strength 3 if and only if it satisfies: for each triple $ijk \in [S_1S_2S_3]$, the intersections of D_3 with hyperplanes $S_1 = i, S_2 = j, S_3 = k$ have exactly 12 points.

We code combinations $000, \dots 111$ by symbols $0, 1, 2, 3, 4, 5, 6, 7$. Then this condition is read off when we put 3 grids $[f|g_1]$, $[f|g_2]$ and $[f|g_3]$ together. That is we superimpose three grids $g_1, g_2, g_3 \in G$ into a *triple superimposed grid* (or *triple grid*) consisting of symbols 0 to 7. We get 6 triple grids with 3 columns. For every $i \in \{0, \dots, 7\}$, if the total number of symbols i from these grids are 12, then we are done. Now by exhaustive search, we find:

PROPOSITION 26. *An orthogonal array* $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^5; 3)$ *exists.*

The five binary columns building up this array are:

S_1	S_2	S_3	S_4	S_5
a_1	a_2	a_7	a_3	a_4
a_1^c	a_2^c	a_7	a_3^c	a_4^c
a_1	a_2	a_7^c	a_6	a_9
a_1	a_2^c	a_7^c	a_6^c	a_9^c
a_1^c	a_2	a_6	a_9^c	a_4
a_1^c	a_2^c	a_6^c	a_9	a_4

Construction of $D_a = \mathrm{OA}(80; 5{\cdot}4{\cdot}2^a; 3)$, $a \leq 6$. We encode of orthogonality between columns as slightly differently from the previous section. We use the rectangular discrete cube $\{0, 1, 2, 3\} \times \{0, 1\}^2$, project the cube onto a plane, and generate 0, 1-grids and their derived grids. Then we try to match as many grids as possible.

View an orthogonal array in 3-dimensional space. We suppose

$$D_a = \mathrm{OA}(80; 5 \cdot 4 \cdot 2^a; 3) = [Z|X|Y|W|S_1| \cdots |S_a]$$

where the factor Z has five levels, X has four levels, and Y, W, S_i have two levels each. The full design $f := \mathrm{OA}(16; 4 \cdot 2^2; 2)$ is the discrete box or parallelotope $\{0, 1, 2, 3\} \times \{0, 1\}^2$. By mapping f (in the 3-dimensional space XYW) onto the plane XY, we identify f with the positions in a 4×4 matrix J, in which the columns represent levels $0, 1, 2, 3$ of X and the rows represent levels 0,1 of Y, W. Note that, in this encoding, we attach the levels of the unique 4-level factor X to columns, not rows; we reserve the rows for the binary factors Y and W. Denote $J(i)$ for the ith row of J, let Y_0, Y_1, W_0, W_1 be sub-grids of J determined by:

$$\begin{aligned} Y_0 &= \{J(1), J(4)\}, \\ Y_1 &= \{J(2), J(3)\}, \\ W_0 &= \{J(3), J(4)\}, \\ W_1 &= \{J(1), J(2)\}. \end{aligned} \tag{3.6.3}$$

These sub-grids represent the levels of the factors Y and W.

Determine the feasible grids for the third binary column in $\mathrm{OA}(16; 4{\cdot}2^2{\cdot}2; 2)$. Let S be a binary column to be added to $f = \mathrm{OA}(16; 4{\cdot}2^2; 2)$ to form an $\mathrm{OA}(16; 4{\cdot}2^2{\cdot}2; 2)$.

REMARK 3.4. Adding S is equivalent to assigning the symbol 0 to exactly 2 points in every column of f such that the number of symbols 0 in each sub-grid Y_0, Y_1, W_0, W_1 is precisely 4. These points are $xyw0 \in XYWS$, and the remaining points represent $xyw1 \in XYWS$ (where $0 \leq x \leq 3, 0 \leq y, w \leq 1$) in the resulting array which is denoted by $[f|S]$.

We find 5 non-isomorphic series of grids to be used for building an $\mathrm{OA}(16; 4\cdot 2^2\cdot 2; 2)$. The general method for obtaining these classes will be detailed in Section 4.2. The first two classes A and B are described in the construction of $\mathrm{OA}(96; 6\cdot 4^2\cdot 2^5; 3)$. The third, fourth and fifth, denoted by C, D, E, consist of 6, 144 and 24 isomorphic grids; but in fact, only 2, 48 and 8 isomorphic grids in C, D, E respectively satisfy Remark 3.4. We list here 3 representatives c_1, d_1, e_1 for the last three classes C, D and E.

$$c_1 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad d_1 = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \qquad e_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix},$$

Let $G := A \cup B \cup C \cup D \cup E$ be the set of all 148 (=18+72+2+48+8) grids.

Form conditions on $F := [f|S]$ *such that 5 copies of* F *form an orthogonal array* $D = \mathrm{OA}(80; 5\cdot 4\cdot 2^2\cdot 2; 3)$.

Condition 1. *A putative fraction* D *must satisfy:*

(i) *each triple* xys, xws *appears exactly 5 times; and moreover,*
(ii) *each triple* yws *appears exactly 10 times in* D,
for all $0 \le x \le 3$, $0 \le y, w \le 1$, *and* $s \in \{0, 1\}$.

For any grid $g \in G$, let $Y_0(g), Y_1(g), W_0(g), W_1(g)$ be the corresponding subgrids (defined in (3.6.3)); let $Y_0(D)$, $Y_1(D)$, $W_0(D)$, $W_1(D)$ be the union of 5 subgrids extracted from component grids of D. Each of the triples xys, xws occurs 5 times in D if and only if the intersections of the plane $\{X = j\}$ with $Y_0(D)$, $Y_1(D)$, $W_0(D)$, or $W_1(D)$ consists of five symbol 0 and 1 for all $0 \le j \le 3$. Using the grid $a_7 \in A$, and applying the column permutations $(1, 3)$ and $(1, 3)(2, 4)$ to a_7, we get

$$a_7 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \qquad a_{7b} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}, \qquad a_{7c} = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix}$$

Lemma 27. *Let* $S = [a, b, c, d, e]^T$ *be a candidate binary column (of* D*) where* $a, b, c, d, e \in G$.

(1) If there are two complement pairs of grids in S *then the fifth grid must be* a_7, a_{7b} *or* a_{7c}.
(2) If there is only one complement pair in S, *say* $S = [a, a^c, c, d, e]^T$ *then the intersections of* $\{X = j\}$, *for* $0 \le j \le 3$, *with grids* $Y_i(c) \cup Y_i(d) \cup Y_i(e)$, $W_i(c) \cup W_i(d) \cup W_i(e)$, *for* $0 \le i \le 1$, *must contain exactly three symbols* 0.

Proof. For any grid $g \in G$, and for each $\{X = j\}$, there are precisely two 0s from the complement pair g, g^c contributing to $Y_0(D)$, $Y_1(D)$, $W_0(D)$, $W_1(D)$. If we use two pairs a, a^c and b, b^c then only one 0 need be found from the fifth grid. Only grids a_7, a_{7b} or a_{7c} have the property that every column $\{X = j\}$ intersects with Y_0, Y_1, W_0, W_1 at one 0 simultaneously, for $0 \le j \le 3$. The second statement is evident. $\square$

Furthermore, triplets $yw0$ and $yw1$ have to occur 10 times in D. In our setting, pairs $yw \in YW$ can be identified with rows of the grid. In more detail,

$$\begin{aligned}
(Y = 0 \quad \text{and} \quad W = 0) \quad &\Longleftrightarrow \quad Y_0 \cap W_0 = J(4),\\
(Y = 0 \quad \text{and} \quad W = 1) \quad &\Longleftrightarrow \quad Y_0 \cap W_1 = J(1),\\
(Y = 1 \quad \text{and} \quad W = 0) \quad &\Longleftrightarrow \quad Y_1 \cap W_0 = J(3),\\
(Y = 1 \quad \text{and} \quad W = 1) \quad &\Longleftrightarrow \quad Y_1 \cap W_1 = J(2).
\end{aligned}$$

If we use the pair X, X^c in column S, then since every grid $g \in$A$\cup B$ has two 0s in every row, Condition 1(ii) is fulfilled.

Build up conditions such that 5 copies of $F = [f|S_1|S_2]$ form an array $D =$ OA$(80; 5 \cdot 4 \cdot 2^2 \cdot 2 \cdot 2; 3)$

CONDITION 2. *Now, a putative fraction D must satisfy: for all $0 \leq x \leq 3$ and $0 \leq y, w \leq 1$,*

(i) *each triple $xs_1s_2 \in XS_1S_2$ occurs 5 times in D,*
(ii) *each triple $ys_2s_2 \in YS_1S_2$ and each triple $ws_2s_2 \in WS_1S_2$ appears 10 times in D, where $s_1, s_2 \in \{0, 1\}$.*

Suppose that two putative binary columns have patterns

$$S_1 = [a_1, \dots, a_5], \qquad S_2 = [b_1, \dots, b_5] \qquad \text{where} \quad a_i, b_i \in G.$$

For each pair $a_i, b_i \in (S_1, S_2)$, let d_i be their superimposed grid, $a_i * b_i$, and let $d_i(j)$ be the j-th column of this grid, where $1 \leq i \leq 5$, $0 \leq j \leq 3$. Recall that the symbols $0, 1, 2, 3$ in d_i denote pairs $00, 01, 10, 11$ in S_1S_2. Then Condition 2(i) means: for each $j = 0, \dots, 3$, the total number of symbols 0 (and 1,2,3 as well) in the union $\bigcup_{1 \leq i \leq 5} d_i(j)$ is exactly 5.

We call an order n grid a *columnar Latin square* of order n if it each of symbol $1, 2, \dots n$ occurs once in each column. It is obvious that a Latin square is also a columnar Latin square. Notice that when every superimposed grid d_i is a columnar Latin square then Condition 2(i) is satisfied. Denote by $Y_0(d_i)$, $Y_1(d_i)$, $W_0(d_i)$, $W_1(d_i)$ the sub-grids extracted from d_i, then Condition 2(ii) says that the number of symbols 0 (1,2,3) in the unions $\bigcup_{1 \leq i \leq 5} Y_s(d_i)$ and $\bigcup_{1 \leq i \leq 5} W_s(d_i)$ is 10 for $s = 0, 1$. We have

LEMMA 28. *Let $S_1 = [a_1, \dots, a_5]$ and $S_2 = [b_1, \dots, b_5]$ (where $a_i, b_i \in G$, $i = 1, \dots 5$) be two columns to be appended to $f =$ OA$(16; 4 \cdot 2 \cdot 2; 2)$. Column X is orthogonal to the pair S_1S_2 if one of the following conditions is satisfied*

(1) all of the five superimposed grids d_i are columnar Latin squares; or
(2) three of the d_i are columnar Latin squares and the remaining two (non columnar Latin squares) are of the form $g * h$, $g * h^c$ or $g * h$, $h^c * g$; or
(3) only one superimposed grid d_i is a columnar Latin square and the remaining four are of the form $g * h$, $g * h^c$ or $g * h$, $h^c * g$, where $g, h \in G$.

PROOF. The implication 'Item (1) is fulfilled implies X is orthogonal to the pair S_1S_2' is obvious. If Item (2) is satisfied, we consider two pairs being of the form $g * h, g * h^c$, where neither $g * h$ nor $g * h^c$ is a columnar Latin square. Each column of $g * h$ has two symbols, i, j, say, each symbol occurs exactly twice. Since each column of $g^c * h$ consists of symbols $(i + 2) \bmod 4$ and $(j + 2) \bmod 4$ occuring exactly twice; every symbol in each column of $g * h^c$ appears twice too, (see the proof of Lemma 22). The same argument is applied for columns of $h^c * g$.

Hence each symbol occurs 5 times in $\bigcup_{1\le i\le 5} d_i(j)$, and 10 times in $\bigcup_{1\le i\le 5} Y_s(d_i)$ and $\bigcup_{1\le i\le 5} W_s(d_i)$. The orthogonality between X and S_1S_2 follows then. The last implication is correct by similar reasoning. □

Applying this reasoning, we get

PROPOSITION 29. *An orthogonal array* $F := \mathrm{OA}(80; 5\cdot 4\cdot 2^6; 3)$ *exists.*

Denote

$$b_2 = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix}$$

which is obtained from grid b_1 (as in (3.6.2)) by applying the column permutation $(3,4)$ to b_1^c, then the row permutation $(1,3,4)$ to the resuting grid. Let $b_3 := b_2^p$ where p is the row permutation $(1,2)$, let $b_4 := b_3^q$ where q is the row permutation $(1,4,2,3)$, and let $b_5 := b_4^r$ where r is the row permutation $(3,4)$. The four binary columns extending an $\mathrm{OA}(80; 5\cdot 4\cdot 2^2; 3)$ to F are determined by:

S_1	S_2	S_3	S_4
c_1^c	a_4	a_2^c	a_8
a_3^c	c_1^c	b_2	a_2
c_1	a_3^c	b_3	b_4
a_9	c_1	a_2	b_5
a_9^c	a_4^c	a_8	a_2^c

3.7. Decomposing arrays using row orbits

This construction uses the concept of the automorphism group of an array, which is introduced later in Section 4.2.

Denote an arbitrary array $\mathrm{OA}(N; r_1\cdot r_2\cdots r_d; t)$ by F. Decompose F into sub-arrays $F_0, F_1, \ldots, F_{s-1}$ each having N/s runs. If each of these sub-arrays has strength $t-1$, then

$$\left[\begin{array}{c|c} \mathbf{0} & F_0 \\ \mathbf{1} & F_1 \\ \vdots & \vdots \\ \boldsymbol{s-1} & F_{s-1} \end{array}\right]$$

is an $\mathrm{OA}(N; s\cdot r_1\cdot r_2\cdots r_d; t)$. Note that if $F_0, \ldots, F_{s-2}$ have strength $t-1$, then F_{s-1} must also have strength $t-1$. In particular, when $s=2$, if we can ensure that F_0 is an $\mathrm{OA}(N/2; r_1\cdot r_2\cdots r_d; t-1)$, then the complementary array F_1 of F_0 in F is obviously an $\mathrm{OA}(N/2; r_1\cdot r_2\cdots r_d; t-1)$ too.

The automorphism group $\mathrm{Aut}(F)$ of F is the set of all products of row permutations, symbol permutations, and column permutations among factors of equal level that preserve F. (Section 4.2 in the next chapter will clarify this concept). To limit the search space for all possible sub-arrays F_0 we can use subgroups of F.

Use of a specific subgroup. Now suppose that $F = \mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; 3)$. Let H be a subgroup of $\mathrm{Aut}(F)$, and let L be the set of all rows of F. We decompose L into the $\mathrm{Aut}(F)$-orbits, denoted by $O_1, O_2, \ldots, O_l$:

$$L = \bigcup_{j=1}^{l} O_j. \tag{3.7.1}$$

Let $y := [y_1, \ldots, y_l]$ be a list of representatives of these orbits, ie, $y_j \in O_j = \mathrm{Orbit}(\mathrm{Aut}(F), y_j)$. We compute the images $\mathrm{Orbit}(H, y_j)$ of these representatives under the action of H. Put

$$F_0 := \bigcup_{j=1}^{l} \mathrm{Orbit}(H, y_j) \subseteq F \tag{3.7.2}$$

If F_0 is $\mathrm{OA}(N/2, r_1 \cdot r_2 \cdots r_d, 2)$ then we can extend F by a binary factor having value 0 on F_0 and value 1 on the other runs.

An application. This method works for $\mathrm{OA}(54; 3^5; 3)$. In total, there are 4 non-isomorphic arrays of this series which we denote by I, II, III, and IV, using the notation of Hedayat et al. [1997]. Applying formulas (3.7.1) and (3.7.2) respectively for array III, with H the commutator subgroup of $\mathrm{Aut}(F)$, we find that the sub-array F_0 is an $\mathrm{OA}(27; 3^5; 2)$. More precisely, in this case, $\mathrm{Aut}(F)$ is a permutation group of size 144 with 5 generators, and H is a permutation group of size 18. The rows of F are partitioned into 2 parts, with particular representatives y_1, y_2 of the $\mathrm{Aut}(F)$-orbit. Then $\mathrm{Orbit}(H, y_1)$ has 9 runs, $\mathrm{Orbit}(H, y_2)$ has 18 runs. And by inspection, F_0 is an orthogonal array $\mathrm{OA}(27; 3^5; 2)$ indeed. The array $G = \left[\begin{smallmatrix} F_0 & \mathbf{0} \\ F_1 & \mathbf{1} \end{smallmatrix}\right]$ is the new array $\mathrm{OA}(54; 3^5 \cdot 2; 3)$, where $F_1 = F \setminus F_0$, and $\mathbf{0}, \mathbf{1}$ are constant vectors of length 27.

3.8. Conclusion

The methods that we have discussed are based only on the definition of orthogonal arrays, and employ some extra assumptions. For instance, we use the linearity assumption in the arithmetic construction of Section 3.5.

Using extra assumptions narrows down the solution set. Another drawback of the methods discussed is that they are combinatorial, mainly based on counting symbols. That means they depend on particular parameter sets. This fact limits the possibility of generalization to other cases. When they work, we get an extension, but we don't know how many extensions can be formed. We need some good ways to find all extensions. These will be discussed in the next chapter.

CHAPTER 4

Enumerating strength 3 orthogonal arrays

4.1. Introduction

This chapter is devoted to finding all isomorphism classes of strength 3 orthogonal array (OAs) with a given parameter set (levels) and run size. In Section 4.2, we use group theory to define the full group of fraction transformations and compute the automorphism group of an orthogonal array. By translating orthogonal arrays to their corresponding colored graphs, we find canonical orthogonal arrays in Section 4.3. That settles the problem of computing representatives of isomorphism classes provided we know all orthogonal arrays with given levels and run size. Another way of enumerating strength 3 OAs which have two distinct levels by *backtrack search* is discussed in Section 4.4. Finally, in Section 4.5, we use *integer linear programming* methods combined with *canonical fractions* to list all non-isomorphic extensions of a strength 3 OA.

4.2. The automorphism group of a fraction

This section is organized as follows: First we provide a general combinatorial setting for the remaining sections. We define the *underlying set* of a fractional factorial design and show how to use it to encode a fraction. The *full group of fraction transformations* G and the *automorphism group of a fraction* F are then described. Finally we provide a scheme for computing G and $\mathrm{Aut}(F)$.

Combinatorial setting. Let $\mathbb{X}$ be the set of all structures of a particular type built on an *underlying set* T. For example, $\mathbb{X}$ could be all the graphs with vertex set T. The subgroup $G := G(T) \leq \mathrm{Sym}(T)$ which acts naturally on $\mathbb{X}$ is called the *(full) group of transformations* of $\mathbb{X}$. Two elements A and B of $\mathbb{X}$ are *isomorphic* if they are in the same G*-orbit*, that is, there exists a permutation g in G such that $A = B^g$. The automorphism group of $S \in \mathbb{X}$ is defined as

$$\mathrm{Aut}(S) := \{g \in G : S^g = S\}. \tag{4.2.1}$$

The number of distinct objects isomorphic to a structure S is the length of the G-orbit of S. By Lagrange's theorem [Nathanson, 2000], this number is:

$$\frac{|G|}{|\mathrm{Aut}(S)|}.$$

EXAMPLE 4.1. Let $V = T$ be a set of size N. Then the set of undirected, *finite graphs* with vertex set V can be defined as the collection of subsets E of $\binom{V}{2}$. Each subset E represents the edges of a particular graph. We define the full group $G := \mathrm{Sym}(V)$, and define E^g by the usual convention that if an edge $e := \{u, v\} \in E$ then the edge $e^g := \{u^g, v^g\} \in E^g$ for any $g \in G$. The automorphism group of a particular graph $X = (V, E)$ is $\mathrm{Aut}(X) := \{g \in \mathrm{Sym}(V) : E^g = E\}$.

EXAMPLE 4.2. Let $P = T$ be a finite set of points, $v := |P|$. Let $k \le v$, and let $\mathcal{B} \subseteq \binom{P}{k}$ be a collection of subsets of P of size k. A pair $X = (P, \mathcal{B})$ is called a t-(v, k, λ) *block design* if every set of t points in P is contained in exactly λ elements of $\mathcal{B}$. Let $\mathbb{X}$ be the set of all t-(v, k, λ) block designs defined on P. We define the full group of block design transformations by $G := \mathrm{Sym}(P)$, and the action of G on $\mathbb{X}$ by $X^g := (P, \mathcal{B}^g)$ for $g \in G$, where $\mathcal{B}^g := \{B^g : B \in \mathcal{B}\}$. The automorphism group of a particular block design $X = (P, \mathcal{B})$ is

$$\mathrm{Aut}(X) := \{g \in G : \mathcal{B}^g = \mathcal{B}\}.$$

EXAMPLE 4.3. Let N be $1, 2$ or a positive multiple of 4 and let

$$T := \{1, 2, \ldots, N\} \times \{1, 2, \ldots, N\} \times \{-1, 1\}.$$

A Hadamard matrix of order N is $H_N := [v_1, v_2, \ldots, v_N]$ in T^N such that $v_i \cdot v_j = 0$ if $i \neq j$; and $v_i \cdot v_j = N$ if $i = j$. Let $\mathbb{X}$ be the set of all Hadamard matrices X of order N. The full group G is a direct product

$$\mathrm{Sym}_N \times \mathrm{Sym}_N \times \mathrm{Sym}(\{-1, +1\})$$

where the first component acts on the rows, the second acts on the columns and the last component acts entrywise on the matrix. The last component is called the *symbol change group*. The automorphism group of a particular Hadamard matrix $X \in \mathbb{X}$ is $\mathrm{Aut}(X) := \{g \in G : X^g = X\}$

Let $U = r_1 \cdot r_2 \cdots r_d = s_1^{a_1} \cdot s_2^{a_2} \cdot s_3^{a_3} \cdots s_m^{a_m}$ be a design type, (as described in Appendix B). Let $\mathcal{F}(U, N)$ be the set of all fractional factorial designs (fractions) having *design type* U and *run size* N. Write $\mathcal{F}$ for $\mathcal{F}(U, N)$ if no ambiguity occurs. We now define the underlying set T and construct the full group G. We divide the columns into sections corresponding to the distinct level sizes $s_1, \ldots, s_m$. So the ith section consists of the a_i columns with s_i levels, and $d = a_1 + a_2 + \cdots + a_m$. For instance, a Placket-Burmann design with $N = 8$ runs ($m = 1$) is represented by $U = s_1^{a_1} = 2^7$. Thus we have one section, and $d = 7$.

We may view $F \in \mathcal{F}$ as an $N \times d$-matrix. The set $\{1, 2, \ldots, d\}$ has a partition into *sections*

$$\begin{aligned}
J_1 &= [1, \ldots, a_1], \\
J_2 &= [a_1 + 1, \ldots, a_1 + a_2], \\
&\vdots \\
J_k &= [a_1 + \cdots + a_{k-1} + 1, \ldots, a_1 + \cdots + a_k], \\
&\vdots \\
J_m &= [a_1 + \cdots + a_{m-1} + 1, \ldots, a_1 + \cdots + a_m = d].
\end{aligned} \tag{4.2.2}$$

Let $Q_k := \{1, 2, \ldots, s_k\}$ for $k = 1, \ldots, m$. Define

$$\begin{aligned}
D : \{1, \ldots, N\} \times \{1, \ldots, d\} &\to \{Q_1, Q_2, \ldots, Q_m\}, \\
(i, j) &\mapsto Q_k \text{ if there exists } k \text{ such that } j \in J_k.
\end{aligned}$$

Notice that D is a surjection but not an injection. We can code all possibilities for the (i, j)-entry of F by triplets $[i, j, s]$, where $i \in I_N$, $j \in [1, 2, \ldots, d]$, and

$s \in D(i,j)$. For a fixed set $\mathcal{F}$ of fractions, the *underlying set* or the *look-up table* T of $\mathcal{F}$, uniquely determined by the run size N and the type U, is

(4.2.3)
$$T = T(U,N) := \big\{[i,j,s] : i \in \{1,\dots,N\},\, j \in \{1,\dots,d\}, \text{ and } s \in D(i,j)\big\}.$$

Encoding of fractions. We view a fraction $F \in \mathcal{F}$ as an $N \times d$ matrix with (i,j)-entry $F[i,j]$. Then F is encoded by

$$S(F) = \big\{[i,j,F[i,j]] : \quad i = 1 \dots N, \quad j = 1 \dots d\big\}. \tag{4.2.4}$$

S is a map $\mathcal{F} \to \mathcal{P}(T)$, since $S(F) \subset T$ and each F has a unique image $S(F)$, called the *encoding map*. This is an injective mapping, but not surjective. Note that $|S(F)| = Nd$ for all fractions $F \in \mathcal{F}$. Let

$$A_i := \big\{[i,j,s] : j \in \{1,\dots,d\} \text{ and } s \in D(i,j)\big\}.$$

Then the image of $\mathcal{F}$ in $\mathcal{P}(T)$ is

(4.2.5)
$$\begin{aligned} S(\mathcal{F}) = \big\{K \subseteq T :\, & |K \cap A_i| = d,\ [i,j,s_1],[i,j,s_2] \in K \text{ implies } s_1 = s_2, \text{ and} \\ & [i,j_1,s],[i,j_2,s] \in K \text{ implies } j_1 = j_2, \text{ for } i = 1,\dots,N, \text{ for } j = 1,\dots,d\big\}. \end{aligned}$$

Moreover,

$$|T| = N \sum_{i=1}^{m} s_i . a_i \qquad \text{and}$$
$$|\mathcal{F}| = \prod_{i=1}^{m} (s_i^{a_i})^N.$$

For example, let $U = 2^3 \cdot 3^1$ and $N = 12$. Then $d = 4$ and the possibilities for the $(12,2)$-entry (of an arbitrary F) are 1 and 2 so the corresponding triplets in T are $[12,2,1]$ or $[12,2,2]$. But the possible triples for the $(1,4)$-entry are $[1,4,1]$, $[1,4,2]$ or $[1,4,3]$. Hence $|T| = 12 \cdot (2 \cdot 3 + 3 \cdot 1) = 108$.

The full group G of fraction transformations. Let $x = [i,j,s] \in T$, where $i = 1,\dots,N$, $j = 1,\dots,d$, and $s \in Q_k$ if $j \in J_k$. To avoid confusion, we use index k when indicating the section and index j when indicating the column.

The *row permutation group* of F, is defined to be $R := \mathrm{Sym}_N$ acting on $\mathcal{F}$ by

$$\boldsymbol{x}^r := \boldsymbol{x}^{\phi_R(r)} = [i^r, j, s]. \tag{4.2.6}$$

The *column permutation group of section k*, for each $k = 1,\dots,m$, is $C_k := \mathrm{Sym}(J_k)$ (where J_k is given in (4.2.2)). The *column permutation group* C is $C := \prod_{k=1}^{m} C_k$. This group acts on $\mathcal{F}$ by the *column exchange action* $\phi_C : C \to \mathrm{Sym}(T)$, defined by

$$\boldsymbol{x}^c := \boldsymbol{x}^{\phi_C(c)} = [i, j^{c_k}, s], \tag{4.2.7}$$

where $\boldsymbol{x} = [i,j,s]$, $j \in Q_k$ and $c = c_1 c_2 \dots c_k \dots c_m \in C := \prod_{k=1}^{m} \mathrm{Sym}(J_k)$.

The *level permutation group* of column j is determined by

$$L_{k,j} := \mathrm{Sym}_{s_k}, \qquad \text{for } j \in J_k$$

acting on the symbols of the jth column. The level permutation group of section k is then defined by

$$L_k := \prod_{j \in J_k} L_{k,j} = (\mathrm{Sym}_{s_k})^{a_k}.$$

Now L_k acts on $\mathcal{F}$ by the level exchange action $\phi_{L_k} : L_k \to \mathrm{Sym}(T)$ defined by

$$\boldsymbol{x}^l := \boldsymbol{x}^{\phi_{L_k}(l)} = [i, j, s^l] = [i, j, s^{l_j}] \tag{4.2.8}$$

where $l = l_1 l_2 \dots l_j \dots l_d \in L := \prod_{k=1}^m L_k$.
The group L switches levels of all columns of F, and we write $L = \prod_{j=1}^d \mathrm{Sym}(r_j)$ if we want to separate the action on each column.

For instance, the column permutation group C_2 permutes columns in the second section, the group $L_{3,2}$ exchanges levels of the second column in the third section and so forth.

Lemma 30. *The groups R, C and L act faithfully on T.*

Proof. We show that, for instance, $\mathrm{Ker}(\phi_R) = \{\mathrm{id}_R\}$. For all $\boldsymbol{x} = [i, j, s] \in T$, $r \in R = \mathrm{Sym}_N$, we have:

$$\phi_R(r) = \mathrm{id} \in \mathrm{Sym(T)}) \iff \forall \boldsymbol{x}, \boldsymbol{x}^{\phi_R(r)} = \boldsymbol{x} \iff [i^r, j, s] = [i, j, s] \iff r = id_R.$$

The last implication is true since only id_R satisfies $i^r = i$ for all $i \in \{1, \dots, N\}$. □

Corollary 31. *We have*

$$R \simeq \phi_R(R) \leq \mathrm{Sym}(T),$$

$$C \simeq \phi_C(C) \leq \mathrm{Sym}(T),$$

$$L \simeq \phi_L(L) \leq \mathrm{Sym}(T).$$

The full group G of fraction transformations is defined by

$$G := \phi_R(R) \times \phi_C(C) \times \phi_L(L) \leq \mathrm{Sym}(T). \tag{4.2.9}$$

This group then acts naturally on $\mathcal{F}$ via $\pi : G \to \mathrm{Sym}(\mathcal{F})$ defined by

$$F^g := F^{\pi(g)} = S^{-1}\big(S(F)^g\big), \quad \forall g \in G, \quad \forall F \in \mathcal{F}.$$

The newly defined group G is indeed a permutation group acting on the space $\mathcal{F}$ of fractions of given type U and run size N. The following lemma shows that π is well-defined.

Lemma 32. *The homomorphism π is a group action. That is, for any permutations $g, h \in G$, and any fraction $F \in \mathcal{F}$, we have:*

$$F^{gh} = (F^g)^h.$$

PROOF. First we show that the function π is well defined. Let $S(F) =: K$ be a subset of $S(\mathcal{F})$. We have

$$K^g = S(F)^g \in S(\mathcal{F})$$

for all $F \in \mathcal{F}$ and $g \in \phi_R(R)$, since $K^g = \big\{[i^g, j, s]\big\} \in S(\mathcal{F})$ as g is a bijection and $K := \big\{[i, j, s]\big\}$ fullfils Conditions (4.2.5). For all $g \in \phi_C(C)$ and $g \in \phi_L(L)$, we also have $S(F)^g \in S(\mathcal{F})$; so $S(F)^g$ is in the image of S for all $g \in G$. Therefore, $F^g = S^{-1}\big(S(F)^g\big) \in \mathcal{F}$ is well defined. Secondly, we have

$$\begin{aligned}(F^g)^h &= \big(S^{-1}(S(F)^g)\big)^h = S^{-1}\big(S(S^{-1}(S(F)^g))^h\big)\\ &= S^{-1}\big((S(F)^g)^h\big) = S^{-1}\big(S(F)^{gh}\big) = F^{gh}.\end{aligned}$$

□

Relations between the three types of permutation and the structure of G.

DEFINITION 33. *The* full automorphism group *of a fraction $F \in \mathcal{F}$ is the normalizer of F in the group G, ie,*

$$\mathrm{Aut}(F) := \{g \in G : F^g = F\}. \tag{4.2.10}$$

Any subgroup $H \leq \mathrm{Aut}(F)$ is called a group of automorphisms of F.

By (4.2.9), the full group G is generated by the *isomorphism images* of the row, column and level permutation groups in $\mathrm{Sym}(T)$. But the structure of G has not yet been determined. To describe it, we need to know the relationship between the three types of permutations. It is clear that the column permutations $c \in C := \prod_{k=1}^m C_k$ and the level permutations $l \in L := \prod_{k=1}^m L_k$ act independently on distinct sections. As expected for isomorphisms, they preserve the strength of a fraction. Therefore there are obvious commutation relations between these permutations described as follows:

PROPOSITION 34 (Properties of G).

(1) Column-Column relation. *Column permutations in distinct sections commute, ie,*
$$[C_k, C_h] = 1$$
for all $k \neq h$.
(2) Level-Level relation. *Level permutations of columns in distinct sections commute, ie,*
$$[L_k, L_h] = 1$$
for $k \neq h$.
(3) Row-Column relation. *Row permutations commute with column permutations, ie,*
$$[R, C] = 1.$$
(4) Row-Level relation. *Row permutations commute with level permutations, ie,*
$$[R, L] = 1.$$

(5) Column-Level relation. *Let $c \in C$ be a column permutation and let $l = l_1 \cdots l_d$ be a level permutation. Then c commutes with l if, and only if, $l_i = l_j$ whenever i and j are in the same cycle of c. So the subgroup generated by column permutations in section k and level permutations in that section is a wreath product*

$$\mathrm{Sym}_{s_k} \wr C_k = L_k \rtimes \mathrm{Sym}_{a_k}.$$

Proof. Items 1 to 2 are obviously true. Item 3 is easily proved by observing that a vertical move of an entry followed by a horizontal move gives the same result as the same moves in the reverse order. Item 4 is true as well, since we get the same fraction if we permute rows first, then switch levels of any column j in any section k, or do it the other way round. That means $r.l_{kj} = l_{kj}.r$; this implies $r.l_k = l_k.r$.

To see the correctness of the last item, first let column permutation $c = (i, j)$ be a transposition inside a section. Let l_i, l_j, l_p be level permutations on columns i, j, p such that $p \neq i$ and $p \neq j$, (p may belong to the same section as i, j or another section). Then

$$c.l_i \neq l_i.c \quad \text{and} \quad c.l_j \neq l_j.c, \tag{4.2.11}$$

but

$$c.l_i = l_j.c \quad \text{and} \quad c.l_j = l_i.c. \tag{4.2.12}$$

However,

$$c.l_i.l_j = l_j.c.l_j = l_j.l_i.c = l_i.l_j.c, \tag{4.2.13}$$

and of course

$$c.l_p = l_p.c \quad \text{for all } p \neq i, j$$

then

$$c.l_i.l_j.l_p = l_i.l_j.c.l_p = l_i.l_j.l_p.c$$

Item 5 now follows from equations (4.2.13) and (4.2). ☐

To summarize, from equations (1), (2), (3) and (4), we see that G is nearly a direct product of symmetric groups and a wreath product of symmetric groups. More precisely, the full group

$$G := R \times (L \rtimes C)$$

where $R := \mathrm{Sym}_N$ is the row permutation group, L and C the level and column permutation groups of $\mathcal{D}$, and $L \rtimes C := \prod_{k=1}^{m} \mathrm{Sym}_{s_k} \wr \mathrm{Sym}_{a_k}$.

Remark 4.1. When applying permutations to a particular fraction F, we apply the level permutations L to all sections first, next we permute the columns in the sections independently, and finally we permute the rows.

Example 4.4. Suppose a fraction has 2 sections, the first with 6 columns, the second with 3. Let $c = c_1.c_2 = (1, 2)(7, 9)$, then

$$c.l_p = l_p.c \qquad \forall p \notin \{1, 2, 7, 9\}.$$

If $p \in \{1, 2, 7, 9\}$, for instance $p = 7$, then

$$c.l_p = c.l_7 = c_1.c_2.l_7 = c_1.l_9.c_2 = l_9.c_1.c_2 = l_9.c,$$

and

$$c.l_7.l_9 = c_1.c_2.l_7.l_9 = c_1.l_9.c_2.l_9 = l_9.c_1.c_2.l_9 =$$

$$= l_9.c_1.l_7.c_2 = l_9.l_7.c_1.c_2 = l_7.l_9.c.$$

However,

$$c.l_1.l_7 = c_1.c_2.l_1.l_7 = l_2.l_9.c_1.c_2 = l_2.l_9.c.$$

In the case of three level permutations acting on 3 columns appearing in c

$$c.l_1.l_7.l_9 = c.l_7.l_9.l_1 = l_7.l_9.c.l_1 = l_7.l_9.l_2.c = l_2.l_7.l_9.c.$$

From Proposition 34 we have

COROLLARY 35. $|G| = N!\, a_1! \cdots a_m!\, (s_1!)^{a_1} \cdots (s_m!)^{a_m}$.

Determining the full group G and the automorphism group $\mathrm{Aut}(F)$. By combining (4.2.3), (4.2.4), and (4.2.9), we now can find an image F^g of a fraction F and compute its automorphism group. To determine the full group G, we calculate the lookup table T; compute the groups R, C, L of row, column, and level permutations; find the *homomorphism images* $\phi_R(R), \phi_C(C)$, and $\phi_L(L)$ of these groups in the symmetric group on $|T|$ points; and form the full permutation group G as a group generated by the generators of these images. Then $G \leq \mathrm{Sym}(\{1, 2, \ldots, |T|\})$ and G acts on $S(\mathcal{F})$.

For any permutation $g \in G$ and any fraction $F \in \mathcal{F}$, we find F^g, the image of F by encoding F by the subset $S(F) \subseteq T$; identifying the index set $f \subset \{1, 2, \ldots, |T|\}$ corresponding to $S(F)$; then $F^g := S^{-1}(f^g)$.

The *automorphism group* $\mathrm{Aut}(F)$, by Definition 33 is:

$$\mathrm{Aut}(F) := \{g \in G : f^g = f\}.$$

Hence, Problem 1 stated at the beginning of this section is now solved. We can also compute the automorphism group $\mathrm{Aut}(F)$ by using the automorphism group of its canonical graph. This will be discussed in Section 4.3.

Testing isomorphism of N-fractions and enumerating isomorphism classes. Given fractions $F, K \in \mathcal{F}$ with the size of G small, we compute the G-orbit of F. Then F is isomorphic to K if and only if F is an element in the G-orbit of K. If the size of G is large, another solution may be translating fractions into canonical graphs, then reducing the isomorphism test to checking the equality of their corresponding graphs; section 4.3 explains this approach. We may also solve the enumeration problem, for small run size designs, by exhaustively making all of non-isomorphic lexicographically-least designs, which is detailed in Section 4.4.

Implementation in GAP. First of all, the homomorphism images $\phi_R(R), \phi_C(C)$, and $\phi_L(L)$ are found with the GAP command `Action(G, T, action-type)`. Now the full automorphism group of a specific fraction F is computed with the GAP command `Stabilizer(G, f, OnSets)`, where $f \subseteq \{1, \ldots, |T|\}$ is the index set of the coding image $S(F) \subseteq T$ of F.

EXAMPLE 4.5. For a 4-runs fraction of a full 2^4-design,

$$F := \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & 2 \\ 1 & 1 & 2 & 2 \\ 1 & 2 & 2 & 1 \end{bmatrix}$$

we have $R = \mathrm{Sym}_4$, $C = \mathrm{Sym}_4$, $L = (\mathrm{Sym}_2)^4$; and the generators of the homomorphism images $\phi_R(R), \phi_C(C), \phi_L(L)$ in $\mathrm{Sym}(\{1, 2, \ldots, |T|\})$ are

$$\begin{aligned}
\phi_R(R) : &(1,9,17,25)(2,10,18,26)(3,11,19,27)(4,12,20,28)\\
&(5,13,21,29)(6,14,22,30)(7,15,23,31)(8,16,24,32),\\
&(1,9)(2,10)(3,11)(4,12)(5,13)(6,14)(7,15)(8,16).\\
\phi_C(C) : &(1,3,5,7)(2,4,6,8)(9,11,13,15)(10,12,14,16)(17,19,21,23)\\
&(18,20,22,24)(25,27,29,31)(26,28,30,32),\\
&(1,3)(2,4)(9,11)(10,12)(17,19)(18,20)(25,27)(26,28).\\
\phi_L(L) : &(1,2)(9,10)(17,18)(25,26).
\end{aligned}$$

Here $|T| = 32$ and

$$\begin{aligned}
T = \{ &[1,1,1],[1,1,2],[1,2,1],[1,2,2],[1,3,1],[1,3,2],[1,4,1],[1,4,2],\\
&[2,1,1],[2,1,2],[2,2,1],[2,2,2],[2,3,1],[2,3,2],[2,4,1],[2,4,2],\\
&[3,1,1],[3,1,2],[3,2,1],[3,2,2],[3,3,1],[3,3,2],[3,4,1],[3,4,2],\\
&[4,1,1],[4,1,2],[4,2,1],[4,2,2],[4,3,1],[4,3,2],[4,4,1],[4,4,2] \}.
\end{aligned}$$

Then G is a permutation group of order 9216 with a generating set consisting of the union of the generators for $\phi_R(R), \phi_C(C), \phi_L(L)$. Although $\phi_L(L)$ has order 2, the wreath product

$$\begin{aligned}
\phi_L(L) \wr \phi_C(C) &= \mathrm{Sym}_2 \wr \mathrm{Sym}_4\\
&= L \rtimes C = (\mathrm{Sym}_2 \times \mathrm{Sym}_2 \times \mathrm{Sym}_2 \times \mathrm{Sym}_2) \rtimes \mathrm{Sym}_4
\end{aligned}$$

contributes $2^4 \cdot 24$ to the order of G. Furthermore,

$$\begin{aligned}
S(F) = \big\{&[1,1,1],[1,2,1],[1,3,1],[1,4,1],[2,1,1],[2,2,2],[2,3,1],[2,4,2],\\
&[3,1,1],[3,2,1],[3,3,2],[3,4,2],[4,1,1],[4,2,2],[4,3,2],[4,4,1]\big\}.
\end{aligned}$$

The index set of the coding image $S(F)$ in T is

$$f = \{1,3,5,7,9,12,13,16,17,19,22,24,25,28,30,31\},$$

and $\mathrm{Aut}(F)$ is a permutation group of size 24 with 3 generators

$$\begin{aligned}
g_1 = &(3,5)(4,6)(9,17)(10,18)(11,21)(12,22)(13,19)(14,20)(15,23)\\
&(16,24)(27,29)(28,30),\\
g_2 = &(3,5,7)(4,6,8)(9,25,17)(10,26,18)(11,29,23)(12,30,24)(13,31,19)\\
&(14,32,20)(15,27,21)(16,28,22),\\
g_3 = &(1,9,17)(2,10,18)(3,13,24)(4,14,23)(5,16,19)(6,15,20)(7,12,22)\\
&(8,11,21)(27,29,32)(28,30,31).
\end{aligned}$$

The first generator of $\mathrm{Aut}(F)$, for example, is composed of the level, the column and the row permutations, respectively

$$l = [(),(),(),()], \quad c = (2,3), \quad \text{and } r = (2,3).$$

The last generator of $\mathrm{Aut}(F)$, is composed of the permutations

$$l = [(),(),(1,2),(1,2)], \quad c = (2,3,4), \quad \text{and } r = (1,2,3)$$

respectively. The number of distinct fractions isomorphic to F, by the Orbit Theorem, is

$$|G|/|\operatorname{Aut}(F)| = 9216/24 = 384.$$

The group $\operatorname{Aut}(F)$ induces a group of permutations on rows of F, so we can talk about the $\operatorname{Aut}(F)$-orbits on rows as well.

4.3. Enumeration of arrays using canonical graphs

We now introduce the concept of *canonical arrays*, then use it to classify *non-isomorphic fractions* of given design type and run size. The idea is to encode an array as a *colored graph*, then use the software package *nauty* [McKay, 2004] to find the *canonical labeling graph* of the colored graph and decode the result to a fraction. Testing isomorphism between orthogonal arrays is then reduced to testing isomorphism between their colored graphs. More precisely, first we describe a way to translate an array to a graph and show how to color that graph. Then we present a method to get back (demerge) an array from a colored graph. Next we find the canonical graph of a colored graph using *nauty*. We close this section by computing the *canonical orthogonal array* of a given orthogonal array.

The graph of an orthogonal array. An orthogonal array D is viewed as a set R of d-tuples $v = (p_1, \ldots, p_d)$, where $p_i \in Q_i$ for level sets $Q_1, \ldots, Q_d$. So each d-tuple from R represents a row of D. A (undirected) graph $G = (V, E)$ is constructed from this OA as

$$V = R \cup S \cup C; \tag{4.3.1}$$

where R is the set of row-vertices (one vertex per row), $S := \bigcup_{i=1}^{d} Q_i$ is the set of levels (symbols) per column (one vertex per level per column), and $C := \{x_1, \ldots, x_d\}$ is the set of columns (one vertex for each column). In total we have

$$|V| = |R| + \big(\sum_{i}^{d} |Q_i|\big) + d = N + \sum_{i}^{d} r_i + d$$

vertices. The edge set is

$$E = E_1 \cup E_2 \subseteq (R \times S) \cup (S \times C) \tag{4.3.2}$$

in which

$$E_1 := \bigcup_{1 \le i \le d} \big\{\{v, p_i\} : v = (p_1, \ldots, p_d) \in R \text{ and } p_i \in Q_i\big\}, \text{ and}$$
$$E_2 := \bigcup_{1 \le i \le d} \big\{\{s, x_i\} : s \in Q_i\big\}.$$

So

$$|E| = d|R| + \sum_{i}^{d} |Q_i| = dN + \sum_{i}^{d} r_i.$$

Since R, S, C are cocliques (ie, vertices in each set are not adjacent with each other), G is a tripartite graph with the vertex partition $R \cup S \cup C$. Let $n_S := |S|$ be the number of symbols, and $N = |R|$ the run size of D. The adjacency matrix A of G has the following pattern:

$$A = \left[\begin{array}{c|c|c} 0 & RS & 0 \\ \hline SR & 0 & SC \\ \hline 0 & CS & 0 \end{array}\right]$$

where RS is the $N \times n_S$-adjacency matrix formed by the row-symbol adjacency, $SR = RS^T$ (the transpose of RS), CS is the $d \times n_S$ adjacency matrix formed by the column-symbol adjacency, and $SC = CS^T$. We call a vertex with valency i an *i-vertex*, and write $V(x)$ for the neighbors of a vertex $x \in V$.

Coloring the graph G. To use *nauty*, we need to number the vertices of G. We number the row-vertices R first, then the symbol-vertices S and finally the column-vertices C. We color the resulting graph G by the following coloring rules:

all vertices of R have color A; here A is called the row color;
all vertices of S have color B; here B is called the symbol color;
$x_1, \ldots, x_d$ have the same color if and only if the corresponding level sets have the same cardinality: $\mathrm{color}(x_i) = \mathrm{color}(x_j) \iff |Q_i| = |Q_j|$.

Recall that $\mathcal{F} = \mathcal{F}_{U,N}$ is the class of all mixed orthogonal arrays of strength $t \geq 1$, of type $U = s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}$ and run size N. If the array $D \in \mathcal{F}$, then the set of column-vertices C is a disjoint union of color classes $C_1, \ldots, C_m$, called the *column-color classes*, and the total number of colors of G is $2 + m$. Also note that each row-vertex is adjacent to precisely d symbol-vertices, and each symbol-vertex is adjacent to exactly one column-vertex. Remark that the partition (R, S, C) is not a color partition, and $d = \sum_{i=1}^{m} |C_i|$. Recall that $n_S = |S|$. We write

$$(4.3.3)\quad f := \Bigg[[1, \ldots, N],\ [N+1, \ldots, N+n_S], \\ [N+n_S+1, \ldots, N+n_S+a_1], \ldots, [N+n_S+1+\sum_{i=1}^{m-1} a_i, \ldots, |V|] \Bigg]$$

for the *color partition* (determining row, symbol and column-vertices, respectively); and denote the colored graph just obtained by G_D.

EXAMPLE 4.6. Let D be the $\mathrm{OA}(4; 2^3; 2)$

$$\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix}.$$

Then $N = 4$, $n_S = 6$, $d = 3$, $m = 1$, the vertices

$$V := R \cup S \cup C = \{1,2,3,4\} \cup \{5,6,7,8,9,10\} \cup \{11,12,13\},$$

and the sizes of color classes are $[4, 6, 3]$ with the partition

$$f := \big\{\{1,2,3,4\}, \{5,6,7,8,9,10\}, \{11,12,13\}\big\}.$$

EXAMPLE 4.7. Let D be the $\mathrm{OA}(6; 3^1 \cdot 2^2; 1)$

$$\begin{bmatrix} 0 & 0 & 1 & 1 & 2 & 2 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}^T.$$

Then $N = 6$, $n_S = 7$, $d = 3$, $m = 2$, and the vertices

$$V = R \cup S \cup C = \{1, 2, \ldots, 6, 7, \ldots 13, 14, 15, 16\}.$$

The color classes have sizes 6, 7, 1, 2, with corresponding vertices

$$f := \big\{\{1, 2, 3, 4, 5, 6\}, \{7, 8, 9, 10, 11, 12, 13\}, \{14\}, \{15, 16\}\big\}.$$

The symbol permutation (0,1) on column 2 of array D is performed by its corresponding permutation $p_S = (10, 11)$ on symbol-vertices 10, 11 of the colored graph G_D. Switching columns 2 and 3 of D has counterpart $p_C = (15, 16)$ on column-vertices. And permuting rows 1 and 2 can be done by the permutations on row-vertices $p_R = (1, 2)$.

Denoting $\mathcal{G}$ the *set of all colored graphs*, we define the map

$$\Phi : \mathcal{F}_{U,N} \to \mathcal{G}, \quad D \mapsto \Phi(D) = G_D,$$

taking an array D to the corresponding colored graph G_D described above.

LEMMA 36. *Φ is an injection.*

PROOF. Notice that the numbering of vertices of G_D does not depend on D but on the design type U and the run size N. So if $F \neq D$ are two distinct arrays, then they must differ at some entry $[i, j]$, hence their adjacencies are different. □

Now we characterize more clearly the image $\Phi(\mathcal{F}_{U,N}) \subseteq \mathcal{G}$. We write $v(u)$ for the valency of a vertex $u \in V$. Recall that $S = Q_1 \cup Q_2 \cup \ldots \cup Q_d$, where $|Q_i| = r_i$ for $i = 1, \ldots, d$; and $C = C_1 \cup \ldots \cup C_m$, where $|C_k| = a_k$, for $k = 1, \ldots, m$.

LEMMA 37. *Let D be an orthogonal array with factors Q_i and with run size N. Then*

(1) G_D is tripartite with the vertex partition (R, S, C) given by (4.3.1) and with $|R| = N$, $|S| = \sum_{k=1}^{m} a_k s_k$, $|C| = \sum_{k=1}^{m} a_k$.
(2) Every vertex $r \in R$ has valency d.
(3) The valency of a column-vertex c in C is s_k, where k is the unique element of $\{1, \ldots, m\}$ such that $c \in C_k$.
(4) The valency of a symbol-vertex: if $s \in S$ then there is a unique $c \in C_k$ such that $\{s, c\} \in E$ for some $k \in \{1, \ldots, m\}$; then

$$v(s) = \frac{N}{v(c)} + 1 = \frac{N}{s_k} + 1$$

[since $t \geq 1$, there are exactly $\frac{N}{s_k}$ rows in array D which have symbol s in column c].
(5) Relationship between R and C: if $r \in R$, and $c \in C$, there exists a unique shortest path of length 2 from r to c through a vertex in S.

DEFINITION 38.

(i) *Given parameters U, N, the colored graphs which satisfy properties* (1)−(5) *of Lemma 37 are called the* colored graphs of type U, N. *They form a subset of $\mathcal{G}$, written $\mathcal{G}_{U,N}$.*
(ii) *By Lemma 37(1), vertices of R, S, C in a graph in $\mathcal{G}_{U,N}$ are called the* row-vertices*, the* symbol-vertices *and the* column-vertices *respectively.*

Demerging a colored graph $g \in \mathcal{G}_{U,N}$. What we want to do now is, firstly, to find the column-vertex set C of g. It may happen that some vertices have the same valency even if they belong to distinct colors (row and column colors, for instance). This can usually be solved by computing the intersection of their neighbor sets. More precisely,

LEMMA 39. *Suppose that $\frac{N}{s_k} \in \mathbb{N}$ for all $k \in \{1, \dots, m\}$, in which case $\frac{N}{s_k} > 1$ for at least one number k. Then, a subset C of the vertex set V of a graph g in $\mathcal{G}_{U,N}$ is the column-vertex set if and only if the valencies of vertices in C are $\{s_1, s_2, \dots, s_m\}$ and their neighbor sets are mutually disjoint subsets of V.*

PROOF. The 'if' is clear by the definition of column-vertex set. Indeed, suppose that C is the column-vertex set of g, for any pair $c_1 \neq c_2 \in C$, we need only check that their neighbors are disjoint, ie, $V(c_1) \cap V(c_2) = \emptyset$. If there is a vertex $s \in V(c_1) \cap V(c_2)$, then $s \notin R$ since g is tripartite, so $s \in S$; Lemma 37(4) implies a contradiction.

Now consider the 'only if' part. Let C be a set of vertices such that their valencies are $s_1, s_2, \dots, s_m$ and their neighbors are mutually disjoint subsets. First they can't be symbol vertices (having nonempty intersections). If there is least one number $\frac{N}{s_k} > 1$, then the neighbors of some pair of row vertices must intersect in a nonempty set. Therefore, C consists only of column vertices. $\square$

EXAMPLE 4.8. The example below is a strength 1 array $F := \mathrm{OA}(4; 4^4; 1)$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 \\ 3 & 3 & 3 & 3 \end{bmatrix}$$

in which $\frac{N}{s_1} = 1$. The row and column vertices of the colored graph G_F are not distinguishable. We will see later that this kind of array requires a subtle treatment to demerge the colored graph.

PROPOSITION 40 (Constructing an array from a colored graph). *Given parameters $U = s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}$ and run size N, such that $\frac{N}{s_k} \in \mathbb{N}$ for all $k \in \{1, \dots, m\}$, and such that there is at least one k for which $\frac{N}{s_k} > 1$, we have*

$$\Phi(\mathcal{F}_{U,N}) = \mathcal{G}_{U,N}.$$

PROOF. We pick a colored graph $g \in \mathcal{G}_{U,N}$. Then g fulfills properties $(1) - (5)$ of Lemma 37. We construct an array $F_g \in \mathcal{F}_{U,N}$ such that $\Phi(F_g) = g$. The process of constructing F_g starts from column-vertices, then locates symbol-vertices, and finally determines row-vertices.

Suppose that $g = (V, E)$. We collect vertices in V that have valencies s_1, s_2, $\dots, s_m$ such that their neighbors are mutually disjoint subsets of V. From Lemma 39, these vertices are uniquely determined and they form column vertices of g. Let C be the set of these column-vertices. For each $c \in C$, we track its neighbors by property 3 of Lemma 37. That is, if $c \in C_k$ for some $k = 1, \dots, m$, then c is adjacent with vertices $V(c) := \{v_1, \dots, v_{s_k}\}$; where $v_i \in V \setminus (C \cup R)$ since g is tripartite and satisfies properties (3) and (5) of Lemma 37. So v_i are symbol-vertices.

Having obtained symbol-vertices $V(c) = \{v_i\}$, we determine the neighbors of each v_i. Only one of them is c, the rest must be the row-vertices, and there are precisely $\frac{N}{s_k}$ such vertices, by properties (4) and (5) of Lemma 37. Each of those row-vertices consist of the same symbol v_i on column c. In this way we can locate all row-vertices together with their neighbors.

Obtaining all row-vertices, we can form the array F_g provided that the neighbors of column-vertices in C have to be numbered increasingly. Hence, $g = \Phi(F_g)$ is in $\Phi(\mathcal{F}_{U,N})$, and $\mathcal{G}_{U,N} \subseteq \Phi(\mathcal{F}_{U,N})$.

On the other hand, by Definition 38(i), it is clear that $\Phi(\mathcal{F}_{U,N}) \subseteq \mathcal{G}_{U,N}$. Hence, $\Phi(\mathcal{F}_{U,N}) = \mathcal{G}_{U,N}$. □

COROLLARY 41. *Provided that $\frac{N}{s_k} \in \mathbb{Z}^\times$ for all $k \in \{1, \dots, m\}$, and that there is at least a number $\frac{N}{s_k} > 1$, with Lemma 36, we have the mapping Φ is a bijection between the set $\mathcal{F}_{U,N}$ of fractions of type U, N and the set $\mathcal{G}_{U,N}$ of colored graphs of type U, N.*

The inverse mapping Φ^{-1} from $\mathcal{G}_{U,N}$ to $\mathcal{F}_{U,N}$ is called the *demerging mapping* of $\mathcal{G}_{U,N}$. Any orthogonal array $D \in \mathcal{F}_{U,N}$ of strength $t \geq 2$ is determined uniquely by its companion graph $G_D \in \mathcal{G}_{U,N}$. Indeed, if strength $t \geq 2$ then $\frac{N}{s_i s_k} \geq 1$ for all $i, k = 1, \dots, m$. So $\frac{N}{s_k} > 1$ for $k = 1, \dots, m$.

LEMMA 42. *Let G_F, G_D be the two colored graphs which are formed by two fractions $F, D \in \mathcal{F} = \mathcal{F}_{U,N}$. Then F and D are isomorphic arrays if and only if G_F and G_D are isomorphic graphs.*

PROOF. If F and D are isomorphic arrays then $D = F^p$ for some permutation p. Now p is a product of a row permutation p_r, a symbol permutation p_s and a column permutation p_c. These permutations induce permutations p_R, p_S and p_C respectively on the disjoint sets R, S and C of vertices. Putting $p^* = p_R\, p_S\, p_C$, we have $G_F^{p^*} = \Phi(F^p) = \Phi(D) = G_D$. It follows that G_F, and G_D are two isomorphic graphs.

The 'only if' part can be seen as follows. If G_F and G_D are isomorphic graphs, we can find a permutation q on vertices (of G_F) such that $G_D = G_F^q$. Now since $G_F, G_D \in \mathcal{G}_{U,N}$, the graphs G_F, G_D satisfy all the conditions in Lemma 37. So they are tripartite and q is a color-preserving permutation. This permutation therefore can be factored as a product of three permutations q_R, q_S, q_C which act on row, symbol and column vertices of G_F independently. Since the numbering of vertices in G_F and G_D are the same, the triple q_R, q_S, q_C induce row, symbol and column permutations q_r, q_s, q_c acting on F. The composed map $q_r\, q_s\, q_c$ takes F to D. □

EXAMPLE 4.9. We construct an OA$(6; 3{\cdot}2^2; 1)$ from the colored graph described by Figure 4.1. Here $m = 2, d = 3, s_1 = 3, s_2 = 2$, the column vertex set $C = \{14, 15, 16\}$ since their neighbor sets $\{7, 8, 9\}, \{10, 12\}$, and $\{11, 13\}$ are mutually disjoint. Vertices $1, 2, \dots 6$, for instance, also have valency 3, but they cannot represent the first column-vertex (3-level column) since their neighbors are not disjoint. Now the first column-vertex is 14, its neighbor $V(14) = \{7, 8, 9\}$ (represent levels 0,1,2 in column 1) lead us to row-vertices 1,2; 3,5 and 4,6 respectively. The symbol vertices are $[[7, 8, 9], [10, 12], [11, 13]]$; those correspond to levels 0,1,2 in column 1, levels 0,1 in column 2 and levels 0,1 in column 3 of F. The array

TABLE 4.1. A counterexample in constructing OA from colored graph

1	:	5	9	13	17
2	:	6	10	14	18
3	:	7	11	15	19
4	:	8	12	16	20
5	:	1	21		
6	:	2	21		
7	:	3	21		
8	:	4	21		
9	:	1	22		
10	:	2	22		
11	:	3	22		
12	:	4	22		
13	:	1	23		
14	:	2	23		
15	:	3	23		
16	:	4	23		
17	:	1	24		
18	:	2	24		
19	:	3	24		
20	:	4	24		
21	:	5	6	7	8
22	:	9	10	11	12
23	:	13	14	15	16
24	:	17	18	19	20

obtained is

$$F = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 0 \\ 2 & 0 & 0 \\ 1 & 1 & 1 \\ 2 & 1 & 1 \end{bmatrix}$$

EXAMPLE 4.10 (counterexample, cf. Example 4.8). We wish to construct an $\mathrm{OA}(4; 4^4; 1)$ from the colored graph with adjacencies as in Table 4.1. Notice that $\frac{N}{s_1} = 4/4 = 1$, so we cannot distinguish between column-vertices and row-vertices. In other words, there are two candidate sets for column-vertices, $\{21, 22, 23, 24\}$ and $\{1, 2, 3, 4\}$. If we choose the first candidate to be column vertex set, then the latter will be row vertex set, and vice versa. Hence, the partition (R, S, C) is not determined uniquely by the colored graph. If we take $\{21, 22, 23, 24\}$ as the column-vertices, and take the partition

$$f = \big\{\{1, 2, 3, 4\}, \{5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20\}, \{21, 22, 23, 24\}\big\}$$

then the result obtained is the array in Example 4.8.

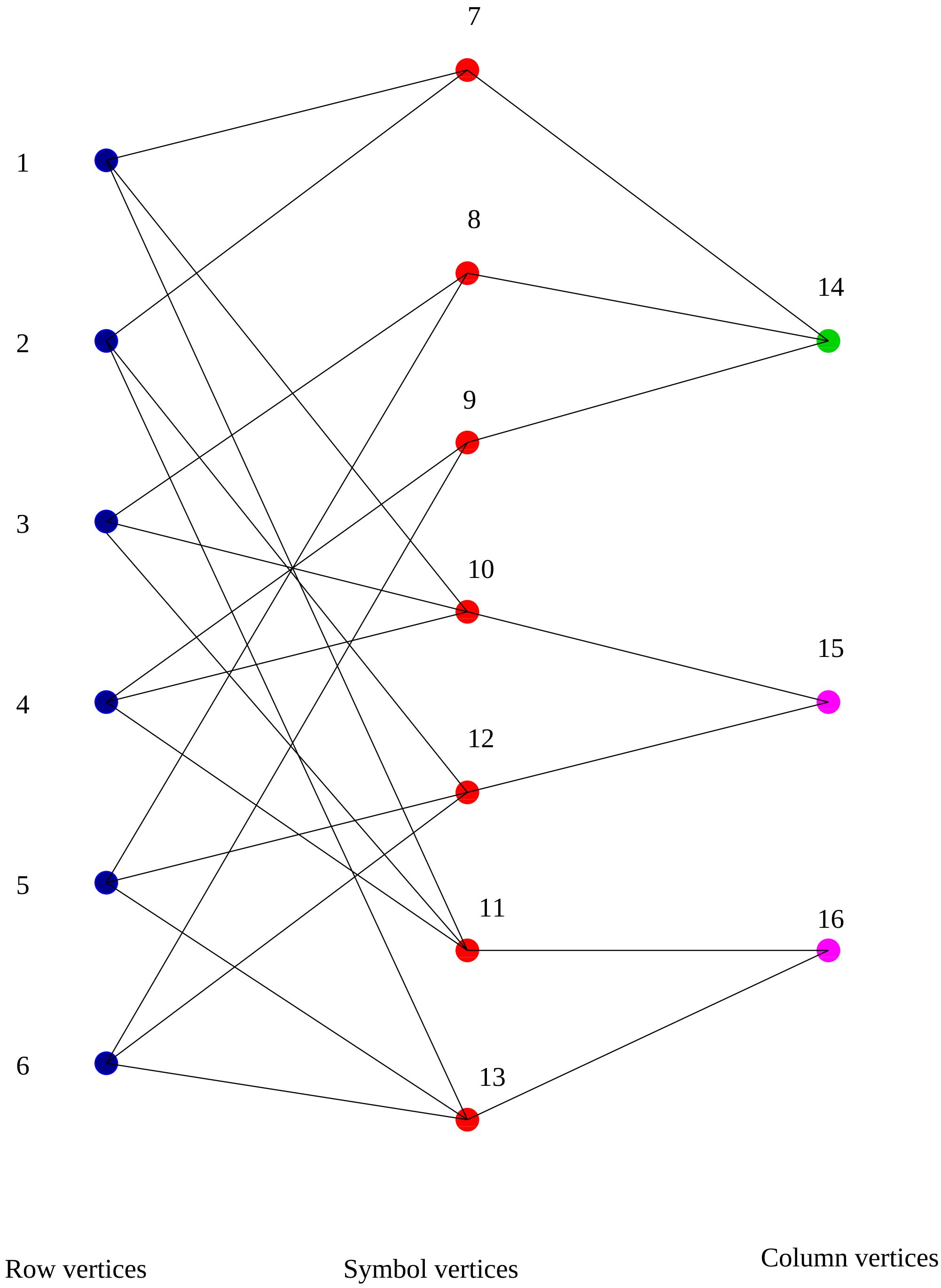

FIGURE 4.1. The colored graph of a 6 runs OA

Finding the canonical graph. For any colored graph G, denote by $\mathrm{canon}(G)$ the *canonical labeling graph* computed using *nauty*. It consists of a vertex relabeling permutation, p, say and new adjacencies. Hence, $\mathrm{canon}(G)$ is determined fully by these adjacencies.

The vertex-relabeling p is of the form

$$p = p_R\ p_S\ p_{C_1}\ p_{C_2} \cdots p_{C_m},$$

where $p_R, p_S, p_{C_1}, p_{C_2}, \ldots, p_{C_m}$ are permutations on the subsets $R, S, C_1, C_2, \ldots, C_m$ respectively. Indeed this fact follows from the requirement of preserving $m+2$ color classes that we input to the *nauty* computation.

Let $G_F := \Phi(F)$ and $G_D := \Phi(D)$ be the colored graphs of arrays F and D respectively. As a result of Lemma 42, we have

COROLLARY 43. *F and D are isomorphic arrays* $\iff$ $\mathrm{canon}(G_F) = \mathrm{canon}(G_D)$.

Notice that if $G \in \mathcal{G}_{U,N}$ then $\mathrm{canon}(G) \in \mathcal{G}_{U,N}$. Let D^* be the *canonical labeling orthogonal array* of an orthogonal array D. Then $G_D \in \mathcal{G}_{U,N}$, and $G_{D^*} \in \mathcal{G}_{U,N}$. Now D^* can be constructed using the scheme below:

$$D \to G_D \to \mathrm{canon}(G_D) \to D^*,$$

in which the first arrow represents the mapping Φ. The third arrow computing D^*, is done by the demerging map Φ^{-1}. For orthogonal arrays of strength $t \geq 2$, the canonical array D^* is uniquely determined by $\mathrm{canon}(G_D)$.

Computing canonical orthogonal array D^*. We may build the orthogonal array D^* from the adjacencies of the graph $\mathrm{canon}(G_D)$ that came from *nauty*. Since the relabeling permutation p preserves color classes, we do not need to rearrange vertices in the canonical graph $\mathrm{canon}(G_D)$. We can apply the demerging scheme (using the demerging mapping). But if we list adjacencies of vertices in G_D in the order: rows R, symbols S, columns C, then we can also do the following:

- Locate column-vertices: Column-vertices in $\mathrm{canon}(G)$, denoted by Cv, occupy rows from $N + n_S + 1$ to $n := |V|$ of B;
- specify row-vertices: row-vertices occupy rows from 1 to N;
- from row-vertices we are able to build up the array D^* row by row by tracking the symbol-vertices which are listed in the corresponding row. Notice that levels of each column must be numbered in the decreasing order, but not necessarily between columns.

EXAMPLE 4.11. Let D be an $\mathrm{OA}(16; 4^1 \cdot 2^2; 2)$.

$$D = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}^T$$

Then $N = 16$, $n_S = 8$, $d = 3$, $m = 2$, the vertices

$$V = R \cup S \cup C = \big\{\{1, 2, \ldots, 15, 16\}, \{17, \ldots 20, 21, 22, 23, 24\}, \{25, 26, 27\}\big\}.$$

The color classes have sizes 16, 8, 1, 2, with the corresponding vertices

$$f := \big\{\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16\},$$
$$\{17, 18, 19, 20, 21, 22, 23, 24\}, \{25\}, \{26, 27\}\big\}.$$

The relabeling permutation is

$$p = (2, 3)(6, 9, 7, 13, 14, 8)(10, 11, 15, 12)(22, 23, 24),$$

the column vertices $Cv = [25, 26, 27]$, and the symbol-vertices

$$Sv = \big[[17, 18, 19, 20], [21, 22], [23, 24]\big].$$

For the row $u = [17, 22, 24]$, we refer to symbol-vertices, ie, symbols 0 in column 1, symbol 1 in column 2, and symbol 1 in column 3. We get back its companion run $[0, 1, 1] \in D^*$. The new adjacencies of the canonical graph are given in Table 4.2.

TABLE 4.2. Adjacency relations of a colored graph

17	21	22						
17	22	24						
17	21	23						
17	23	24						
18	21	22						
19	21	22						
20	21	22						
18	21	23						
18	22	24						
19	22	24						
20	22	24						
19	21	23						
20	21	23						
18	23	24						
19	23	24						
20	23	24						
1	2	3	4	25				
5	8	9	14	25				
6	10	12	15	25				
7	11	13	16	25				
1	3	5	6	7	8	12	13	26
1	2	5	6	7	9	10	11	27
3	4	8	12	13	14	15	16	27
2	4	9	10	11	14	15	16	26
17	18	19	20					
21	24							
22	23							

4.4. Finding lexicographically-least $\mathrm{OA}(N; s_1^a \cdot s_2^b; t)$

In this part, we consider a specific class of designs $\mathcal{F}$ having two sections. That means its design type is $U = s_1^a \cdot s_2^b$, and its fractions F have run size N for suitable N. Recall that for $1 \le j \le a + b =: d$, r_j is the number of symbols of the jth column. That is $r_j = s_1$ for $1 \le j \le a$, and $r_j = s_2$ for $a+1 \le j \le a+b$. Recall that $\boldsymbol{p} = (p_1, p_2 \dots p_j, \dots, p_d)$ is an arbitrary run in F, and that G is the full group of fraction transformations. We fix the notation $G, U, N, F^G, \mathcal{F}, R, C, L, m, d, r_j$ for the remainder of this section. Here F^G is the G-orbit of a fraction F.

Definition 44 (Column lexicographically-least fractions).

- *For two vectors u and v of length N, we say u is lexicographically less than v, written $u < v$, if there exists an index $j = 1, \dots, N-1$ such that $u[i] = v[i]$ for all $1 \le i \le j$ and $u[j+1] < v[j+1]$.*
- *Let $F = [c_1, \dots, c_d]$, $F' = [c'_1, \dots, c'_d]$ be any pair of fractions where c_i, c'_i are columns. We say F is column-lexicographically less than F', written $F < F'$, if and only if there exists an index $j \in \{1, \dots, d-1\}$ such that $c_i = c'_i$ for all $1 \le i \le j$ and $c_{j+1} < c'_{j+1}$ lexicographically.*
- *Fix $F \in \mathcal{F}$. The fraction F_0 which is smallest with respect to the column-lexicographical ordering in the orbit F^H for some subgroup H of G is called the H-lexicographically-least fraction, denoted $\mathrm{LLF}_H(F)$.*
- *If H is a subset of G then $\mathrm{LLF}_H(F)$ is defined to be the smallest fraction (with respect to the column-lexicographical ordering) in the image set $\{F^h : h \in H\}$.*
- *We call the G-lexicographically-least fraction of F its* lexicographical-least fraction, *and denote it by $\mathrm{NF}(F)$.*

We use a backtrack search to list all fractions $\mathrm{NF}(F) \in \mathcal{F}$. We start with a description of the problem in graph language and we conclude with an algorithm which is presented by a pseudo-pascal description.

Definition 45.

(1) *For $1 \le i \le N$, $1 \le j \le d$, denote by F_{ij} the subset of entries of a putative fraction F consisting of $j-1$ columns completely made, and column j built only to row i. We call it a partial fraction up to the jth column and up to the ith row. For convenience, let $F_{0,0}$ be the empty fraction.*
(2) *A full-partial fraction, denoted F_j, of a putative fraction F, is a partial fraction $F_{N,j}$. So the first j columns have been built, for $j = 1, 2, \dots, d$.*
(3) *In a partial fraction F_{ij}, a hth row $F_{ij}[h, -] = (p_1, p_2, \dots, p_j)$, for $h = 1, \dots, i$, is called a partial row, where $1 \le p_l \le r_l$ for $l = 1, \dots, j$.*

Notice that $F_{N,j}$ has strength $\min(j, t)$. So F_d is the fraction that we want to make. We visualize each partial fraction F_{ij} by a vertically colored leaf, (ie, a leaf composed of N *stripes*, colored up to ith stripe) in the jth layer of a rooted tree, denoted by T. The depth of T equals to the number of columns d. So the root of T is F_{00}, and full-partial fractions F_j are leaves of T at the layer for which the distance from the root is j.

For example, let $U := 4^1 \cdot 2^3$, $N = 16$; $i = 5$, $j = 4$. Then F_{54} is given below, where the symbol x indicates symbols that have not yet been found. A partial row in F_{54} is $F_{54}[3,-] = 0101$.

$$F_{54} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & x & x & x & x & x & x & x & x & x & x & x \end{bmatrix}^T$$

The basic idea is to extend column by column from full-partial fractions having $j-1$ columns (ie, completely colored leaves in a built $(j-1)$th layer of the search tree), for each $j = t+1, \ldots, d$. Each column is built by adding symbols one by one and counting corresponding frequencies. Whenever a symbol is added, a (partial) row is formed. During this process, looking at a particular leaf F_{ij} of a jth layer (being built), two possibilities occur:

(1) the orthogonality (strength 3 condition) is violated, because some t-tuples have exceeded the allowed frequency for some $i < N$; then the whole subtree from that leaf is discarded;
(2) the number of (partial) rows i reach the run size N, that is N stripes of that leaf have been fully colored. We start to build a new column (or return that leaf) if the current full-partial fraction is already lexicographical-least. Otherwise, the whole subtree from that leaf is discarded.

The problem now is reduced to determining all *fully colored leaves* which have distance d from the root.

REMARK 4.2. *Up to the first t columns, T has only one leaf for each layer.*

EXAMPLE 4.12. Find $F = \mathrm{OA}(16; 4^1 \cdot 2^3; 3)$. In the first four layers, including the root, of the tree T, there is only one leaf. Let us build F step by step.
Layer 0: $F_{0,0} = []$.
Layers 1,2,3: Columns 1,2,3 are made trivially.
Layer 4: A (4,2,2)-triple occurs once, and a (2,2,2)-triple occurs twice, so there is only one possibility for building the leaf $F_{16,4}$ in this layer. This gives a unique solution for this design, given by (4.4.1).

$$F = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \end{bmatrix}^T \tag{4.4.1}$$

This example reveals that there are two possibilities in making F_{ij}.

(i) At each layer $j = t+1, \ldots, d$ and at each (partial) row i, there exists a unique symbol for entry $F[i,j]$ (as in previous example). In this case we get a unique solution.
(ii) There exist at least two symbols for entry $F[i,j]$, for some $j \in \{t+1, \ldots, d\}$ and some $i \in \{2, \ldots, N\}$.

Furthermore, at some layer, a leaf can be split several times.

DEFINITION 46. *Let $n_{i,j} \geq 1$ be the number of symbols that can be plugged into position $F[i,j]$, and let $X_{i,j} = \{x_1, x_2, \ldots, x_{n_{i,j}}\}$ be the set of these symbols, for*

$1 \le i \le N$, $1 \le j \le d$. *At the first jth layer of the tree T such that there exist a row-index i and $n_{i,j} \ge 2$, we create a stack*

$$\text{Branches}(T) := \Big[J := [(i, x_l); j] : x_l \in X_{i,j}\Big].$$

We call (i, j) a branching point*, and each $J \in$ Branches(T) a* branching leaf *at layer j having symbol x_l at row i.*

Branches(T) is declared globally to store branching leaves during depth-first search. The general strategy is: if we find a branching point, then we add branching leaves to the stack, and follow one of these ramifying leaves. Then either new branching points are found and their branching leaves are updated into Branches(T); or rows can be formed without extending Branches(T) until the whole column has been built. More clearly, during branching at layer j on each leaf $J := [(i, x_l); j]$, if we detect another row-index i_2 such that $n_{i_2,j} \ge 2$, then we replace J in Branches(T) by $n_{i_2,j}$ new branching leaves of the form $[(i, x_l), (i_2, y_k); j]$ where $y_k \in X_{i_2,j} \ldots$ Whenever a leaf F_j in layer j is fully colored, we call that leaf *inspected*. Then we delete the corresponding branching leaf in Branches(T) (not in tree T), and start forming column $j + 1$ from F_j. Hence Branches(T) can consist of branching leaves on distinct layers.

At the first t layers (see Remark 4.2) where branching happens at row i, we initialize

$$\text{Branches}(T) := \Big[J = \big[(i, x_l); j\big] : x_l \in X_{i,j} \text{ and } 1 \le j \le t\Big].$$

From then, the stack Branches(T) may be updated several times: adding new branching leaves (simultaneously with dropping out their father-leaf), and/or deleting its last entry whenever that leaf was inspected. We continue like that until Branches(T) is empty, then all branching points in the search tree have been inspected already. Furthermore, if all fully colored leaves in layer d are lexicographically least in their isomorphic class, then they form the set of all solutions that we want. Indeed, we have

PROPOSITION 47. *For $j = t + 1, \ldots, d$, a* fully colored leaf *$F_{N,j}$ in the layer j is lex-least in its isomorphic class, if we follow the two following operations during constructing $F[-, j]$:*

1. *For any pair of adjacent partial rows, u and v, say, of $F_{N,j}$, where the jth column $F[-, j]$ has not been formed yet from row v, we choose $v[j] \in \{v[j-1], \ldots, r_j\}$ if $u[k] = v[k]$ for all $1 \le k \le j - 1$, otherwise we choose $v[j] \in \{1, \ldots, r_j\}$.*
2. *When column $F[-, j]$ is formed completely, ie, $F_{N,j}$ is made, we permute this column with each of the previous columns (with the same number of levels) and sort rows of the resulting fraction.*
   If the sorted fraction is lexicographically less than $F_{N,j}$ then we discard $F_{N,j}$, (subtree from that leaf has no descendant on layer d); otherwise we accept $F_{N,j}$.

PROOF. Operation 1. makes sure that column $F[-, j]$ is lex least in all candidates for column j up to row and level permutations. Then Operation 2. assures that $F_{N,j}$ which passed through the test of permuting columns and rows is really the smallest in its its isomorphic class. $\square$

If employ these operations, we have

COROLLARY 48.

1. *A solution $F_{N,d}$, ie, a fully-colored leaf at layer d in T, is the lexicographically least fraction in its isomorphic class.*
2. *The set of all fully-colored leaves at layer d in the search tree T gives us all non-isomorphic fractions.*

PROOF. Using Proposition 47 with $j = d$ tells us that Assertion 1. is correct. Now suppose that there are two distinct fully-colored leaves at layer d in T, say F, K, which are isomorphic, and $F < K$. It implies that there is a non-trivial permutation p such that $K^p = F$. By Assertion 1., $K < K^p$, so $F < K^p$, contradiction. Assertion 2. follows. □

To formulate the backtrack algorithm computing all non-isomorphic fractions we use the procedure EXTEND-COLUMN below that extends a column from a fully determined fraction.

Algorithm 2 Backtrack algorithm extends a column

Input: F_{j-1} a fully-colored leaf in layer $j-1$ and
Branches(T), the global stack of branching points.
Output: A fully-colored leaf F_j in layer j.

function EXTEND-COLUMN(F_{j-1}, Branches(T)))
    Compute $n_{i,j}$,
        ▷ # symbols which can be plugged into $F[i, j]$, Definition 46
    if $\exists i : n_{i,j} \geq 2$ **then**
        ▷ detect feasible branching points
        split the leaf F_{j-1} into $n_{i,j}$ branches
            ▷ where the newly-formed leaves are different only at entry $F[i, j]$
        add to Branches(T) leaves $J = [(i, x_l); j]$ in which $x_l \in X_{i,j}$
    else
        form a unique leaf $F[i, j]$ at layer j
    end if
        ▷ depth-first form column j
    repeat
        build up (rows of) each of leaves in layer j from the row $i + 1$
        update Branches(T) during the process
    until $i = N$,
        ▷ a fully-colored leaf F_j in the layer j has been made
    Return F_j
        ▷ see Definition 45(2)
end function

Using this procedure we extend the tree T from a fully-colored leaf, until the number of columns j meets d. We record that solution, go back to the nearest branching point of that solution (ie, its parent), and try its next sibling. These tasks are described in the following algorithm LEX-LEAST-FRACTIONs.

Algorithm 3 Backtrack algorithm computes all non-isomorphic fractions

Input: Design type U, run size N, and strength t.
Output: All non-isomorphic fractions $\mathrm{NF}(F) \in \mathcal{F}$.

function LEX-LEAST-FRACTIONS(U, N, t)
  Initialize a rooted tree T having $t+1$ layers,
  ▷ each layer has only one leaf
  Let F_t denote the leaf at layer $(t+1)$
  ▷ it has t columns
  Let $j := t+1$; Branches(T) := [] (global variable); $K := F_t$;
  while Branches(T) $\neq$ [ ] or $j < d$ **do**
    Compute $K :=$ EXTEND-COLUMN(K, Branches(T))
    if K is at distance d to root of T **then**
      record K as a solution on T;
    end if
  end while
  Return all leaves at layer d of the tree T.
end function

Note that this algorithm could be generalized to more than two section fractions. However, our C code [Brouwer, 2003] presently deals with two section fractions only.

4.5. Use of integer linear programming and symmetry

In this section, we formulate necessary algebraic conditions for the existence of a new factor X in the extension problem of orthogonal arrays.

An algebraic formulation of the problem. Let $F = \mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; 3)$ be a known array having columns $S_1, \ldots, S_d$, in which S_i has r_i levels ($i = 1, \ldots, d$). An s-level factor X is orthogonal to a known factor S_i, denoted as $X \perp S_i$, if the frequency of every symbol pair $(a, x) \in [S_i, X]$ in $\mathrm{OA}(N; r_1 \cdots r_d \cdot s; 3)$ is $N/(r_i s)$. We say X is orthogonal to a pair of known factors S_i, S_j, written $X \perp [S_i, S_j]$, if the frequency of all tuples $(a, b, x) \in [S_i, S_j, X]$ is $N/(r_i r_j s)$. Extending F by X means constructing an $\mathrm{OA}(N; r_1 \cdots r_d \cdot s; 3)$, denoted by $[F|X]$. By the definition of orthogonal arrays, $[F|X]$ exists if and only if X is orthogonal to any pair of columns of F.

OBSERVATION 1 (Transformation rules). We can find a set of necessary constraints P for the existence of $[F|X]$ in terms of polynomials in the coordinate indeterminates of X by: a) calculating frequencies of 3-tuples, locating positions of symbol pairs of (S_i, S_j); and b) equating the sums of coordinate indeterminates of X (corresponding to these positions) to the product of those frequencies with the constant $0 + 1 + 2 + \ldots + s - 1 = \frac{s(s-1)}{2}$.

The number of equations of the system P then is $\sum_{i\neq j}^{d} r_i r_j$, since each pair of factors (S_i, S_j) can be coded by a new factor having $r_i r_j$ levels. When $s = 2$, the constraints P are in fact the sufficient conditions for the existence of X.

EXAMPLE 4.13. Let $F = \mathrm{OA}(16; 4 \cdot 2^2; 3) = [S_1|S_2|S_3]$:

$$F = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}^T.$$

We form a set of constraints P for the extension of F to $D = [F|X] = \mathrm{OA}(16; 4 \cdot 2^3; 3)$, where $X := [x_1, x_2, \ldots, x_{16}]$ is a binary factor ($x_i = 0, 1$). First of all, the system P of linear equations for computing X has $\sum_{i\neq j}^{3} r_i r_j = 2(4 \cdot 2) + 2 \cdot 2 = 16 + 4 = 20$ equations. The frequency of each tuple (a, b, x) in $S_1 \times S_2 \times X$ and $S_1 \times S_3 \times X$ is $\lambda = 1$; that of each tuple $(b, c, x) \in S_2 \times S_3 \times X$ is $\mu = 2$. The pair $[S_1, S_2]$ is coded by an 8-level factor, Y, say; and the pair $[S_2, S_3]$ by a 4-level factor, Z, say. The positions of the pair $[0, 0] \in S_1 \times S_2$ are 1,2; ..., of $[3, 1] \in S_1 \times S_2$ are 15,16. The positions of the pair $[1, 1] \in S_2 \times S_3$ are 4,8,12,16 ... Step a) of Observation 1 is applied. In Step b), the sums of coordinates of X corresponding to the Y symbols and the Z symbols must equal a multiple of the appropriate frequencies. That means: $X \perp [S_1, S_2]$ iff $X \perp Y$ iff $x_1 + x_2 = x_3 + x_4 = \ldots = x_{15} + x_{16} = \lambda \cdot (0 + 1) = 1, \ldots$ and $X \perp [S_2, S_3]$ iff $X \perp Z$ iff $x_1 + x_5 + x_9 + x_{13} = \ldots = x_4 + x_8 + x_{12} + x_{16} = \mu \cdot (0 + 1) = 2$. One solution of P is given in the last row of the matrix below:

$$\left[\begin{array}{cccccccccccccccc} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ \hline 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \end{array}\right]$$

REMARK 4.3. Although the constancy of frequencies is a necessary and sufficient condition (by definition) for the existence of X, we observe that the linear constraints P found using rules of Observation 1 forms a set of necessary conditions.

For instance, appending a blocking factor X (see the definition in Section 5.4) with 4 levels to an array $\mathrm{OA}(16; 4 \cdot 2^3; 3)$ means constructing an $\mathrm{OA}(16; 4 \cdot 2^3 \cdot 4; 2)$. We have $s = 4$, X is orthogonal to S_1 if and only if each pair $(a, x) \in [S_1, X]$ occurs once ($\frac{16}{4 \cdot 4} = 1$). This implies that $x_1 + x_2 + x_3 + x_4 = 1 \cdot (0 + 1 + 2 + 3) = 6$, $x_i \in \{0, 1, 2, 3\}$. Of the two possibilities $[0, 1, 2, 3]$ and $[0, 3, 0, 3]$ only the first is valid, the second is discarded since the frequencies of 0 and 3 are 2 in $\mathrm{OA}(16; 4 \cdot 4; 2)$, which is prohibited.

Generic approach solves the extension problem using canonical orthogonal arrays. We now consider extending strength 3 OAs. Let $m_1 := \sum_{i\neq j}^{d} r_i r_j$ be the number of equations in P. Then the system P of linear equations with integer coefficients can be described by the matrix equation

$$AX = b,$$

in which $A \in \mathrm{Mat}_{m_1,N}(\mathbb{N})$, $b \in \mathbb{N}^{m_1}$, and

$$X = (x_1, \ldots, x_N) \in \{0, 1, \ldots, s - 1\}^N \subseteq \mathbb{N}^N \tag{4.5.1}$$

is a variable vector. The vector b is formed by counting frequencies of triples involving two known columns in F and the unknown column X as in Observation

1. Since each orthogonal array is isomorphic to an array having the first row zero, we let $x_1 = 0$ throughout. By Gaussian elimination, we get the reduced system

$$M\,X = c, \tag{4.5.2}$$

in which $M \in \mathrm{Mat}_{m,N}(\mathbb{Z})$, $c \in \mathbb{Z}^m$, and $X = (0, x_2, \ldots, x_N) \in \mathbb{Z}^N$.

Our general approach to solving the extension problem consists of iterations of the following 3 steps:

(1) build the system (4.5.2) using Observation 1;
(2) find all solution vectors $X = (x_1, \ldots, x_N)$ in $\{0, 1, 2, \ldots, s-1\}^N$;
(3) collect non-isomorphic, canonical orthogonal arrays of the set of all arrays $[F|X]$ into a set L; if L is empty, conclude F has no extension; otherwise go back to Step 1 for each array in L until the number of factors meets the number of columns required.

The first step is already done. The method to solve the last step was given in Section 4.3. What we need to find in Step 2, in fact, are the non-isomorphic vectors X (under row-index permutations) in the whole solution set. We show how to find them in the next sections. We then discuss how to combine the automorphism group $\mathrm{Aut}(F)$ of F in finding non-isomorphic vectors X. Notice that, when extending OAs, the group size tends to grow proportionally with the number of solutions.

Another backtrack approach. The system P described by (4.5.2) can be solved over $\mathbb{N}_{\geq 0}$ by depth-first branching at the variables x_i ($i = 2, \ldots, N$). If P has no solution, then F is not extendable; we try another array having the same parameters as F but not isomorphic to F. We identify P with its polynomials, ie, $P = \{f_1, f_2, \ldots, f_m\}$, in which the f_i are linear polynomials in the indeterminates $x_2, \ldots, x_N$. In particular, when the x_is are binary, we can use the following fact.

Lemma 49 (Finding binary solutions of an integral polynomial). *Let f be an arbitrary polynomial in P, and put the polynomial $p = f \bmod 2$. Denote by V_f, V_p the sets of indeterminates occurring in f and p, respectively. Put $C = V_f \setminus V_p$, $n_f = |V_f|$, $n_p = |V_p|$, $n_C = |C|$. We denote the set of solutions of the equation $f = 0$ by S_f, and the set of solutions of the equation $p = 0 \bmod 2$ by S_p. Let S_p^i be the solution set of the equation $p = i$ for $i = 0, \ldots, n_p$. Then $S_f \subseteq S_p$, and S_p is a disjoint union of $\frac{n_p}{2}$ sets S_p^i, for odd (even) integers $i = 0, \ldots, n_p$ if the constant coefficient of f is odd (even). Moreover, the maximum number of solutions of $f = 0$ is $2^{n_f - 1}$.*

Proof. The first statement is clear. The last follows from the fact that each set S_p^i is precisely the vectors having weight i in the Hamming space $H(n_p, 2)$. □

With this approach, the problem of enumeration of strength 3 OAs can be solved if there are few arrays having one column less. But if N is large, and the system P is symmetric, the branching approach is not strong enough, since there are many isomorphic vector solutions X in each extension. The next subsection deals with these difficulties.

Using the automorphism group to prune the solution set. Suppose that there exists $D := [F|X] = \mathrm{OA}(N; r_1 \cdots r_d \cdot s; t)$, an extension of a known array $F = \mathrm{OA}(N; r_1 \cdots r_d; t)$ by a column X having s levels, where $t \geq 2$. Let $g \in \mathrm{Aut}(F)$. Then g induces a permutation g_1 in the full group G_D of D. Let g_R be the row permutation component of g, then g_R is also the row permutation component of g_1. [Recall from Formula (4.2.9) and Definition 33 that any permutation g acting on F has the decomposition $g = g_R\, g_C\, g_S$ where g_C and g_S are the column and symbol permutations acting on F, respectively].

LEMMA 50. *For $g \in \mathrm{Aut}(F)$, g induces $g_1 \in G_D$ and generates the image D^{g_1} which is isomorphic to D.*

PROOF. We have

$$D^{g_1} = [F|X]^{g_1} = [F^g|X^{g_R}] = [F|X^{g_R}] \tag{4.5.3}$$

since g fixes F, and since only the component g_R really acts on the column X by moving its coordinates. □

Fix $I_N := [1, 2, \ldots, N]$ the row-index list of F, and recall that $r_1 \geq r_2 \geq \ldots \geq r_d$. We explicitly distinguish I_N with $\{1, 2, \ldots, N\}$ for this section.

Localizing the formation of vector solutions X. Let $G := \mathrm{Row}(\mathrm{Aut}(F))$ be the group of all row permutations g_R extracted from the group $\mathrm{Aut}(F)$. We call G the *row permutation group* of F. Then G acts naturally on indices of the vector $X = [x_1, x_2, \ldots, x_N]$. By convention, we say a row permutation $g_R \in G$ *acts fixed-point free*, or globally on X if it moves every indices. Otherwise, we say that g_R *acts locally.*

The first step is to localize the formation of a vector X of the form (4.5.1) by taking the derived designs of strength $t-1$. We get the r_1 derived designs $F_1, \ldots, F_{r_1}$, each of which is an $\mathrm{OA}(r_1^{-1}N; r_2 \cdots r_d; t-1)$. Clearly, if a solution vector X exists, then it is formed by r_1 sub-vectors u_i of length $\frac{N}{r_1}$:

$$X = [u_1; u_2; \ldots; u_{r_1}], \text{ where } u_i = \left(x_{\frac{(i-1)N}{r_1}+1}, \ldots, x_{\frac{iN}{r_1}} \right). \tag{4.5.4}$$

Denote by V_i the set of all sub-vectors u_i which can be added to the ith derived design F_i to form an $\mathrm{OA}(r_1^{-1}N; r_2 \cdots r_d \cdot s; t-1)$. Let $V = V_1 \times V_2 \times \ldots \times V_{r_1}$ (the Cartesian product) and let $\tau := \mathrm{Sym}_s$ be the group of symbol permutations acting on the coordinates of X. A simple way to find all non-isomorphic solution vectors $X \in V$ is: find all candidate sub-vectors $u_i \in V_i$, $i = 1, \ldots, r_1$; discard (prune) them as many as possible by using subgroups of G; plug those u_is together, then find the representatives of the $G \times \tau$-orbits in V. By recursion, the process of building X can be brought back to strength 1 derived designs. We can prune the solution set, denoted $\mathrm{Z}(P)$, from those smallest sub-designs by finding some subgroups of G acting on strength 1 derived designs. Those subgroups must have the property that they act separately on the row-index sets corresponding to the derived designs.

Permutation subgroups associated with the derived designs. Recall that we view $F \in \mathcal{F}$ as an $N \times d$-matrix with the $[l, j]$-entry is written as $F[l, j]$. For each derived design F_i with respect to the first column of F, the row-index set of F_i, denoted by $\mathrm{RowInd}(F_i)$ for $1 \leq i \leq r_1$, is defined as

$$\mathrm{RowInd}(F_i) := \big\{ l \in \{1, 2, \ldots, N\} : F[l, 1] = i \big\}.$$

Define the stabilizer in G of F_i by

$$\begin{aligned} N_G(F_i) &:= \text{Normalizer}\big(G, \text{RowInd}(F_i)\big) \\ &= \big\{h \in G : \text{RowInd}(F_i)^h = \text{RowInd}(F_i)\big\}. \end{aligned} \tag{4.5.5}$$

In this way, we find r_1 subgroups of G corresponding to the derived designs F_i. But it can happen that $\text{RowInd}(F_l)^h \neq \text{RowInd}(F_l)$ for some $h \in N_G(F_i)$ and $0 \le l \neq i \le r_1 - 1$. To make sure that the row permutations act independently on the F_i, we define the group of row permutations acting locally on each F_i as:

$$L(F_i) := \text{Centralizer}\big(N_G(F_i), J(F_i)\big), \tag{4.5.6}$$

where $J(F_i) := I_N \setminus \text{RowInd}(F_i)$ is the sublist of I_N consisting of elements not in $\text{RowInd}(F_i)$. The group $L(F_i)$ acts on the row-indices of F_i and fixes pointwise any row-index outside F_i. We call these subgroups L_i (of G) the *row permutation subgroups associated with strength 2 derived designs* . These subgroups can be determined further as follows.

For an integer $m = 1, \ldots, t-1$ and for $j = 1, 2, \ldots m$, denote by

$$F_{i_1,\ldots,i_m} = \text{OA}\left(\frac{N}{r_1 r_2 \cdots r_m}; r_{m+1} \cdots r_d; t - m\right) \tag{4.5.7}$$

the derived designs of F taken with respect to symbols $i_1, \ldots, i_m$, where symbol i_j in column j and $i_j = 1, \ldots, r_j$. Define the row-index set of $F_{i_1,\ldots,i_m}$ by

$$\text{RowInd}(F_{i_1,\ldots,i_m}) := \bigcap_{j=1}^{m} \big\{l \in \{1, 2, \ldots, N\} : F[l, j] = i_j\big\}. \tag{4.5.8}$$

Let $J(F_{i_1,\ldots,i_m}) := I_N \setminus \text{RowInd}(F_{i_1,\ldots,i_m})$. We define,

$$\begin{aligned} N_G(F_{i_1,\ldots,i_m}) &:= \text{Normalizer}\big(G, \text{RowInd}(F_{i_1,\ldots,i_m})\big), \\ L(F_{i_1,\ldots,i_m}) &:= \text{Centralizer}\big(N_G(F_{i_1,\ldots,i_m}), J(F_i)\big), \text{ for } 1 \le i_j \le r_j. \end{aligned}$$

Definition 51. *$L(F_{i_1,\ldots,i_m})$ is called the subgroup associated with the derived design $F_{i_1,\ldots,i_m}$, for $1 \le i_j \le r_j$, $j = 1, 2, \ldots m$. We say $L(F_{i_1,\ldots,i_m})$ acts locally on the derived design $F_{i_1,\ldots,i_m}$, and write $L_{i_1,\ldots i_m} := L(F_{i_1,\ldots,i_m})$ if no ambiguity occurs.*

For $t = 3$, we compute these subgroups for $m = 1$ and $m = 2$. For $m = 1$, we have s_1 subgroups $L(F_i)$ acting locally on strength 2 derived designs; and for $m = 2$, we have $s_1 s_2$ subgroups $L(F_{i,j})$ acting locally on strength 1 derived designs.

Using the subgroups $L_{i_1,\ldots,i_m}$. Recall that $\mathrm{Z}(P)$ is the set of all solutions X. From (4.5.3), the vector X^g can be pruned from $\mathrm{Z}(P)$, for any solution X and any permutation $g \in \text{Aut}(F)$. This follows from the fact that D^g is an isomorphic array of $D = [F|X]$. For a fixed m-tuple of symbols $i_1, \ldots, i_m$, let $V_{i_1,\ldots,i_m}$ be the set of solutions of $F_{i_1,\ldots,i_m}$ (being an $\text{OA}((r_1 r_2 \cdots r_m)^{-1} N; r_{m+1} \cdots r_d; t - m))$ for $1 \le m \le t - 1$. For any sub-vector $u \in V_{i_1,\ldots,i_m}$, from (4.5.8) and (4.5.4), let

$$\begin{aligned} &I(u) := \text{RowInd}(F_{i_1,\ldots,i_m}); \quad J(u) := I_N \setminus I(u); \text{ and} \\ &\mathrm{Z}(u) := \big\{(x_j) : j \in J(u) \text{ and } \exists X \in \mathrm{Z}(P) \text{ such that } X[I(u)] = u\big\}, \end{aligned}$$

here $X[I(u)] := (x_i : i \in I(u))$. For instance, if $m = 1$ and $u \in V_1$ then

$$\mathrm{Z}(u) = \big\{ [u_2; \ldots; u_{r_1}] : X = [u; u_2; \ldots; u_{r_1}] \in \mathrm{Z}(P) \big\}.$$

PROPOSITION 52. *For any pair of sub-vectors* $u, v \in V_{i_1,\ldots,i_m}$*, if* $v = u^{g_R}$ *for some* $g_R \in L_{i_1,\ldots,i_m}$*, we have* $\mathrm{Z}(u) = \mathrm{Z}(v)$*.*

We prove this proposition in the next two lemmas. In Lemma 53, without loss of generality, it suffices to give the proof for the first strength 2 derived array. The induction step will be presented in Lemma 55.

LEMMA 53 (Case $m = 1$).
Let u_1 *and* v_1 *be two arbitrary sub-solutions in* V_1*, ie, they form strength 2 OAs* $[F_1|u_1]$ *and* $[F_1|v_1]$ *of the form* $\mathrm{OA}(r_1^{-1}N; r_2 \cdots r_d \cdot s; 2)$*. Let*

$$\mathrm{Z}_X(u_1) = \left\{ [u_2; \ldots; u_{r_1}] : X = [u_1; u_2; \ldots; u_{r_1}] \in \mathrm{Z}(P) \right\},$$
$$\mathrm{Z}_Y(v_1) = \left\{ [v_2; \ldots; v_{r_1}] : Y = [v_1; v_2; \ldots; v_{r_1}] \in \mathrm{Z}(P) \right\}.$$

Suppose that there exists a nontrivial subgroup, say $L(F_1)$*, and if* $v_1 = u_1^h$ *for some* $h \in L_1$*, we have* $\mathrm{Z}_X(u_1) = \mathrm{Z}_Y(v_1)$*.*

PROOF. Pick up a nontrivial permutation h in $L(F_1)$. Then it acts locally on $\mathrm{RowInd}(F_1)$. By symmetry, we only check that $\mathrm{Z}_X(u_1) \subseteq \mathrm{Z}_Y(v_1)$. We choose any sub-vector $\boldsymbol{u}^* := [u_2; \ldots; u_{r_1}] \in \mathrm{Z}_X(u_1)$, then $X = [u_1; u_2; \ldots; u_{r_1}]$ is in $\mathrm{Z}(P)$. We view $h \in \mathrm{Aut}(F)$, so

$$\begin{aligned} D^h = [F|X]^h &= \left[F^h|\, X^h\right] = \left[F|\, X^h\right] = \left[F|\, [u_1; u_2; \ldots; u_{r_1}]^h\right] \\ &= \left[F|\, [u_1^h; u_2; \ldots; u_{r_1}]\right] = \left[F|\, [v_1; u_2; \ldots; u_{r_1}]\right]. \end{aligned}$$

This implies that $[v_1; u_2; \ldots; u_{r_1}]$ is a solution, hence $u^* \in \mathrm{Z}_Y(v_1)$. □

COROLLARY 54. *We can wipe out all solutions* $Y = [v_1; v_2; \ldots; v_{r_1}] \in \mathrm{Z}(P)$ *if* $v_1 \in u_1^{L_1}$*, the* L_1*- orbit of* u_1 *in* V_1*. In other words, if* $V_1 \neq \emptyset$*, then it suffices to find the first sub-vector of vector* X *by selecting* $|V_1|/|L_1|$ *representatives* u_1 *from the* L_1*- orbits in* V_1*.*

Furthermore, the above proof is independent of the original choice of derived design. Hence it can be done simultaneously at all solution sets $V_1, V_2, \ldots, V_{r_1}$*, using the subgroups* $L_1, \ldots, L_{r_1}$*.*

We call this procedure the *local pruning process* using strength 2 derived designs. Notice that we can use the row orbits of G when G is very large. These subgroups can be defined similarly, just replace the derived designs by the G-row orbits in the set of rows of F.

Next, if $t \geq 3$ we extend the proof of Proposition 52 for $2 \leq m \leq t-1$.

LEMMA 55 (Case $m > 1$). *For any pair of sub-vectors* $u, v \in V_{i_1,i_2}$*, if* $v = u^{g_R}$ *for some* $g_R \in L_{i_1,i_2}$*, we have* $\mathrm{Z}(u) = \mathrm{Z}(v)$*.*

PROOF. We prove this result for $t = 3$ and $m = 2$ only. For arbitrary $t > 3$, and $m > 2$, the proof is a straightforward generalization. Similar to the proof of Lemma 53, without loss of generality, we consider the first derived design $F_1 = \mathrm{OA}(n; r_2 \cdots r_d; 2)$ where $n = N/r_1$. Taking derived designs of F_1 with respect to the second column (having r_2 levels), we get r_2 strength 1 arrays, denoted by

$$f_1 := F_{1,1}, f_2 := F_{1,2}, \ldots, f_{r_2} := F_{1,r_2},$$

each is an $\mathrm{OA}(r_2^{-1}n; r_3 \cdots r_d; 1)$. Any element u_1 in V_1 can be written as

$$u_1 \;=\; [u_{1,1}; u_{1,2}; \ldots; u_{1,r_2}],$$

a concatenation of r_2 sub-vectors $u_{1,j}$ of length $\frac{n}{r_2}$, where

$$u_{1,j} = \left(x_{\frac{(j-1)n}{r_2}+1}, \ldots, x_{\frac{jn}{r_2}} \right) \quad \text{for } j = 1, \ldots, r_2.$$

From (4.5.8) and Definition 51, we know $L(f_j) :=$ Centralizer $\big(N_G(f_j), J(f_j)\big)$ consists of row permutations acting locally on

$$\mathrm{RowInd}(f_j) = \left\{ \frac{(j-1)n}{r_2} + 1, \ldots, \frac{jn}{r_2} \right\}, \quad \text{for each } j = 1, \ldots, r_2.$$

That means the subgroup $L(f_j)$ fixes $J(f_j) = [1, \ldots, N] \setminus \mathrm{RowInd}(f_j)$ pointwise. Because V_1 is the Cartesian product of the subsets $V_{1,j} := \{ u_{1,j} \}$, we prune $V_{1,j}$ by using $L(f_j)$, for $j = 1, \ldots, r_2$.

We start with $j = 1$. Let $u_{1,1}$ and $v_{1,1}$ be two arbitrary sub-vectors in $V_{1,1}$ (ie, they can be used to make strength 1 arrays $[f_1|u_{1,1}]$ and $[f_1|v_{1,1}]$ being of the form $\mathrm{OA}(r_2^{-1}n; r_3 \cdots r_d \cdot s; 1)$. Let

$$\mathrm{Z}_X(u_{1,1}) := \Big\{ \big[[u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big] : X = [u_1; u_2; \ldots; u_{r_1}] \in \mathrm{Z}(P) \Big\},$$

$$\mathrm{Z}_Y(v_{1,1}) := \Big\{ \big[[v_{1,2}; \ldots; v_{1,r_2}]; v_2; \ldots; v_{r_1} \big] : Y = [v_1; v_2; \ldots; v_{r_1}] \in \mathrm{Z}(P) \Big\},$$

where $v_1 = [v_{1,1}; v_{1,2}; \ldots; v_{1,r_2}] \in V_1$. We prove that if $v_{1,1} = u_{1,1}^h$ for some $h \in L(f_1)$, then we have $\mathrm{Z}_X(u_{1,1}) = \mathrm{Z}_Y(v_{1,1})$. In fact, we only need to have $\mathrm{Z}_X(u_{1,1}) \subseteq \mathrm{Z}_Y(v_{1,1})$. Let any sub-vector

$$\boldsymbol{u}^* := \big[\ [u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big] \in \mathrm{Z}_X(u_{1,1}),$$

and $h \in L(f_1)$. Then we have $X = [u_1; u_2; \ldots; u_{r_1}] \in \mathrm{Z}(P)$, and

$$\begin{aligned} D^h = [F|X]^h = F^h|\, X^h = F|\, X^h &= F|\, [\, u_1^h; u_2; \ldots; u_{r_1} \,] \\ &= F|\, \big[[u_{1,1}^h; u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big] \\ &= F|\, \big[[v_{1,1}; u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big]. \end{aligned}$$

Hence, $Y = \big[[v_{1,1}; u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big]$ is a solution vector and $\boldsymbol{u}^* \in \mathrm{Z}_Y(v_{1,1})$. In F_1, the choice of f_j does not affect to the proof, so the pruning process can be applied at the same time for all f_j, $j = 1, \ldots, r_2$. □

Operations on derived designs. Recall from (4.5.7) that the symbols $i_1, \ldots, i_m$ (where $1 \leq i_j \leq r_j$) indicate the derived design having symbol i_j in column j, for $j = 1, \ldots, m$. Let

$$\sigma := G \times \tau \tag{4.5.9}$$

be the *direct product* of G and τ, where $\tau := \mathrm{Sym}(s)$ is the group acting on the symbols of column X.

We consider each derived design as an agent that receives data from its lower strength derived designs, make some appropriate operations, then pass the result to its parent design. Notice that strength 1 and strength t designs require special operations. Recall from Definition 51 that $L_{i_1,\ldots,i_m}$ are the subgroups associated with the derived designs $F_{i_1,\ldots,i_m}$ having strength $t-m$. When $m = t-1$, we write $L_{i_1,\ldots,i_{t-1}}$ for the subgroup associated with the strength 1 derived design $F_{i_1,\ldots,i_{t-1}}$. The agents of derived designs can be described as follows.

(1) At designs $F_{i_1,\dots,i_{t-1}}$ (Initial step when $m = t-1$):
Input: $F_{i_1,\dots,i_{t-1}}$;
Operation: form $V_{i_1,\dots,i_{t-1}}$, the set of all strength 1 vectors of length $(r_1 r_2 \cdots r_{t-1})^{-1}N)$ being appended to $F_{i_1,\dots,i_{t-1}}$, compute $L_{i_1,\dots,i_{t-1}}$, and find the representatives of $L_{i_1,\dots,i_{t-1}}$ - orbits in the set $V_{i_1,\dots,i_{t-1}}$;
Output: these representatives, ie, solutions of $F_{i_1,\dots,i_{t-1}}$.

(2) At strength k derived designs ($1 < k \le t-1$): let $m := t-k$, we have
Input: the vector solutions (of length $(r_1 r_2 \cdots r_m{\cdot}r_{m+1})^{-1}N)$ of strength $k-1$ sub-designs; and $L_{i_1,\dots,i_m}$;
Operation: form sub-vector solutions (of length $(r_1 r_2 \cdots r_m)^{-1}N)$ of $F_{i_1,\dots,i_m}$, prune these solutions by $L_{i_1,\dots,i_m}$;
Output: representatives of the $L_{i_1,\dots,i_m}$- orbits in the set $V_{i_1,\dots,i_m}$.

(3) At the (global) design F:
Input: the sub-vectors from strength $t-1$ derived designs;
Operation: find the representatives of σ-orbits in the Cartesian product $V = V_1 \times V_2 \times \ldots \times V_{r_1}$, where V_i had been already pruned by the subgroup L_i $(i = 1, 2, \dots, m)$;
Output: solution vectors X which are non-isomorphic up to $\sigma = G \times \tau$, defined in (4.5.9).

We propose the following three-step procedure:

function PRUNING-USES-SYMMETRY(F, d)
Input: F is a strength t design; d is the number of columns required
Output: All non-isomorphic extensions of F
$\diamond$ Step 1: *Local pruning at strength k derived designs.*
1a) Find sub-vectors of $F_{i_1,\dots,i_m}$, for $m := t-k$, and $k = 1, \dots, t-1$,
1b) prune these sub-vectors locally and simultaneously by using $L_{i_1,\dots,i_m}$,
1c) concatenate these sub-vectors to get sub-vectors in $V_{i_1,\dots,i_{m-1}}$.
$\triangleright$ For strength $t = 3$, in Step 1), we form subvectors
$\triangleright$ $u_{i,j} \in V_{i,j}$ simultaneously at the $r_1 r_2$ sets $V_{i,j}$, then
$\triangleright$ concatenate $u_{i,j}$ $(1 \le i \le r_1, 1 \le j \le r_2)$ to get $u_i \in V_i$.

$\diamond$ Step 2: *Pruning at strength t design F.*
2a) Select the representative vectors X from the σ-orbits of V,
$\triangleright$ V consists of vectors of length N, being
$\triangleright$ formed by sub-vectors found from Step 1
2b) append vectors X to F to get strength t orthogonal arrays $[F|X]$,
2c) compute and store their canonical arrays into a list Lf, return Lf.

$\diamond$ Step 3: *Repeating step.*
if # current columns $<$ d **then**
Call PRUNING-USES-SYMMETRY(f, d) for each $f \in Lf$
else
Return Lf
end if
end function

EXAMPLE 4.14. Let $U := \big[[3,1],[2,3]\big]$, $F = \mathrm{OA}(24; 3.2^3; 3)$,

$$F = \begin{bmatrix} 0&0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&2&2&2&2&2&2&2&2 \\ 0&0&0&0&1&1&1&1&0&0&0&0&1&1&1&1&0&0&0&0&1&1&1&1 \\ 0&0&1&1&0&0&1&1&0&0&1&1&0&0&1&1&0&0&1&1&0&0&1&1 \\ 0&0&1&1&1&1&0&0&0&1&0&1&0&1&0&1&1&1&0&0&0&0&1&1 \end{bmatrix}^T.$$

$\mathrm{Aut}(F)$ has order 12288. Compute $G = \mathrm{Row}(\mathrm{Aut}(F))$, and update it by $G = \mathrm{Stabilizer}(G, [1])$, which is a permutation group of size 768. The three strength 2 derived designs give 8, 8, and 16 candidates respectively, so we have to check $8.8.16 = |V| = 1024$ possibilities.

The row permutation subgroups of the three strength 2 derived designs are

$L_0 = [(), (7,8), (5,6), (5,6)(7,8), (3,4), (3,4)(7,8), (3,4)(5,6), (3,4)(5,6)(7,8)]$,

$L_1 = [()]$, and

$$\begin{aligned} L_2 = [&(), (23,24), (21,22), (21,22)(23,24), (19,20), (19,20)(23,24), \\ &(19,20)(21,22), (19,20)(21,22)(23,24), (17,18), (17,18)(23,24), (17,18)(21,22), \\ &(17,18)(21,22)(23,24), (17,18)(19,20), (17,18)(19,20)(23,24), \\ &(17,18)(19,20)(21,22), (17,18)(19,20)(21,22)(23,24)] \end{aligned}$$

with corresponding orders 8,1,16. And the subspaces are pruned to 1,8, and 1 vectors respectively. That is we need to check 8 cases now.

Observe that $\mathrm{Aut}(F)$ decomposes the rows of F into row-orbits $O_1, \ldots, O_l$. If $\mathrm{Aut}(F)$ acts intransitively on the rows of F, then $l > 1$. For each of the orbits O_j, let $\mathrm{RowInd}(O_j) \subseteq \{1, \ldots, N\}$ be the row indices of O_j in F. We can define the normalizers and the centralizers of O_j as in (4.5.5) and in (4.5.6). But the subgroups found in this way help reducing isomorphic vectors only when the group G has very large size. This is not the case when arrays have many columns.

A mixed approach using linear algebra and symmetries. Recall that the extension of an orthogonal array F with run size N to a new array $[F|X]$ is reduced to solving a linear system P having matrix form (4.5.2):

$$M.X = c.$$

Recall that $G = \mathrm{Row}(\mathrm{Aut}(F))$ is the group of all row permutations induced by the automorphism group $\mathrm{Aut}(F)$, and that $\mathrm{Z}(P)$ is the set of solutions of (4.5.2) over the set $\{0, 1, \ldots, s-1\}$ as a subset of $\mathbb{N}$. Denote by $\mathbb{Q}^N$ the vector space of dimension N over the rationals. For any solution X, we view $X \in S$, where S is the solution set of (4.5.2) over $\mathbb{Q}$. The set S in fact is an affine space in $\mathbb{Q}^N$; and $\mathrm{Z}(P) = S \cap \{0, 1, \ldots, s-1\}^N$. Moreover, $\mathrm{Z}(P)$ is a subset of $\bigcap_{g \in G} S^g$. Indeed, since $\mathrm{Z}(P)^g = \mathrm{Z}(P)$ for all $g \in G$, we have $\mathrm{Z}(P) \subseteq S^g$, for all $g \in G$. We call the intersection $\bigcap_{g \in G} S^g$ the *G-invariant core* of $\mathrm{Z}(P)$, (by definition it is the maximal G-invariant subset of S). The G-invariant core $\bigcap_{g \in G} S^g$ of $\mathrm{Z}(P)$ is still an affine space since the image S^g of S is an affine space, and intersecting two affine spaces results in again an affine space. The idea is that even though S has large dimension, it is likely that the G-invariant core of $\mathrm{Z}(P)$ could have smaller dimension.

EXAMPLE 4.15. Consider extending array $\mathrm{OA}(72; 6{\cdot}3{\cdot}2^2; 3)$ to $\mathrm{OA}(72; 6{\cdot}3{\cdot}2^3; 3)$. The solution space has dimension 36, using G we can reduce it to dimension 20.

Computing the G-invariant core of the solution set $\mathrm{Z}(P)$. First we compute the intersection of two affine spaces. We identify S with the pair $[v, B]$, where v is a specific vector in S and B is a basis of S (over $\mathbb{Q}$). Let $n := N-$ rank(M) be the dimension of S, then $|B| = n$, and

$$S = v + \langle B \rangle = v + \sum_{i=1..n} b_i B_i, \text{ where indeterminates } b_i \in \mathbb{Q}. \tag{4.5.10}$$

Observation 2. Let $p \in G$, the affine image S^p can be determined by the vector v^p and the basis $B^p := \{u^p : u \in B\}$. In other words,

$$S^p = v^p + \langle B^p \rangle = v^p + \sum_{i=1..n} c_i B_i^p, \text{ where } c_i \in \mathbb{Q}. \tag{4.5.11}$$

Moreover, $S \cap S^p \neq \emptyset$ if and only the system

$$\begin{aligned} v^p - v &= \sum_{i=1..n} b_i B_i - \sum_{i=1..n} c_i B_i^p \\ &= \big[B_1 | B_2 | \dots | B_n | - B_1^p | - B_2^p | \dots | - B_n^p\big] [b_1, \dots, b_n, c_1, \dots, c_n]^t \end{aligned}$$

has solution $b_1, \dots, b_n, c_1, \dots, c_n$.

Hence, if $S \cap S^p \neq \emptyset$, its basis and specific vector can be found by substituting $b_1, \dots, b_n$ back into (4.5.10), (or $c_1, \dots, c_n$ into (4.5.11)). We prune the integral solution set Z(P) by computing its G-invariant core. Let H be a set of generators of G. We compute $\bigcap_{g \in G} S^g$ using the following procedure.

Algorithm 4 Computing G-invariant core

```
    Input: the affine solution space S of (4.5.2), and the generators H;
    Output: the affine space ⋂_{g∈G} S^g.
  function Find-G-invariant-core( S, H )
      Set Y := S;
      repeat
          W := Y;
          update Y := ⋂_{g∈H} Y^g ∩ Y;
      until Y = W;
      return Y.
  end function
```

Proof. Let Y_0 be the output of the procedure, we show that $Y_0 = \bigcap_{g \in G} S^g$. The space Y_0 has property $Y_0 = \bigcap_{g \in H} Y_0^g \cap Y_0$. Therefore, $Y_0 = Y_0^p$ for all $p \in H$. Since any permutation $g \in G$ is a product of $p \in H$, $Y_0 = Y_0^g$. $\square$

Having obtained the G-invariant core $Y_0 =: [u, C]$ of Z(P), we update $S := Y_0$, and update the dimension n to a possibly smaller dimension $n := n_0 = dim(Y_0)$. The integral vector solution X (viewed as column vector) now is computed by:

$$X^T = (0, x_2, x_3, \dots, x_N)^T = u + \sum_{i=1..n} y_i C[i], \tag{4.5.12}$$

where pivotal variables $y_i \in \mathbb{Z}$. Hence, solving P in terms of indeterminates $(x_j) \in \{0, 1, \dots, s-1\}^N$ $(j = 1, \dots, N)$ is reduced to finding all integral (pivotal) tuples $(y_i) \in \mathbb{Z}^n$ $(i = 1, \dots, n)$ such that each coordinate x_j is in $\{0, 1, \dots, s-1\}$.

Although very often $n < N$, this approach is useful if a few more inequalities would be found and used to delete out some (not all) isomorphic vectors in each isomorphic class retaining the non-isomorphic vectors. From that point, the search for non-isomorphic vectors becomes feasible.

Imposing extra constraints on the system. For each generator p of G such that at least one of its cycles has even length, we extract those *even length cycles* into a set K. We do not use odd length cycles of p. Then, for each $h \in K$, we form an extra inequality whose left hand side is the sum of X's coordinates with odd indices, and the right hand side is the sum of X's coordinates with even indices of the cycles in h. In more details, we have

LEMMA 56. *If $K \neq []$, for each $h \in K$ having the form*

$$h = \prod_i (i_1, i_2) \quad \prod_j (j_1, j_2, j_3, j_4) \dots$$

where $1 \leq i_1 \neq i_2 \neq j_1 \neq j_2 \neq j_3 \neq j_4, \dots \leq N$, we can add the following inequality

$$x_{i_1} + x_{j_1} + x_{j_3} + \dots \leq x_{i_2} + x_{j_2} + x_{j_4} + \dots \tag{4.5.13}$$

into the original system P without missing any non-isomorphic vector solution X.

PROOF. Suppose $h = \prod_i (i_1, i_2) \quad \prod_j (j_1, j_2, j_3, j_4) \dots \in K$, and $Z = [z_1, z_2, z_3, \dots, z_N]$ is a solution so that

$$z_{i_1} + z_{j_1} + z_{j_3} + \cdots \geq z_{i_2} + z_{j_2} + z_{j_4} + \cdots$$

We prove that Z is isomorphic with a solution $X = [x_1, x_2, x_3, \dots, x_N]$ which fulfills

$$x_{i_1} + x_{j_1} + x_{j_3} + \cdots \leq x_{i_2} + x_{j_2} + x_{j_4} + \cdots$$

The vector $X := Z^h$ indeed satisfies Condition (4.5.13). $\square$

For example, let $h = (1, 2)(7, 8, 9, 10)(13, 16)$ be a permutation in K, ($h^{-1} = (1, 2)(7, 10, 9, 8)(13, 16)$), we can impose the following inequality

$$x_1 + x_7 + x_9 + x_{13} \leq x_2 + x_8 + x_{10} + x_{16}$$

on the original system P. Indeed, suppose that $Z = [z_1, z_2, z_3, \dots, z_{16}]$ is a solution, and

$$(*) \dots z_1 + z_7 + z_9 + z_{13} \geq z_2 + z_8 + z_{10} + z_{16}.$$

The image

$$X = (x_i) = Z^h = (z_{i^{h^{-1}}}) = (z_2, z_1, z_3, z_4, z_5, z_6, z_{10}, z_7, z_8, z_9, z_{11}, z_{12}, z_{16}, z_{14}, z_{15}, z_{13});$$

satisfies the constraint (4.5.13), since (*) means

$$x_2 + x_8 + x_{10} + x_{16} \geq x_1 + x_9 + x_7 + x_{13}.$$

Finding pivotal variables y_i such that $X \in \{0, 1, \dots, s-1\}^N$. Having obtained Formula (4.5.12) of X, and found extra inequalities (using Lemma 56), we now find integral (pivotal) tuples $(y_i) \in \mathbb{Z}^n$ by a recursive procedure. Let $ExtraS$ be the set of these extra inequalities, and let Y be the set of coordinates of X in terms of $(y_i)_{i=1,\dots,n}$. We split Y into 3 subsets:

$$\begin{aligned} &Y_1 := \{\text{ monomials}\}, \\ &Y_2 := \{\text{ monomials with constant, and be grouped with respect to } y_i\}, \\ &Y_3 := \{\text{ polynomials with at least two indeterminates } y_i\}. \end{aligned} \tag{4.5.14}$$

For $t = 3$ we cut vector X into $r_1 r_2$ sub-vectors

$$L_X := \Big[\big(x_1, \dots, x_{\frac{N}{r_1 r_2}}\big), \dots, \big(x_{\frac{(r_1 r_2 - 1)N}{r_1 r_2}}, \dots, x_N\big)\Big];$$

for $t = 2$ we cut vector X into r_1 sub-vectors

$$L_X := \Big[\big(x_1, \dots, x_{\frac{N}{r_1}}\big), \dots, \big(x_{\frac{(r_1 - 1)N}{r_1}}, \dots, x_N\big)\Big].$$

We use *ExtraS* and L_X as *certificates* to prune vector solutions during the search. That is, whenever we find a sub-vector (or partial vector) by using Y, we substitute it into *ExtraS* to check whether $ExtraS \leq 0$ (ie, each polynomial p in *ExtraS* must be less than or equal 0), and to L_X to see whether all of its components have strength 1. Note that components in L_X are still considered valid when they depend on variables y_i; the same reasoning is applied for non-positiveness of polynomials in *ExtraS*. If all conditions are all right, we enlarge the sub-vector (in all feasible possibilities) until the length of vectors equals to n. Then the column vector X is found back by (4.5.12). A combination of depth-first and breath-first schemes to find all solutions $(y_i) \in \mathbb{Z}^n$ is presented in the following algorithm.

Algorithm 5 Recursive computing of $(y_i) \in \mathbb{Z}^n$

Input: Y; *ExtraS* and L_X
Output: All vectors $(y_i)_{i=1,\dots,n} \in \mathbb{Z}^n$

```
function COMPUTE-PIVOTALS(Y, ExtraS, L_X )
    repeat
        split Y = Y_1 ∪ Y_2 ∪ Y_3 by (4.5.14),

        form all partial vectors by making the hypercube from variables of Y_1,

        prune them using ExtraS ≤ 0, and L_X;

        substitute each valid partial vector back to Y,
    until Y_1 = ∅;        ▷ only keep intermediate valid nodes in the search tree;

    ◇ Since Y = Y_2 ∪ Y_3,
    extend the valid partial vectors made above by all possible vectors of Y_2


    collect the full vector solutions whose lengths equal n
    ◇ always certificate newly extended nodes using ExtraS and L_X

    return the representatives in the σ := G × τ-orbits (4.5.9) of Z(P).
end function
```

EXAMPLE 4.16. Extending $F = \mathrm{OA}(16; 2^3; 3)$ to $[F\ X] = \mathrm{OA}(16; 2^3 \cdot 4; 3)$. Here $N = 16$, the group of row permutations G has size 768, generated by the following permutations:

$$\big[(15,16),(13,14),(11,12),(9,10),(7,8),(5,6),(3,4),(3,6)(4,5)$$
$$(9,10)(11,14)(12,13),(3,10,5,4,9,6)(7,11,14)(8,12,13)\big],$$

from which we find 169 extra inequalities . After reducing the affine solution space by these symmetries, we get an 8-dimensional G-core S, and the solution vector $X \in \{0, 1, 2, 3\}^{16}$ in terms of $(y_i) \in \mathbb{Z}^8$ $(n = 8)$ is

$$\begin{aligned} X = (x_j) =&(0, y_1 + 6, y_2 + 6, -y_1 - y_2 - 6, y_3, -y_1 - y_3, y_4, y_1 - y_4 + 6,\\ &y_5, -y_1 - y_5, y_6 + 6, y_1 - y_6, y_7 + 6, y_1 - y_7, y_8, -y_1 - y_8) \end{aligned}$$

We want to find all $(y_1, \ldots, y_8) \in \mathbb{Z}^8$ such that $X \in \{\,0, 1, 2, 3\,\}^{16}$ by splitting

$$\begin{aligned} Y = \{&y_1 + 2, y_2 + 2, -y_1 - y_2 - 2, y_3, -y_1 - y_3, y_4, y_1 - y_4 + 2, y_5, -y_1 - y_5, y_6 + 2,\\ &y_1 - y_6, y_7 + 2, y_1 - y_7, y_8, -y_1 - y_8\} \end{aligned}$$

into $Y_1 = \{y_3, y_4, y_5, y_8\}$; $\quad Y_2 = \big\{[y_1 + 6], [y_6 + 6, y_2 + 6], [y_7 + 6]\big\}$; and

$$Y_3 = \{-y_1 - y_8, -y_1 - y_5, -y_1 - y_3, -y_1 - y_2 - 6, y_1 - y_7, y_1 - y_6, y_1 - y_4 + 6\}.$$

We form all partial solutions from Y_1, pruning at each those sub-vectors (having length 4) by using 169 inequalities of $ExtraS$, and by employing the fact that each of the four vectors $(0, y_1 + 6, y_2 + 6, -y_1 - y_2 - 6)$, $\quad (y_3, -y_1 - y_3, y_4, y_1 - y_4 + 6)$, $(y_5, -y_1 - y_5, y_6 + 6, y_1 - y_6)$, $\quad$ and $(y_7 + 6, y_1 - y_7, y_8, -y_1 - y_8)$ has strength 1. At each iteration, when ever $Y_1 = \emptyset$, we generate all valid partial solutions from Y_2, concatenate them with partial solutions of y_3, y_4, y_5, y_8, and prune again. This results in 35 vectors; of these only one vector forms an $\mathrm{OA}(16; 2^3 \cdot 4; 3)$.

4.6. Conclusion

The main concern of this chapter is generating strength 3 fractions. The concepts of transformations of fractions and the automorphism group of a fraction introduced in Section 4.2 play a vital role. To distinguish two non-isomorphic fractions, for instance, we can compute their automorphism groups and compare the orders. But that is not strong enough to discriminate them. The canonical array of an orthogonal array then can be found using the canonical labeling graph of its companion colored graph. This technique was discussed in Section 4.3.

Formulating the column extension of a 3-balanced array in terms of a linear system with integer coefficients, and employing the row symmetries of the automorphism group are alternatives to approach the problem. This is the theme of Section 4.5. Combining these together with computing canonical arrays, we solved the problem of making 3-balanced arrays in this chapter. Furthermore, in the special case of two section arrays, the algorithm Lex-Least-Fractions in Section 4.4 generates all non-isomorphic fractions faster than the combined approaches above. Together, all of the methods help in listing all non-isomorphic fractions of strength 3. But we postpone the listing until Chapter 6. Instead, in the next chapter, we show how to pick the 'good' design out of a set of non-isomorphic designs. This becomes necessary and interesting when there are several non-isomorphic ones.

CHAPTER 5

Selecting strength 3 orthogonal arrays

5.1. Introduction

In the early stages of industrial experimentation, scientists may want to detect what factors affect the properties of some product or process. Frequently, there is an extensive list of candidate factors, of which only a few turn out to be active. When interactions between the active factors can be considered negligible, it makes sense to estimate the main effects with an orthogonal array (OA) of strength 2. In arrays with $t = 2$, for any factor A, all possible levels of any other factor appear equally often at each of the levels of A. As a consequence, the main effect of any factor can be deduced from the corresponding set of s_i means of the experimental results. This property follows only if interactions are indeed negligible. Otherwise, the mean of the first level of A, say, could be distorted by a particular combination of two other factors, and it is hard to disentangle the main effects from the 2-factor interactions.

OAs with $t = 3$ and $N \leq 100$ can be used fruitfully if there are substantial interactions between the experimental factors, while their identity is not known in advance. Contrary to the $t = 2$ case, the estimates of the main effects are not distorted by interactions between other factors. However, the main effect of a factor involved in interactions depends on the identity of the other factors in the array. If factor A interacts with factor X, the main effect of A obviously depends on the inclusion of X in the array. So, for a practical investigation, we would want to include a fairly complete list of factors that could interact.

With an OA of $t = 3$, estimates of interaction components can be affected by the presence of other interaction components. Indeed, such an OA does not have every level pair of factors appearing equally often against every pair of settings of two other factors. In addition, the degrees of freedom available for the estimation of interaction components may not be sufficient to estimate them all simultaneously. So there could be a problem of interpreting an active interaction component.

For the specific case of the 24-run array constructed by folding over a 12-run Plackett-Burman scheme (Plackett and Burman [1946]), Miller and Sitter [2001] studied a way out of the above problem. They proposed a two-stage approach to detect active main effects and interactions. First, activity of the main effects is detected by standard methods. The strength of the array ensures that important main effects will not be extinguished by one or more interactions. The second stage uses all-possible-subsets methods to discriminate between models containing active and those containing inactive interactions. The two-stage approach is generalizable to any orthogonal array of strength 3.

There is much literature on constructing OAs with $t = 2$; see Wu and Hamada [2000], Hedayat et al. [1999], and the references therein contained. Indeed, Sloane's web site gives a table of all orthogonal arrays with $t = 2$ and $N \leq 100$; see Sloane [2005]. The large amount of literature will partly be due to the popularity of the designs advocated by Taguchi [1959, 1987], where interactions not of direct interest are assumed absent. An appealing aspect of these designs is their run-size economy. For example, in the Taguchi L_{16}, one can investigate the main effects of 15 two-level factors in just 16 runs.

The OAs with $t = 3$ have received much less attention in the literature than have those with $t = 2$. Exceptions are the regular prime-level designs of resolution IV (see, eg, Wu and Hamada [2000]). The purpose of this chapter is to study the selection of non-regular OAs with $t = 3$ for practical experimentation. In Brouwer et al. [2005], results were presented for all mixed arrays with $t = 3$ and $N \leq 64$. The selection issue in the present chapter is exemplified with $3^a \cdot 2^b$ arrays, extending the run-size limit to $N \leq 72$. The rest of the chapter is organized as follows. In Section 5.2, we apply the algorithm LEX-LEAST-FRACTIONS from Section 4.4 to obtain sets of all non-isomorphic OA$(48; 3 \cdot 2^9; 3)$, OA$(54; 3^5; 3)$, OA$(54; 3^5 \cdot 2; 3)$. The number of distinct arrays were found to be 3, 4, 4. For series OA$(72; 3^2 \cdot 2^7; 3)$ and OA$(72; 3^2 \cdot 2^8; 3)$, the numbers of distinct arrays are at least 1304, and 379, respectively. The four non-isomorphic OA$(54; 3^5; 3)$ were obtained earlier by Hedayat et al. [1997]. However, these authors did not consider the selection issue. In Section 5.3, we turn to the selection problem. We present some simple criteria, and we use these to study the aforementioned sets. In Section 5.4, we develop some methodology of blocking a strength 3 OA and we explore our designs of special interest as to their capability for blocking. A brief discussion concludes the chapter.

5.2. Enumeration

Using the algorithm LEX-LEAST-FRACTIONS we obtain all non-isomorphic array OA$(N; 3^a \cdot 2^b; 3)$s. Henceforth, we will use the notation $N.a.b.z$ to denote the zth array in a set of OA$(N; 3^a \cdot 2^b; 3)$s. Table 5.1 gives minimum run sizes for all cases with $t = 3$, $a + b \leq 10$, and $N \leq 100$.

Designs with $a = 0$ correspond with two-level designs. Those with up to 8 factors can be constructed using regular design theory. The designs with 9 and 10 factors, respectively, can be obtained by deleting columns from the folded-over 12-run Plackett-Burman design. In fact, there can be a folded-over design with $N = 24$ and $t = 3$ for up to 12 factors.

Designs with $b = 0$ are three-level designs. Those with 3, 4, and 6–10 factors can be constructed using regular design theory [Wu and Hamada, 2000]. Hedayat et al. [1997] give 4 non-isomorphic 54-run designs with 5 three-level factors, and show that these are the only ones. These are of special interest here as the problem of selecting one of them for practical use has not yet been addressed. To emphasize the special interest, we mark the corresponding entries in Table 5.1 with a bold typeface.

Of the 19 pairs (a, b) in the table for which $a \geq 1$ and $b \geq 1$, 13 can be derived from those with either $a - 1$ three-level factors or $b - 1$ two-level factors. Of the six remaining ones, the (a, b) pairs (1,9), (5,1), (2,7), and (2,8) are also marked as special interest designs. We will see later that designs (2,6) and (2,5) may well be constructed by deleting columns from certain (2,7) arrays. For this reason, they are not marked in the present table.

TABLE 5.1. Min. run sizes of $3^a \cdot 2^b$ arrays with $a+b \leq 10$, and $N \leq 100$

b	a						
	0	1	2	3	4	5	6 – 10
0	-	-	-	27	27	**54**	81
1	-	-	18	54	54	**54**	
2	-	12	36				
3	8	24	72				
4	8	24	72				
5	16	48	72				
6	16	48	72				
7	16	48	**72**				
8	16	48	**72**				
9	24	**48**					
10	24						

NOTE: bold-faced entries indicate designs of special interest.

Using the above algorithm, we obtained 3 non-isomorphic $\mathrm{OA}(48; 3 \cdot 2^9; 3)$, and four $\mathrm{OA}(54; 3^5 \cdot 2; 3)$; these are given in the Appendix. There are at least 1304 distinct $\mathrm{OA}(72; 3^2 \cdot 2^7; 3)$, and at least 379 distinct $\mathrm{OA}(72; 3^2 \cdot 2^8; 3)$. For the current study, we use the first 1304 distinct OAs of the series $\mathrm{OA}(72; 3^2 \cdot 2^7; 3)$, and use the first 379 distinct OAs of the series $\mathrm{OA}(72; 3^2 \cdot 2^8; 3)$. Selected examples are given in Appendix A; the full lists are electronically available at Nguyen [2005]. The construction of mixed two-and-three level designs was attempted earlier by Connor and Young [1961]. The run-sizes of each of the designs, together with the strength t of the designs when viewed as orthogonal arrays, is given in Table 5.2.

All of the designs permit simultaneous estimation of all the main effects and all the interactions. The table shows that for many cases this comes at the cost of run-size or strength. We believe that our mixed designs of special interest give a useful alternative with smaller run-sizes or greater strength. In particular, our $\mathrm{OA}(48; 3 \cdot 2^9; 3)$ and our $\mathrm{OA}(54; 3^5; 3)$ series have smaller run sizes. Further, as we will see later, a few of our $\mathrm{OA}(72; 3^2 \cdot 2^7; 3)$ arrays have all their interactions estimable, while they also have smaller run-size and greater strength.

5.3. Selection

Orthogonal arrays of strength 3 can be used in practice for collecting data to identify active main effects in the presence of strong interactions, and to identify some, or possibly all, active two-factor interactions. The identification can be carried out by comparing the fit of statistical models to the data. We propose a model building approach for strength 3 arrays that consists of two stages; it is adapted from Miller and Sitter [2001]. In the first stage, only the main effects are considered. Assuming that interactions involving 3 or more factors are negligible, many of the arrays under study have degrees of freedom left to estimate random error; some of them even have error degrees of freedom from duplicate runs. These can be used to test the statistical significance of the main effects. If there are insufficient degrees of freedom for random error, we may judge the main effects

TABLE 5.2. $3^a \cdot 2^b$ arrays from Connor and Young

a	b	N	t	a	b	N	t
1	4	36	1	4	3	162	1
	5	48	3		4	162	1
	6	48	3		5	216	1
	7	96	3		6	324	1
	8	96	3	5	1	162	4
	9	128	0		2	162	1
2	3	36	2		3	216	2
	4	72	3		4	324	1
	5	72	2		5	432	2
	6	96	1	6	1	243	0
	7	144	2		2	486	1
	8	144	3		3	486	1
3	2	54	1		4	486	1
	3	72	2	7	1	243	0
	4	108	1		2	486	1
	5	144	2		3	486	1
	6	288	2	8	1	243	0
	7	432	2		2	486	1
4	1	81	0	9	1	243	0
	2	162	1				

with a robust estimate of the standard error constructed from the main effects themselves (Lenth [1989], Schoen and Kaul [2000], Loeppky and Sitter [2002]).

For the second stage in the model building process, we construct the set of all components of the two-factor interactions. We then use all-possible-subsets procedures [Miller and Sitter, 2001] to look at the best few models consisting of all main effects and k two-factor interactions, for a range of values of k. When considering an interaction, we want to include all of its components. We presuppose that an experimenter cannot specify in advance which subset of all the possible interactions contain the active ones. Thus, he would want to be able to entertain as many models as are possible. We will now discuss various criteria that might be used to quantify the model-building potential of an array and thus will help with the selection of an array for practical use.

Rank of selected model matrices. Consider an $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; 3)$, F, say. Call the columns in F original columns. Replace any original column of r_i levels with $r_i - 1$ orthogonal columns, and call these the main effect columns. Add to the left a column $\mathbf{1}$ and call the matrix of the new set of columns M_1. As the arrays are orthogonal, we know that M_1 has full rank. Construct the p-extended model matrix M_p by extending M_1 with columns formed by the entry-wise products of $2, \ldots, p$ of the main effect columns for $p = 2, \ldots, d$. Do not form products of main effect columns obtained from the same original column.

We propose to characterize the non-isomorphic arrays $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; 3)$ for given values of N and $r_1, r_2, \ldots, r_d$ by the following rank-based quantities:

$$n_2 = r(M_2) - r(M_1),\ n_+ = r(M_d) - r(M_2),\ \text{and}\ n_{pe} = N - r(M_d).$$

Quantity n_2 corresponds to the maximum number of estimable components of 2-factor interactions in a model based on the array. This quantity may be refined further by looking at the ranks for meaningful subsets of the 2-factor interactions. For example, one could be specifically interested in interactions among 2-level factors. In addition, we quantify with n_+ the additional higher-order interaction components that are estimable. Finally, in some arrays there are duplicate runs; n_{pe} gives the number of degrees of freedom obtained from such runs. In general, we would prefer arrays with large n_2. Table 5.3 shows rank-based characteristics of the 48-run and 54-run designs of special interest. It is remarkable that 54.5.0.4 has almost all its interaction components estimable. For the sets of 1304 $\mathrm{OA}(72; 3^2 \cdot 2^7; 3)$ and 379 $\mathrm{OA}(72; 3^2 \cdot 2^8; 3)$, Table 5.4 shows the distribution of the distinct values of n_2. The total number of 2-factor interaction-components is 53 and 64, respectively. Interestingly, there are 4 non-isomorphic $\mathrm{OA}(72; 3^2 \cdot 2^7; 3)$ arrays that have all components of 2-factor interaction estimable. In view of the strength of the arrays, the interaction estimates must be correlated.

TABLE 5.3. Rank-based characteristics for arrays of special interest

	$\mathrm{OA}(48; 3 \cdot 2^9; 3)$	54.5.0.1	54.5.0.2	54.5.0.3	54.5.0.4	$\mathrm{OA}(54; 3^5 \cdot 2; 3)$
n_2	36	31	36	35	39	41
(n_2)	(18)	(9)	(4)	(5)	(1)	(9)
n_+	0	10	6	8	4	1
n_{pe}	0	2	1	0	0	0

NOTE: Bracketed figures bear on non-estimable components of 2-factor interactions.

Minimum forbidden sub-configurations. Consider a model $\mathcal{M}$ containing all components of k 2-factor interactions. The set of all these components is called a minimum forbidden sub-configuration (MFS) if

(1) $\mathcal{M}$ contains at least 1 non-estimable component.
(2) Deleting all components of any of the k 2-factor interactions would result in an estimable model.

Augmentation of $\mathcal{M}$ with other interactions also results in a model that is not fully estimable. For an orthogonal array of strength 3, the set of all MFS for $k = 1, 2, \ldots, \binom{n}{2}$ permit an assessment of models that can be estimated with the particular array. The set can be found by calculating the ranks of sub-matrices of $M_2 \setminus M_1$, the 2-extended model after excluding the columns of the 1-extended model. We excluded main effects from consideration, because they are orthogonal to the 2-factor interactions. Thus, the non-estimability of 2-factor interactions is solely due to the structure of the space spanning the corresponding components.

To explore the set of MFS, we used graphs with the factors as nodes and the (non-estimable) interactions as edges. We also tabulated numbers of MFS according to the number of $s_i \times s_j$ interactions in the sub-configuration.

Estimation Capacity. Consider, for some strength 3 OA with n columns, all $\binom{c}{v}$ v-interaction models with $c = \binom{n}{2}$. The estimation capacity for v two-factor interactions, denoted EC_v, is defined as the fraction of these models that are estimable

TABLE 5.4. Values for n_2 for OA$(72; 3^2 \cdot 2^7; 3)$s and OA$(72; 3^2 \cdot 2^8; 3)$s

n_2	OA$(72; 3^2 \cdot 2^7; 3)$	OA$(72; 3^2 \cdot 2^8; 3)$
37	2	1
38	28	9
39	304	266
40	4	2
41	15	3
42	202	39
43	2	0
44	24	0
45	89	0
46	47	1
47	121	31
48	416	16
49	5	2
50	13	6
51	7	0
52	21	2
53	4	0
54	0	1

[Cheng et al., 1999]. We can compare orthogonal arrays by making tables of EC_v for $v = 1, 2, \ldots, c$. For mixed arrays, it is useful to classify the results in more detail according to the number of $s_i \times s_j$ interactions in the model.

Extensions of resolution and aberration to non-regular arrays. Xu and Wu [2001] propose the concept of generalized word-length pattern (GWLP) to classify symmetrical as well as asymmetrical orthogonal arrays. The GLWP of an array is calculated as follows. First, replace each s-level column in an array with $s - 1$ columns orthogonal to each other and to the vector of ones. Second, normalize the columns such that they all have squared length N. Third, define p-factor interactions as products between p main effect columns. Finally, define A_p with

$$A_p = N^{-2} \sum_{k=1}^{n_p} \left| \sum_{i=1}^{N} x_{ik}^{(q)} \right|^2 . \tag{5.3.1}$$

The GWLP is the vector $(A_1, A_2, \ldots, A_n)$. For all designs, the A_j are independent of the choice of orthonormal contrasts [Dey and Mukerjee, 1999].

Resolution is defined as the smallest p such that $A_p > 0$. Designs with a high resolution are preferable to those with a low resolution. To discriminate among several maximum resolution designs, Xu and Wu use a generalized aberration (GA) criterion as follows. Consider designs D_1 and D_2, say. D_1 is said to have less aberration than D_2 is there exists a p, $1 \le p \le n$, such that $A_p(D_1) < A_p(D_2)$ and $A_j(D_1) = A_j(D_2)$ for $j = 1, \ldots, p-1$. D_1 is said to have generalized minimum aberration, denoted GMA, if there is no other design with less aberration than D_1.

Xu and Wu [2001] motivate the use of the GA criterion by proving that minimization of this criterion sequentially minimizes the contamination of non-negligible j-factor interactions on the estimation of main effects for $j = 2, \ldots, e$, where e

equals the number of factors for symmetrical designs and the strength for asymmetrical designs. This implies that a minimum GA array with $t = 3$ has minimum contamination of its main effect estimates with 3-factor interactions. Note that minimization of GA also minimizes the sum of squared correlations among two-factor interaction components. Using the criterion to judge the first 1304 OA$(72; 3^2 \cdot 2^7; 3)$, we find that array OA$(72; 3^2 \cdot 2^7; 3)$ no. 588 with $A_4 = 4.525$ is the single GMA array. The rank for the 2fi columns, however, is 51, which is 3 less than the maximum. So we would miss the maximum rank arrays if we would rely on GA alone. Thus, for $t = 3$, we would also want to consider rank-based characteristics.

The approach of Xu and Wu [2001] generalizes the concept of resolution and aberration to non-regular designs. However, the resolution is still an integer number. Deng and Tang [2002] define a generalized resolution in the context of their study of Hadamard matrices D of strength 2. The generalized resolution of D is defined as

$$R(D) = r + \left[1 - \max_{|s|=r} J_r(s)/N\right] \tag{5.3.2}$$

In their notation, $J_r(s)/N$ is the absolute value of the element-wise sum of the product of a subset s of r columns of an array, $|s|$ is the size of the subset, and r is the smallest integer such that $\max_{|s|=r} J_r(s) > 0$. $J_4(s)/N$ can be interpreted as the correlation between the two-factor interactions i_1, i_2 and $s - \{i_1, i_2\}$, where $\{i_1, i_2\} \subset s$. For $t = 3$, $r = 4$. If there are two interaction components fully aliased, they will have $J_4(s)/N = 1$, and the generalized resolution will be exactly 4. In our set of 1304 non-isomorphic arrays, 1098 arrays have a Hadamard part with resolution 4.667; for the remaining 206 arrays, the resolution is 4.444. There are arrays with resolution 4.667 that have the rank of the 2×2 interaction part as low as 11. On the other hand, some arrays with resolution 4.444 have a maximum rank for the estimation of 2×2 interactions. This demonstrates that generalized resolution as defined by Deng and Tang [2002] must not be used as the sole criterion to discriminate among resolution 4 designs.

Orthogonality of subspaces. In an $s_i^a s_j^b$ array, the spaces spanned by $s_i \times s_j$, $s_i \times s_i$, and $s_j \times s_j$ interactions may of may not be orthogonal to each other. If they are, we can build models by considering the subspaces one at a time. This decreases computational effort and increases interpretability of interaction effects. We checked the orthogonality of subspaces in our sets of OA$(72; 3^2 \cdot 2^7; 3)$ and OA$(72; 3^2 \cdot 2^8; 3)$ arrays. All of the arrays had the 3×3 interaction space orthogonal to the 2×3 interaction space. The set with 7 two-level factors had 441 arrays with the 2×2 interactions orthogonal to the 2×3 interactions. For the set with 8 two-level factors, this number was 314. These arrays thus have the attractive property that the 2×3 interactions are orthogonal to all remaining interactions.

Discussion. In our definitions of MFS and EC, we consider estimability of models $\mathcal{M}$ containing all components of k 2-factor interactions. If an array has at least one factor at more than two levels, we could also consider models for which some of the individual interaction components are estimable. We prefer the former option, because the designs considered here will be mainly used for categorical factors. It is unlikely that an interaction between such factors can be modeled using a subset of the interaction components.

Our preference for models containing full sets of interaction components only applies to irregular designs - as are the designs of special interest considered here. For regular designs, components of an interaction are defined by modular arithmetic (see, eg, Wu and Hamada [2000]). While it remains unlikely that an interaction between categorical factors can be fully modeled using only one component, the components form mutually orthogonal sets whose activity can be judged by standard methods.

The weighing of the multiple criteria to judge the quality of an OA will very much depend on the practical context of the experiment. We should want to restrict attention to the arrays that have good combined properties regarding these criteria. Following Sun et al. [1997], we discard inadmissible arrays. Let c be the number of criteria studied. An array is inadmissible according to c criteria if there is another array that is strictly better according to at least one of these c criteria and equally good according to the remaining criteria. Otherwise, the array is called admissible according to these c criteria.

Detailed results. A major issue in comparing non-isomorphic arrays concerns the computational feasibility of the criteria. This depends on the number of non-isomorphic arrays as well as on the number of possible interaction models. For the four OA$(54; 3^5; 3)$ arrays, the total number of k-interaction models, $k = 0, \ldots, 10$ is 2^{10}. Extension of the arrays with an additional two-level factor gives a total of 2^{15} models to consider. These quantities as well within what can be done on a fast PC. This permits the study of MFS and EC criteria. However, our OA$(48; 3 \cdot 2^9; 3)$ and our sets of 72-run arrays just have too many factors to permit all possible models to be considered. Thus it is not feasible to study all MFS. For the first 1304 OA$(72; 3^2 \cdot 2^7; 3)$, we tabulated ranks of selected sub-matrices. For the four OA$(48; 3 \cdot 2^9; 3)$ and the first 379 OA$(72; 3^2 \cdot 2^8; 3)$, we considered the EC of 1000 randomly selected models with k_1 2×2 and k_2 2×3 interactions and all feasible combinations of k_1 and k_2. For the first OA$(72; 3^2 \cdot 2^8; 3)$ set, we also considered for every configuration of 2×2 and 2×3 interactions models that either did or did not include the single 3×3 interaction. The results were tabulated according to the included numbers of interactions of each type.

OA$(54; 3^5; 3)$. Our study of the arrays 54.5.0.1 and 54.5.0.2 is based on the original arrays of Hedayat et al. [1997]. For the study of arrays 54.5.0.3 and 54.5.0.4, we used our lexicographical minimal arrays because of representational convenience: these arrays are extended with a two-level factor in Table A.2. Table 5.5 shows EC, expressed as a percentage of the total number of k-interaction models, and the values of A_4. The arrays 54.5.0.1 and 54.5.0.2 have identical estimation capacities and A_4 values. Also, the non-estimable models in either of the arrays have exactly the same specifications. There are 25 MFS, all having 6 interaction terms. They fall apart into two classes, whose graph representations are given as Figure 5.1. The first class of MFS consists of the 15 possible models whose graph representation is isomorphic to the left graph in the figure; the second class consists of the 10 possible models whose graph is isomorphic to the right graph in the figure.

The graphs in Figure 5.1 do not match the following specifications: (1) models containing at most 5 interactions; (2) models containing interactions among 4 out of the 5 factors only; (3) models containing interactions between any factor and at most 2 of the other factors.

TABLE 5.5. EC and A_4-values of OA$(54; 3^5; 3)$s

k	I = 54.5.0.1	II = 54.5.0.2	III = 54.5.0.3	IV = 54.5.0.4
1	100	100	100	100
2	100	100	97.8	100
3	100	100	93.3	100
4	100	100	86.7	99.5
5	100	100	77.8	97.6
6	88.1	88.1	64.8	92.9
7	0	0	40.0	83.3
8	0	0	0	66.7
9	0	0	0	40.0
10	0	0	0	0
A_4	3.056	3.056	3	3

So it would seem save to use I or II to estimate the parameters for these models. However, estimability of all models containing k interactions does not guarantee that we can distinguish between these models. This is because several models may lead to the same set of fitted values [Miller and Sitter, 2001]. Srivastava [1975] studies conditions for which one can identify the true model from all the models containing main effects and k interactions. Assuming observations without error, he showed that a necessary and sufficient condition (of this identification) is the estimability of all models containing $2k$ interactions. (His actual formulation was more general. Here we apply his results to strength 3 arrays assuming that we always want to estimate all the main effects.) A design that fulfills the condition is said to be strongly resolvable with resolving power k.

We conclude that arrays I and II permit identification of any model with two interactions, provided that these are sufficiently large as compared with experimental error. The arrays can also be used to identify models with more than 2 interactions, but additional experimentation may be required to identify the true model; see Miller and Sitter [2001] for further argumentation. We note finally that I is inadmissible if n_2 is used as a criterion additional to k or A_4; see Table 5.3.

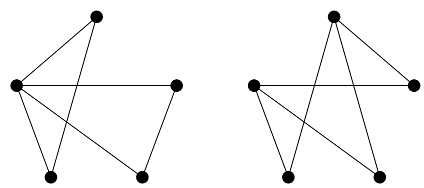

FIGURE 5.1. Minimum forbidden sub-configurations in array I, II of OA$(54; 3^5; 3)$

There are a total of 5 MFS in array III; see Figure 5.2. One MFS has 2 interactions; the remaining 4 contain 6 interactions. Thus, the array is inadmissible if k, A_4, and n_2 are used as criteria.

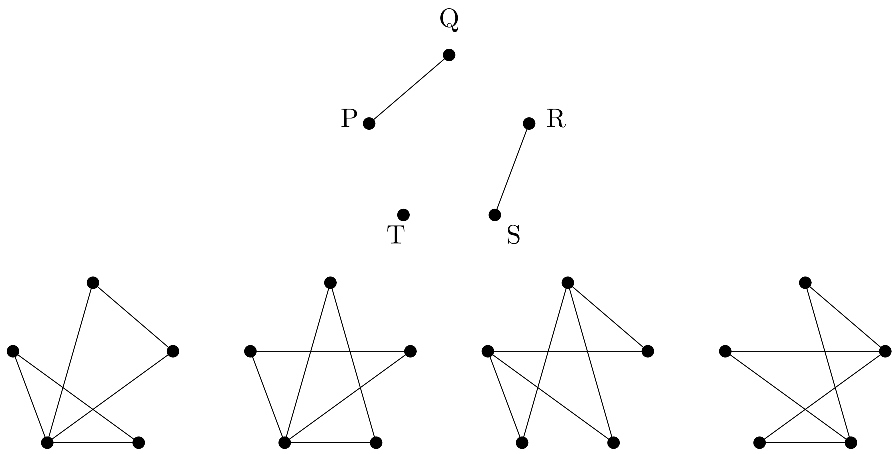

FIGURE 5.2. Minimum forbidden sub-configurations in array III of OA($54; 3^5; 3$)

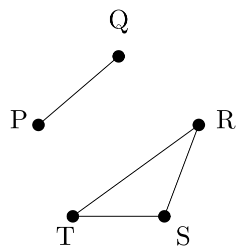

FIGURE 5.3. Minimum forbidden sub-configurations in array IV of OA($54; 3^5; 3$)

The EC results of array IV, finally, are fully explainable by a single MFS, which is shown in Figure 5.3. It contains the interactions PQ, QT, TP and RS. If we can assume absence of any of these interactions, the remaining interactions can all be estimated. This leads us to prefer 54.5.0.4 in general. We prefer 54.5.0.2 if the following three conditions apply simultaneously: first, it is not possible to appoint some interaction as negligible; second, additional experimentation is not feasible; third, there are at most 2 active interactions. Note that selection on the basis of A_4 alone would leave the matter undecided between 54.5.0.4 and 54.5.0.3.

OA($54; 3^5 \cdot 2; 3$). Arrays 54.5.1.1 and 54.5.1.2 are non-isomorphic extensions of 54.5.0.3; 54.5.1.3 and 54.5.1.4 were obtained by extending 54.5.0.4. All arrays have an A_4 of 5.667. In Table 5.6, we give the numbers of MFS according to the number of 3×3 interactions (rows) and 2×3 interactions (columns). The results in the Table lead us to prefer 54.5.1.3, because it has a total of two 4-interaction MFS, as opposed to one 2-factor interaction MFS for 54.5.1.1 and 54.5.1.2, and four 4-interaction MFS for 54.5.1.4. The MFS of 54.5.1.3 that has 2 interactions of each type consists of $\{RS, RT, AP, AQ\}$, with A denoting the two-level factor. The 2 MFS with three 3×3 interactions and two 2×2 interactions contain $\{AP, AQ\}$ and either $\{PQ, RS, ST\}$ or $\{PQ, RT, ST\}$. Combining this result with the MFS with four 3×3 interactions of Figure 5.1, if one can point out an unlikely interaction of either type, we can assign the factors in such a way that the array is strongly resolvable with resolving power 4. A table with detailed results on all MFS of the 4 arrays is available upon request.

OA$(48; 3 \cdot 2^9; 3)$. We checked the EC for sets of 1000 randomly selected models with k_1 2×2 interactions, k_2 2×3 interactions and all feasible values of k_1 and k_2. The results are summarized below.

Array	$EC_{..}$	$EC_{.0}$	$n_{2(.0)}$	A_4
1	447	665	28	8.222
2	403	598	28	8.222
3	549	733	33	8.556

The EC results are expressed as the number of estimable models among the 1000 selected ones. The characteristics shown are the mean EC over all 37×10 (k_1, k_2) pairs, the mean EC over all 37 $(k_1, 0)$ pairs, and the n_2 value when the 2×3 interactions are not considered. The results clearly let us to discard arrays 1 and 2 as inadmissible under these criteria. However, 48.1.9.1 is admissible if A_4 is used as an additional criterion.

TABLE 5.6. Numbers of MFS in OA$(54; 3^5 \cdot 2; 3)$s

54.5.1.1

0	0	0	0	0	0
0	0	0	0	0	0
1	0	1	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
4	0	18	0	0	0
0	0	0	0	0	0

54.5.1.2

0	0	0	0	0	0
0	0	0	0	0	0
1	0	2	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
4	0	16	0	0	0
0	0	0	0	0	0

54.5.1.3

0	0	0	0	0	0
0	0	0	0	0	0
0	0	1	0	0	0
0	0	2	0	0	0
1	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	3	0	0	0
0	0	3	6	0	-
0	3	0	-	-	-

54.5.1.4

0	0	0	0	0	0
0	0	0	0	0	0
0	0	3	0	0	0
0	0	0	0	0	0
1	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	3	0	0	0
0	0	3	6	0	-
0	3	0	-	-	-

OA$(72; 3^2 \cdot 2^7; 3)$. We studied the list of OA$(72; 3^2 \cdot 2^7; 3)$ arrays using the following criteria for selecting OAs

(1) the rank of the matrix with all components of the 2-factor interactions, $n_{2(\ldots)}$,

(2) the rank of the interaction matrix excluding the components of the 3×3 interaction, $n_{2(..0)}$,
(3) the rank of the matrix of just the 2×2 interactions, $n_{2(.00)}$,
(4) the rank of just the 2×3 interactions, $n_{2(0.0)}$,
(5) the value of A_4 (the fourth component of GWLP given in (5.3.1)), and
(6) the orthogonality of the 2×3 interactions to the remaining interactions, respectively. We also included
(7) the minimum decrease in n_2 in case the design was to be blocked in 6 blocks, df_6, and
(8) the minimum decrease for the 12 blocks case, df_{12}.

A full discussion of the blocking issue is given in Section 5.4. Under the aforementioned criteria, only 17 of the designs are admissible. Properties of the admissible designs are give in Table 5.7. We noted earlier the existence of 4 arrays with the

TABLE 5.7. Admissibility among the first 1304 OA($72; 3^2 \cdot 2^7; 3$)s

Array	$n_{2(...)}$	$n_{2(..0)}$	$n_{2(.00)}$	$n_{2(0.0)}$	A_4	df_6	df_{12}
178	51	48	21	27	5.17	3	-
552	46	42	16	26	5.50	3	5
588	51	47	21	26	4.53	3	-
822	45	41	16	27	5.83	3	9
824	45	41	16	27	5.83	3	9
1024	51	47	21	28	5.53	3	-
1078	53	49	21	28	5.15	-	-
1079	53	49	21	28	5.15	-	-
1080	53	49	21	28	5.15	-	-
1081	53	49	21	28	5.15	-	-
1157	47	43	20	28	5.44	4	10
1187	48	46	21	28	4.98	5	11
1189	48	46	21	28	4.98	5	11
1230	52	48	21	28	5.13	4	-
1253	52	48	21	28	5.13	4	-
1294	48	46	21	28	5.25	4	11
1296	45	41	16	27	5.67	3	10

NOTES: Array numbers printed in bold have 2×3 interactions orthogonal to all remaining interactions

maximum possible value of $n_{2(...)}$. For these arrays we calculated a determinant D as $D = |\mathbf{X}'\mathbf{X}|^{1/53}/72$, where $\mathbf{X}$ is the 72×53 matrix of all 53 components of the two-factor interactions, normalized to squared length 72. The values of D are 0.5393, 0.5391, 0.5393, and 0.5406 for the arrays 1078, 1079, 1080, and 1081, respectively. Thus, array 1081 is slightly better than the three other arrays. The remaining 13 arrays are all worse in their rank-based criteria, but better in either the blocking, the contamination or the orthogonality criteria. There are three pairs of equally good arrays. Finally, the arrays with the space of the 2×3 interactions orthogonal to the remaining interactions do not have a full rank of the 2×3 interaction matrix.

The list of admissible arrays reduces the problem of choosing from 1304 arrays to the problem of choosing from 17 arrays. If no blocking is required, we would generally suggest array 1081; it is given in Table A.3. A possible disadvantage of this array is a slightly more pronounced correlation between the two-factor interactions as exhibited by larger A_4 values and the 2×3 subspace being in-orthogonal to the other interactions. However, we would take this risk and solve ambiguities by follow-up experimentation, as this permits all subsets of the interactions to be studied. We note that the best arrays according to the EC criterion cannot be blocked in 6 or 12 blocks. There are several arrays that permit an arrangement in 6 blocks with 48 remaining degrees of freedom to estimate interactions. As regards arrangements in 12 blocks, array 552, given in full in Table A.3, is the best option in view of the 41 remaining degrees of freedom for the interactions.

If there are less than seven 2-level factors required, we would suggest omitting columns from array 1081. However, it may be possible that there are maximum-rank $\mathrm{OA}(72; 3^2 \cdot 2^a; 3)$ with $a = 5$ or 6 that have better values of the model matrix's determinant, and full series of these arrays are required to pick up the best one.

$\mathrm{OA}(72; 3^2 \cdot 2^8; 3)$. We studied the $\mathrm{OA}(72; 3^2 \cdot 2^8; 3)$ using criteria (1) up to (8) from the study of the $\mathrm{OA}(72; 3^2 \cdot 2^7; 3)$. As there were no arrays with a full rank of the interaction sub-matrix ($n_2 = 64$), it is of interest to include further criteria based on a more detailed assessment of the estimation capacity. So we also included

(9) the mean estimation capacity over all models with 0 up to 45 two-factor interactions, $EC_{(\ldots)}$,
(10) the mean estimation capacity of the interaction models excluding the components of the 3×3 interaction, $EC_{(..0)}$,
(11) the mean estimation capacity of models involving just the 2×2 interactions, $EC_{(.00)}$,
(12) the mean estimation capacity of just the 2×3 interactions, $EC_{(0.0)}$,
(13) the maximum number of 2×2 interactions for which all 1000 models not containing any other interaction are estimable, and
(14) the corresponding value for the 2×3 interactions.

Under these criteria, 36 $\mathrm{OA}(72; 3^2 \cdot 2^8; 3)$ are admissible. Properties of the admissible designs are give in Tables 5.8 and 5.9. We would generally prefer array 379 if no blocking is required, see Table A.3. Its estimation capacities are superior to those of the remaining arrays. The remaining arrays are also admissible because they either have orthogonal 2×3 subspaces or have larger values of $m_{(2\times 3)}$. However, the EC value for ten 2×3 interactions in arrays 379 is 993. So we do not expect problems here. As in the previous case, the best array according to the EC criterion cannot be blocked in 6 or 12 blocks. The arrays 19, 95, 104, 130, and 246 permit an arrangement in 6 blocks with 45 remaining degrees of freedom to estimate interactions. Arrays 264 and 280 give a 12-block arrangements with 33 degrees of freedom left for the interactions; the latter array is given in Table A.3.

5.4. Blocking

Methodology. Randomization of the runs of an OA protects the effect-estimates against contamination with unknown sources of extraneous variation. However, if these sources are known, one tries to block the experimental runs into groups to

TABLE 5.8. Selected OA($72; 3^2 \cdot 2^8; 3$)s: rank and estimation capacities

Array	$n_{2(\ldots)}$	$n_{2(..0)}$	$n_{2(.00)}$	$n_{2(0.0)}$	$EC_{(\ldots)}$	$EC_{(..0)}$	$EC_{(.00)}$	$EC_{(0.0)}$
19	48	44	18	26	382	382	493	772
68	39	35	11	24	287	287	384	747
70	39	35	11	24	290	290	384	756
84	39	35	11	24	287	287	385	745
95	48	44	18	26	373	373	495	751
104	48	44	18	26	360	360	496	728
118	42	38	14	24	338	338	472	717
130	48	44	18	26	360	360	494	729
138	39	35	11	24	288	288	385	749
157	39	35	11	24	286	286	384	744
177	42	38	14	24	351	351	472	744
180	39	35	11	24	290	290	384	755
183	39	35	11	24	289	289	383	754
195	39	35	11	24	290	290	383	755
199	39	35	11	24	288	288	385	748
236	47	44	19	25	429	431	592	731
239	48	44	18	26	384	384	493	778
241	52	50	24	26	525	527	667	791
246	48	44	18	26	360	360	495	728
253	39	35	11	24	289	289	383	753
264	42	38	14	24	346	346	474	734
272	39	35	11	24	287	287	385	748
273	39	35	11	24	288	288	384	753
274	39	35	11	24	288	288	384	750
277	39	35	11	24	282	282	386	736
278	39	35	11	24	278	278	384	722
280	42	38	14	24	342	342	471	727
286	39	35	11	24	288	288	385	749
297	39	35	11	24	289	289	384	753
347	39	35	11	24	288	288	383	751
374	47	44	19	28	516	516	611	855
375	47	44	19	28	516	517	611	855
376	47	44	19	28	516	516	608	856
377	47	44	19	28	516	516	610	855
378	42	38	14	25	350	350	472	746
379	54	51	28	30	814	815	1000	837

NOTES: Admissibility arrays based on the first 379 cases. EC based on 1000 randomly selected models for each of k_1 2×2 and k_2 2×3 interactions. Array numbers printed in bold have 2×3 interactions orthogonal to all remaining interactions

eliminate the variation without biasing the effect-estimates. In fact, blocking is a classical device treated in all the standard textbooks, such as the one by Box et al. [1978]. Most of the theory on blocking concentrates on regular designs (see, eg, Sun et al. [1997], Sitter et al. [1997], and Cheng and Wu [2002]). The main concern is to construct a blocking factor whose main effect is orthogonal to all the main

TABLE 5.9. Selected OA$(72; 3^2 \cdot 2^8; 3)$s: further properties

Array	$m_{(2\times2)}$	$m_{(2\times3)}$	A_4	df_6	df_{12}
19	6	7	10.94	3	-
68	5	9	14.89	3	-
70	6	9	15.11	3	-
84	6	8	15.11	3	-
95	7	7	10.94	3	-
104	7	4	10.83	3	-
118	7	8	14.64	3	-
130	8	4	11.27	3	-
138	6	9	15.67	3	-
157	7	8	15.22	3	-
177	6	9	13.09	3	-
180	5	10	15.33	-	-
183	7	10	14.89	-	-
195	5	10	14.44	-	-
199	5	10	15.33	3	-
236	9	7	12.48	-	-
239	7	9	10.72	-	-
241	8	8	10.23	-	-
246	6	4	10.83	3	-
253	6	9	15.33	3	9
264	5	7	14.09	3	9
272	6	8	15.00	3	9
273	6	9	15.33	3	9
274	6	9	15.00	3	9
277	6	5	15.33	3	9
278	6	6	14.67	3	9
280	7	5	13.09	3	9
286	6	9	15.22	3	-
297	6	10	14.67	3	-
347	5	10	14.67	3	9
374	7	11	13.49	-	-
375	6	10	13.10	-	-
376	7	10	13.49	-	-
377	8	10	13.10	-	-
378	6	8	14.83	5	-
379	28	8	11.28	-	-

NOTES: Admissibility arrays based on the first 379 cases. EC based on 1000 randomly selected models for each of k_1 2×2 and k_2 2×3 interactions. Array numbers printed in bold have 2×3 interactions orthogonal to all remaining interactions

effects of the experimental factors, and also orthogonal to as many of the 2-factor interactions as is possible. In this section, we give some blocking methodology for orthogonal arrays of strength t, and apply the methodology to the arrays of special interest. We start with the following.

DEFINITION 57. *An* orthogonally blocked orthogonal array $\mathrm{OAB}(N; r_1 \cdots r_d; b; t_1, t_2)$, $t_1 \geq t_2$, *is an* $\mathrm{OA}(N; r_1 \cdots r_d; t_1)$ *with an additional column* B *containing* b *symbols such that the resulting array is an* $\mathrm{OA}(N; r_1 \cdots r_d, b; t_2)$.

It follows immediately from the definition that the block size in such an array must be divisible by $\mathrm{lcm}(r_1, \ldots, r_d)$. If $t_1 = t_2$, the problem of finding factor B is equivalent to finding an additional treatment factor while maintaining the strength of the array. If $t_1 > t_2$, a new class of problems emerges. For arrays with $t_1 = 3$ and $t_2 = 2$, we propose to search for blocking factors in 2 stages. First, we search for basic blocking factors (BBFs) defined by the following procedure.

(1) Include in the set of BBFs all s-level components of 2-factor interactions between s-level factors, calculated by modular arithmetic, for all distinct values of s present in the array.
(2) Augment the set of BBFs with factors from the orthogonal array that are not used as treatment factors.
(3) For each p-tuple of s-level factors and each distinct value of s in the array, use modular arithmetic to calculate s-level potential blocking factors (PBFs). Here, $p = 3, \ldots, k_s$, and k_s is the maximum value of p for which components of the p-factor interaction are still estimable after allowing for all interactions of order up to $p - 1$.
(4) Discard PBFs that are not orthogonal to all the main effects.
(5) Discard PBFs of order $p > 2$ if they are fully aliased with components of interactions of order up to $p - 1$.
(6) Augment the set of BBFs with the PBFs not discarded in the previous steps.

The numbers of levels of the BBFs are a subset from those of the original factors in the array. In the second stage of the search for blocking factors, we construct compound blocking factors (CBFs) with levels outside this subset. To do so, we combine two ore more BBFs by the method of grouping [Wu, 1989] and check whether the resulting factor is orthogonal to the main effects. As a special case, we can always construct 4-level blocking arrangements in arrays with more than two binary factors by using any pair of interactions that share a common factor.

To illustrate the construction of the set of BBFs, consider array 54.5.1.1. There are a total of 10 2-factor interactions of 4 degrees of freedom each. Each interaction can be decomposed into 2 orthogonal components $X + aY = c \pmod 3; a = 1, 2$. Thus, after step 1 of the procedure, there are a total of 20 3-level factors in the set of BBFs. Further, the two-level factor of the array need not be used. If this is indeed the case, the array of the treatment factors is equivalent to 54.5.0.3, and the two-level factor is added to the set of BBFs; see step 2 of the procedure. The space spanned by the 3-factor interactions has 8 degrees of freedom (see Table 5.3). There are a total of 10 possible 3-factor interactions. Each of these consists of 4 orthogonal components of the type $X + aY + bZ = c \pmod 3; a, b = 1, 2$. Thus, step 3 results in a total of 40 PBFs of order 3. We discarded 22 of these because they were not orthogonal to the main effects (step 4). In step 5, a further 6 components were discarded because they were fully aliased with 2-factor interactions. The set $\{PQ^2T, PQ^2T^2, PRT, PRT^2, PST, PST^2, QRT, QRT^2, QST, QST^2, RS^2T, RS^2T^2\}$ remains. This set is joined with the 2-factor components and the two-level factor to arrive at the final set of BBFs.

To construct a 6-level CBF, we check all possible ways to group the two-level BBF with a 3-level BBF. The BBFs $PQ^2T, PQ^2T^2, PQ, RS, PT^2, QT^2, RS^2$, combined with the two-level factor, give orthogonal blocking with a drop in n_2 of 0, 0, 2, 2, 2, 2, and 3, respectively.

Any BBF or CBF can be used to block the array orthogonally to the main effects. Among equally-leveled blocking factors, we prefer the one that causes the lowest possible drop in n_2, and, if possible, is orthogonal to the 2-factor interactions. In the 6-level blocking case, we clearly would prefer using PQ^2T or PQ^2T^2.

The procedure could be refined by decomposing any factor whose number of levels is not a prime into prime-leveled pseudo-factors, and using these to define PBFs. For example, a 4-level factor can be decomposed in 3 single-degree-of-freedom pseudo-factors. For our designs of special interest, this is clearly not applicable.

Results. $\mathrm{OA}(48; 3 \cdot 2^9; 3)$. For these arrays, block sizes have to be a multiple of 6. Thus, we want to search for $2 \times 24, 4 \times 12$, or 8×6 arrangements. All PBFs of order 3 and higher are fully aliased with the 2-factor interactions. For arrays 48.1.9.1 and 48.1.9.2, the 4-level CBFs can only be constructed by grouping pairs of interactions sharing a common factor. There were no 8-blocks arrangements found for these arrays. For array 48.1.9.3, there are 9 additional ways to create an arrangement in 4 blocks. These are defined by any pair of interactions not sharing a common factor from $\{B, C, D, J\}$, or from $\{B, C, E, G\}$, or from $\{B, C, F, H\}$. The array further has 48 different ways to create 8 blocks of 6 units each. These are given by taking 3 independent interactions from any single set from the above sets of factors.

$\mathrm{OA}(54; 3^5; 3)$ and $\mathrm{OA}(54; 3^5 \cdot 2; 3)$. The arrays 54.5.0.1 and 54.5.0.2 cannot be extended to an $\mathrm{OA}(54; 3^5 \cdot 2; 3)$. So it is not possible to construct an $\mathrm{OAB}(N; 3^5; 2; 3, 3)$ from these arrays. We found an $\mathrm{OAB}(N; 3^5; 2; 3, 2)$ by exploiting the fact that the arrays have index 2. For the first 3 factors in the first block, we wrote down a complete 3^3. For each run in the second block, the factor levels of the first three factors were chosen complementary to those in the first block. The settings of the remaining 2 factors were added in such a way that each run indeed occurred in the 3^5 array. By counting frequencies and exchanging runs, we arrived at the arrangements given in Table 5.10; these do not cause a drop in n_2. There were no BBFs consisting of higher-order interaction components. The set of BBFs, including the heuristically found two-level BBF, could not be combined to a multi-level blocking arrangement.

Table 5.11 gives recommended blocking arrangements for 54.5.1.1 up to 54.5.1.4, and for their parental $\mathrm{OA}(54; 3^5; 3)$ arrays. Here, factor A denotes the two-level factor. If A is used as a treatment factor, potential blocks have 6 or 18 runs. These cases are labeled — *1*. The Table shows that there is no appreciable difference in arrays 1–4 regarding the impact of the blocking on estimability of 2-factor interactions. We conclude that array 54.5.1.3 remains the preferred array if blocking is called for.

If A is not employed as a treatment factor, blocks may have 3, 6, 9, or 18 runs. The corresponding rows in the table are labeled — *0*. The table shows that our generally recommended 54.5.0.4 cannot be arranged in 18 blocks of 3 runs. So for this case we have to resort to 54.5.1.2, using factor A as a BBF. This revokes the previous judgment of inadmissibility for the 18-block case. In all other blocked

TABLE 5.10. Orthogonal blocking of 54.5.0.1 and 54.5.0.2 in 2 blocks

54.5.0.1		54.5.0.2	
block 1	block 2	block 1	block 2
0 0 0 1 1	0 0 0 2 2	0 0 0 0 0	0 0 0 0 0
0 0 1 0 1	0 0 2 0 2	0 0 1 1 1	0 0 2 1 2
0 0 2 2 0	0 0 1 1 0	0 0 2 2 1	0 0 1 2 2
0 1 0 0 1	0 2 0 0 2	0 1 0 1 2	0 2 0 1 1
0 1 1 0 0	0 2 2 0 0	0 1 1 0 2	0 2 2 0 2
0 1 2 2 1	0 2 1 1 2	0 1 2 2 0	0 2 1 0 1
0 2 0 2 0	0 1 0 1 0	0 2 0 2 2	0 1 0 2 1
0 2 1 2 1	0 1 2 1 2	0 2 1 2 0	0 1 2 0 1
0 2 2 1 1	0 1 1 2 2	0 2 2 1 0	0 1 1 1 0
1 0 0 0 1	2 0 0 0 2	1 0 0 1 1	2 0 0 1 2
1 0 1 2 2	2 0 2 1 1	1 0 1 2 0	2 0 2 0 2
1 0 2 1 2	2 0 1 2 1	1 0 2 0 1	2 0 1 1 0
1 1 0 2 2	2 2 0 1 1	1 1 0 2 0	2 2 0 2 0
1 1 1 1 1	2 2 2 2 2	1 1 1 0 0	2 2 2 2 2
1 1 2 0 2	2 2 1 0 1	1 1 2 1 2	2 2 1 0 0
1 2 0 1 2	2 1 0 2 1	1 2 0 0 2	2 1 0 1 0
1 2 1 0 2	2 1 2 0 1	1 2 1 1 2	2 1 2 0 0
1 2 2 0 1	2 1 1 0 2	1 2 2 0 0	2 1 1 2 1
2 0 0 2 0	1 0 0 1 0	2 0 0 2 1	1 0 0 2 2
2 0 1 1 2	1 0 2 2 1	2 0 1 0 1	1 0 2 1 0
2 0 2 0 0	1 0 1 0 0	2 0 2 2 0	1 0 1 0 2
2 1 0 1 2	1 2 0 2 1	2 1 0 0 2	1 2 0 1 0
2 1 1 2 0	1 2 2 1 0	2 1 1 2 2	1 2 2 2 1
2 1 2 1 0	1 2 1 2 0	2 1 2 1 1	1 2 1 2 1
2 2 0 0 0	1 1 0 0 0	2 2 0 0 1	1 1 0 0 1
2 2 1 1 0	1 1 2 2 0	2 2 1 1 2	1 1 2 2 2
2 2 2 2 2	1 1 1 1 1	2 2 2 1 1	1 1 1 1 1

cases, the arrays derived from 54.5.0.4 have more degrees of freedom available to estimate interactions.

$OA(72; 3^2 \cdot 2^7; 3)$ and $OA(72; 3^2 \cdot 2^8; 3)$. The 72-run arrays can potentially be blocked in 2, 3, 4, 6, or 12 blocks. There were no higher-order interactions among two-level factors that were orthogonal to all the main effects. This is an interesting observation, because there exist three 72.2.12, and the additional main effects in these arrays must somehow employ the higher-order interaction space of arrays with less two-level factors. Clearly, our approach does not result in all possible blocking arrangements. A more complete enumeration of blocking arrangements would be quite interesting. However, we believe that such an enumeration would be computationally much more cumbersome than our present approach.

We enumerated the blocking arrangements for the series of $OA(72; 3^2 \cdot 2^7; 3)$ and $OA(72; 3^2 \cdot 2^8; 3)$ arrays employing just their 2-factor interaction components. The arrangements in 2, 3 and 4 blocks can be constructed trivially from the BBFs. In many arrays, the BBFs could not be combined to a 6-level or a 12-level CBF.

TABLE 5.11. Selected blocking arrangements for OA($54; 3^5 \cdot 2; 3$)s

Arrangement	54.5.1.1		54.5.1.2		54.5.1.3, 54.5.1.4	
	BBFs	Δn_2	BBFs	Δn_2	BBFs	Δn_2
$2 \times 27 \mid 0$	A	0	A	0	A	0
$3 \times 18 \mid 0$	PQ^2T	0	PQ^2T	0	PRS	2
$\mid 1$	2fi	2	2fi	2	2fi	2
$6 \times 9 \mid 0$	A, PQ^2T	0	A, PQ^2T	2	A, PQ	2
$9 \times 6 \mid 0$	PQ^2T, PQ	6	PQ^2T, PQ	6	PRT^2, PT	8
$\mid 1$	PQ^2T, PQ	8	PQ^2T, PQ	8	PRT^2, PT	8
$18 \times 3 \mid 0$	-	-	A, PQ^2, PR^2	15	-	-

For arrays that did allow for such CBFs, we searched for the CBF that minimized the drop in degrees of freedom for the 2-factor interaction space. This gives us the two additional properties to list the admissible designs of the Tables 5.7, 5.8 and 5.9.

5.5. Conclusion

This chapter featured selection of an orthogonal array from a set of non-isomorphic OA($N; r_1 \cdot r_2 \cdots r_d; 3$) to use as an experimental design. We proposed methodology to reduce to much smaller sets of admissible arrays. Finally, we addressed the question of how to group the runs of an array in equally sized blocks. For this purpose, we defined orthogonally blocked orthogonal arrays (OABs) and we studied OAB($N; r_1 \cdots, r_d; b; 3, 2$) by exploiting components of 2-factor interactions.

Using an algorithm to generate series of arrays gives little information on succinct ways to construct individual arrays. Knowledge of an explicit construction method may well lead to more insight into the best way to analyze the results of an experiment. We would therefore welcome a more extensive study of the arrays developed. As the set of two-level factors in many of the arrays developed here could be subsets of Hadamard matrices, we would particularly welcome further elucidation of the relation of the present arrays with these matrices.

CHAPTER 6

A collection of strength 3 orthogonal arrays

6.1. Introduction

This chapter is organized as follows. Section 6.2 recalls known results and presents parameters of strength 3 orthogonal arrays (OAs) with $8 \le N \le 100$. Section 6.3 presents the construction of OAs with $72 \le N \le 100$. Finally, we use the methods of Chapter 4 to obtain a table of many isomorphism classes of OAs with run size at most 100 in Section 6.4. For convenience, we abbreviate methods used for constructing and enumerating orthogonal arrays. The abbreviations are listed in Table 6.1. It is also convenience to use abbreviations for specific lower bounds and for particular nonexistence proofs. These too are listed in Table 6.1.

Notation	Name	Reference
(A)	Arithmetic	3.5
(B)	Backtrack search for $s_1^a s_2^b$ OAs	4.4
(C)	Colored graphs	4.3
(Con)	Concatenation	3.3
(D)	Decomposing sub-arrays	3.7
(La)	Latin squares	3.6
(H)	Hadamard construction	3.3
(I)	Integer linear programming (ILP)	4.5
(IS)	ILP with symmetry	4.5
(J) and (L)	Juxtaposition and Linear code	3.3
(M) and (O)	Multiplication and Even sum	,,
(O'), (Br)		Brouwer [2004]
(Q)	Quasi-multiplication	3.3
(S) and (T)	Split and Trivial design	,,
(X), (X_6)		Brouwer et al. [2005]
(X_3), (X_4), (X_5)	explicit constructions	,,
(X_1), (X_7), (***)	mixed additive codes	,,
(3^5)		Hedayat et al. [1997]
(Rao)	the *generalized Rao bound*	Rao [1947]
(Del)	the *Delsarte bound*	Delsarte [1973]
(Div)	the divisibility condition	
(5.1)	$\nexists\,$OA$(24; 3 \cdot 2^5; 3)$, Sec. 5.1	Brouwer et al. [2005]
(5.9)	$\nexists\,$OA$(64; 4^5 \cdot 2^3; 3)$, Sec. 5.9	,,
(5.10)	$\nexists\,$OA$(64; 4^3 \cdot 2^9; 3)$, Sec. 5.10	,,

TABLE 6.1. An overview of constructions, lower bounds on run sizes

6.2. Parameter sets of OAs with run size $8 \le N \le 100$

The *divisibility condition* for the run size of an orthogonal array F gives a necessary condition for the existence of F in terms of its parameters.

LEMMA 58. *In an* $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; t)$*, the run size N must be divisible by the least common multiple* (lcm) *of all numbers* $\prod_{i \in I} r_i$ *where* $|I| = t$.

PROOF. This says that the t times derived design has an integral run size. □

For example, in an $\mathrm{OA}(N; 3^5 \cdot 2; 3)$, N must be a multiple of $\mathrm{lcm}(3 \cdot 3 \cdot 3, 2 \cdot 3 \cdot 3) = 54$. By this criterion, there is no strength 3 OA with N greater 64 and less than 72.

In Brouwer et al. [2005], we constructed all orthogonal arrays of strength 3 with run sizes N at most 64. The main result of that paper is

THEOREM 59. *For every set of parameters $N, r_1, r_2, \ldots, r_d$ and $N \le 64$ such that an orthogonal array* $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; 3)$ *exists, we construct at least one such array. More precisely, if $d = 3$ such an array is trivial, and if $d > 3$ a construction is presented or a proof of nonexistence is given.*

The result is presented in Table 6.2.

Table 6.2: Parameters of OAs of strength 3 with $N \le 64$

N	Type	Existence	Construction	Nonexistence
8	2^a	$a \le 4$	(H)	
16	$2^a \cdot 4$	$a \le 3$	(M)	
16	2^a	$a \le 8$	(H)	
24	$2^a \cdot 6$	$a \le 3$	(M)	
24	$2^a \cdot 3$	$a \le 4$	(M)	$a = 5$
24	2^a	$a \le 12$	(H)	
27	3^b	$b \le 4$	(L)	$b = 5$
32	$2^a \cdot 8$	$a \le 3$	(M)	
32	$2^a \cdot 4^2$	$a \le 4$	(X_1)	
32	$2^a \cdot 4$	$a \le 7$	(M)	
32	2^a	$a \le 16$	(H)	
36	$2^2 \cdot 3^2$		(T)	
40	$2^a \cdot 10$	$a \le 3$	(M)	
40	$2^a \cdot 5$	$a \le 6$	(X)	$a = 7$
40	2^a	$a \le 20$	(H)	
48	$2^a \cdot 12$	$a \le 3$	(M)	
48	$2^a \cdot 4 \cdot 6$	$a \le 2$	(M)	$a = 3$
48	$2^a \cdot 6$	$a \le 7$	(M)	
48	$2^a \cdot 3 \cdot 4$	$a \le 4$	(X_3)	$a = 5$
48	$2^a \cdot 4$	$a \le 11$	(M)	
48	$2^a \cdot 3$	$a \le 9$	(X_4)	$a = 10$
48	2^a	$a \le 24$	(H)	
54	$3^b \cdot 6$	$b \le 3$	(M)	$b = 4$
54	$2^a \cdot 3^b$	$a \le 1$, $b \le 5$	(X_5)	$(a, b) = (0, 6)$
56	$2^a \cdot 14$	$a \le 3$	(M)	
56	$2^a \cdot 7$	$a \le 6$	(J)	$a = 7$

continued on next page

Table 6.2 (continued)

N	Type	Existence	Construction	Nonexistence
56	2^a	$a \le 28$	(H)	
60	$2^2 \cdot 3 \cdot 5$		(T)	
64	$2^a \cdot 16$	$a \le 3$	(M)	
64	$2^a \cdot 4 \cdot 8$	$a \le 4$	(M)	
64	$2^a \cdot 8$	$a \le 7$	(M)	
64	4^c	$c \le 6$	(L)	
64	$2^a \cdot 4^5$	$a \le 2$	(S)	$a = 3$
64	$2^a \cdot 4^4$	$a \le 6$	(X_6)	
64	$2^a \cdot 4^3$	$a \le 8$	(S)	$a = 9$
64	$2^a \cdot 4^2$	$a \le 12$	(X_7) or (Q)	
64	$2^a \cdot 4$	$a \le 15$	(M)	
64	2^a	$a \le 32$	(H)	

LEMMA 60. *The following are the only nontrivial parameter sets for mixed orthogonal arrays of strength 3 and run size at most 100 allowed by* (Div), (Rao), and (Del).

$\mathrm{OA}(4m; 2^a; 3)$	$4 \le a \le 2m$, m even, $2 \le m \le 24$,
$\mathrm{OA}(4m; m \cdot 2^3; 3)$	m even, $2 \le m \le 24$,
$\mathrm{OA}(8m; m \cdot 2^a; 3)$	$3 \le a \le 7$, $3 \le m \le 12$,
$\mathrm{OA}(8m; m \cdot 4 \cdot 2^a; 3)$	$2 \le a \le 4$, m even, $4 \le m \le 12$,
$\mathrm{OA}(9m; m \cdot 3^b; 3)$	$3 \le b \le 4$, $m = 3, 6, 9$,
$\mathrm{OA}(36; 3^2 \cdot 2^a; 3)$	$1 \le a \le 2$,
$\mathrm{OA}(48; 3 \cdot 2^a; 3)$	$3 \le a \le 15$,
$\mathrm{OA}(48; 4 \cdot 3 \cdot 2^a; 3)$	$2 \le a \le 9$,
$\mathrm{OA}(48; 4 \cdot 2^a; 3)$	$3 \le a \le 11$,
$\mathrm{OA}(54; 3^b \cdot 2^a; 3)$	$a = 0, 1$, $b \ge 1$, $a + b \ge 4$, $a + 2b \le 19$,
$\mathrm{OA}(60; 5 \cdot 3 \cdot 2^a; 3)$	$a = 2$,
$\mathrm{OA}(64; 4^c \cdot 2^a; 3)$	$a \ge 0$, $c \ge 1$, $a + c \ge 4$, $a + 3c \le 18$,
$\mathrm{OA}(72; 6^2 \cdot 2^a; 3)$	$1 \le a \le 6$,
$\mathrm{OA}(72; 6 \cdot 3^b \cdot 2^a; 3)$	$0 \le b \le 1$, $1 \le a \le 11$,
$\mathrm{OA}(72; 4 \cdot 3^2 \cdot 2^a; 3)$	$a = 1$,
$\mathrm{OA}(72; 3^b \cdot 2^a; 3)$	$1 \le b \le 2$, $1 \le a \le 23$,
$\mathrm{OA}(80; 5 \cdot 4^b \cdot 2^a; 3)$	$0 \le b \le 1$, $1 \le a \le 15$,
$\mathrm{OA}(80; 4 \cdot 2^a; 3)$	$2 \le a \le 19$,
$\mathrm{OA}(81; 9 \cdot 3^b; 3)$	$b \le 4$,
$\mathrm{OA}(81; 3^b; 3)$	$3 \le b \le 14$,
$\mathrm{OA}(84; 7 \cdot 3 \cdot 2^a; 3)$	$a \le 2$,
$\mathrm{OA}(90; 5 \cdot 3^2 \cdot 2^a; 3)$	$a = 1$,
$\mathrm{OA}(96; 8 \cdot 6^b \cdot 2^a; 3)$	$0 \le b \le 1$ $a + b \ge 3$, $a \le 11$,
$\mathrm{OA}(96; 8 \cdot 3^b \cdot 2^a; 3)$	$0 \le b \le 1$ $a + b \ge 3$, $a \le 11$,
$\mathrm{OA}(96; 6 \cdot 4^b \cdot 2^a; 3)$	$1 \le b \le 2$, $a + b \ge 3$, $3b + a \le 15$,
$\mathrm{OA}(96; 4^c \cdot 3^b \cdot 2^a; 3)$	$0 \le b \le 1$, $0 \le c \le 2$, $a + b + c \ge 4$, $3(c-1) + 2b + a \le 23$,
$\mathrm{OA}(100; 5^2 \cdot 2^a; 3)$	$1 \le a \le 2$.

PROOF. The cases with N at most 64 were given in Brouwer et al. [2005]. The first five cases depending on parameters m were also determined there. We consider now cases with $72 \leq N \leq 100$.

(i) Applying (Rao) to $\mathrm{OA}(12, 6 \cdot 2^a; 2)$ of $\mathrm{OA}(72; 6^2 \cdot 2^a; 3)$ gives $1 \leq a \leq 6$.
$\mathrm{OA}(72; 6 \cdot 3^b \cdot 2^a; 3)$ with $0 \leq b \leq 1$, $1 \leq a \leq 11$: When $b = 1$, we use the derived designs $\mathrm{OA}(12, 3 \cdot 2^a; 2)$, and find $a \leq 9$. When $b = 0$, we use the derived designs $\mathrm{OA}(12, 2^a; 2)$, which leads to $a \leq 11$.
Applying (Div) to $\mathrm{OA}(18, 3^2 \cdot 2^a; 2)$ of $\mathrm{OA}(72; 4 \cdot 3^2 \cdot 2^a; 3)$ we find $a = 1$.
$\mathrm{OA}(72; 3^b \cdot 2^a; 3)$ with $1 \leq b \leq 2$: Applying (Rao) to $\mathrm{OA}(24, 3^{b-1} \cdot 2^a; 2)$s, we have $24 \geq 1 + 2(b-1) + a$. In other words:

$$1 \leq b \leq 2, \quad a + b \geq 4 \text{ (to avoid trivial designs) and } a + 2b \leq 25.$$

Hence $3 \leq a \leq 23$ for $b = 1$, and $2 \leq a \leq 21$ for $b = 2$. If $b = 2$ then $a \leq 20$ by (Del) [Hedayat et al., 1999, Section 9.2].

(ii) $\mathrm{OA}(80; 5 \cdot 4^b \cdot 2^a; 3)$ with $a \geq 8$: Applying (Rao) to the derived designs $\mathrm{OA}(16; 4^b \cdot 2^a; 2)$ of $\mathrm{OA}(80; 5 \cdot 4^b \cdot 2^a; 3)$, the parameters must satisfy:

$$0 \leq b \leq 1, \quad a + b \geq 3 \text{ and } 3b + a \leq 15.$$

If $b = 0$, $a \leq 15$; and if $b = 1$ then $a \leq 12$.

(iii) $\mathrm{OA}(81; 9 \cdot 3^b; 3)$: $b \leq 4$ by applying (Rao) to $\mathrm{OA}(9, 3^b; 2)$.
$\mathrm{OA}(81; 3^b; 3)$: the derived designs $\mathrm{OA}(27; 3^{b-1}; 2)$ must satisfy that $27 \geq 1+2(b-1)$, ie, $b \leq 14$.

(iv) $\mathrm{OA}(84; 7 \cdot 3 \cdot 2^a; 3)$: we have $a \leq 2$ by applying (Div).

(v) $\mathrm{OA}(90; 5 \cdot 3^2 \cdot 2^a; 3)$: we have $a \leq 1$ by applying (Div).

(vi) $\mathrm{OA}(96; 8 \cdot 6^b \cdot 2^a; 3)$ with $0 \leq b \leq 1$ $a + b \geq 3$, $a \leq 11$: applying (Rao) to $\mathrm{OA}(12; 6^b \cdot 2^a; 2)$, we get $a + b \geq 2$, $12 \geq 1 + 5b + a$, or $a + 5b \leq 11$. If $b = 0$, $a \leq 11$, and if $b = 1$, $a \leq 6$.
$\mathrm{OA}(96; 8 \cdot 3^b \cdot 2^a; 3)$ with $0 \leq b \leq 1$ $a + b \geq 3$, $a \leq 11$. Indeed, the derived designs $\mathrm{OA}(12; 3^b \cdot 2^a; 2)$ shows that $a \leq 11$ if $b = 0$; and $a \leq 4$ if $b = 1$.
$\mathrm{OA}(96; 6 \cdot 4^b \cdot 2^a; 3)$ and $b > 0$. Use (Rao) for $\mathrm{OA}(16; 4^b \cdot 2^a; 2)$ to see that the parameters must satisfy

$$1 \leq b \leq 2, \quad a + b \geq 3, \text{ and } 3b + a \leq 15.$$

When $b = 2$, $a \leq 9$; and when $b = 1$, $a \leq 12$.
$\mathrm{OA}(96; 4^c \cdot 3^b \cdot 2^a; 3)$ with $b + c > 0$. When $c > 0$, use Rao for $\mathrm{OA}(16; 4^{c-1} \cdot 3^b \cdot 2^a; 2)$; when $c = 0$, use Rao for $\mathrm{OA}(32; 3^{b-1} \cdot 2^a; 2)$. The parameters must satisfy

$$0 \leq b \leq 1, \quad 0 \leq c \leq 2, \quad a + b + c \geq 4, \text{ and } \quad 3(c-1) + 2b + a \leq 23.$$

That is, when $c = 2$, if $b = 1$, $a \leq 18$; if $b = 0$, $a \leq 20$. When $c = 1$, if $b = 1$, $a \leq 21$; if $b = 0$, $a \leq 20$.

(vii) By (Div), $a < 3$ in $\mathrm{OA}(100; 5^2 \cdot 2^a; 3)$. □

N	Levels	Existence	Construction	Upper bound	Nonexistence
72	$18 \cdot 2^a$	$a \leq 3$	(M)	3	
72	$9 \cdot 2^a$	$a \leq 6$	(IS)	7	$a = 7$, (X)
72	$6^2 \cdot 2^a$	$a \leq 2$	(IS)	3	$a = 3$, (O)
72	$6 \cdot 3 \cdot 2^a$	$a \leq 4$	(IS)	5	$a = 5$, (O')
72	$6 \cdot 2^a$	$a \leq 11$	(M)	11	
72	$4 \cdot 3^2 \cdot 2^a$	$a \leq 1$	(T)	13	$a = 2$, (Div)
72	$3^2 \cdot 2^a$	$a \leq 12$	(B) and (IS)	20	$a = 13$?
72	$3 \cdot 2^a$	$a \leq 12$	(B) and (IS)	23	$a = 13$?
80	$20 \cdot 2^a$	$a \leq 3$	(M)	3	
80	$10 \cdot 4 \cdot 2^a$	$a \leq 2$	(O)	4	$a = 3$, (O)
80	$10 \cdot 2^a$	$a \leq 7$	(M)	7	
80	$5 \cdot 4 \cdot 2^a$	$a \leq 6$	(A), (La), (IS)	8	$a = 7$?
80	$5 \cdot 2^a$	$a \leq 9$	(B)	15	$a = 10$?
80	$4 \cdot 2^a$	$a \leq 19$	(M)	19	
81	$9 \cdot 3^b$	$b \leq 4$	(***)	4	
81	3^b	$b \leq 10$	(L)	14	$b = 11$,
84	$7 \cdot 3 \cdot 2^a$	$a \leq 2$	(M)	4	$a = 3$, (Div)
88	$22 \cdot 2^a$	$a \leq 3$	(M)	3	
88	$11 \cdot 2^a$	$a \leq 6$	(IS)	7	$a = 7$, (X)
90	$5 \cdot 3^2 \cdot 2^a$	$a = 1$	(T)	6	$a = 2$, (Div)
96	$24 \cdot 2^a$	$a \leq 3$	(M)	3	
96	$12 \cdot 4 \cdot 2^a$	$a \leq 4$	(IS) and (L)	4	
96	$12 \cdot 2^a$	$a \leq 7$	(M)	7	
96	$8 \cdot 6 \cdot 2^a$	$a \leq 2$	(IS) or (O)	3	$a = 3$, (O)
96	$8 \cdot 3 \cdot 2^a$	$a \leq 4$	(IS) or (J)	5	$a = 5$, (O')
96	$8 \cdot 2^a$	$a \leq 11$	(M)	11	
96	$6 \cdot 4^2 \cdot 2^a$	$a \leq 6$	(La), (IS)	9	$a = 7$?
96	$6 \cdot 4 \cdot 2^a$	$a \leq 8$	(S)	12	$a = 9$?
96	$6 \cdot 2^a$	$a \leq 15$	(M)	15	
96	$4^2 \cdot 3 \cdot 2^a$	$a \leq 7$	(S)	18	$a = 8$?
96	$4^2 \cdot 2^a$	$a \leq 20$	(Q)	20	
96	$4 \cdot 3 \cdot 2^a$	$a \leq 9$	(S)	21	$a = 10$?
96	$3 \cdot 2^a$	$a \leq 16$	(J)	31	$a = 17$?
100	$5^2 \cdot 2^a$	$a \leq 2$	(T)	15	$a = 3$, (Div)

TABLE 6.3. Parameters of OA$(N; s_1^c \cdot s_2^b \cdot s_3^a; 3)$s with $72 \leq N \leq 100$

6.3. Constructing OAs with run size $72 \leq N \leq 100$

Since there is no OA of strength 3 with run size larger 64 and less than 72, we list parameters for OAs with $72 \leq N \leq 100$ in Table 6.3. In the fourth column of Table 6.3 we show the constructions for OAs with $72 \leq N \leq 100$ whose parameters were indicated in Lemma 60. We skip all cases found by Construction (M). When the gap between the total number of known columns with the upper bound is positive, we mention the next open cases. The question marks ? written in the last column of Table 6.3 indicate that we have not proved yet the nonexistence of OAs with corresponding values.

Basic constructions. We consider case by case with respect to the run sizes.

(i) $N = 72$: OA$(72; 9 \cdot 2^a; 3)$ with $2 \leq a \leq 6$: this has the form OA$(8m; m \cdot 2^a; 3)$ where $3 \leq a \leq 7$, $3 \leq m \leq 12$. Since $m = 9$ is an odd number, using Construction (X) we get $a = 6$.
OA$(72; 6^2 \cdot 2^a; 3)$ exists for $a \leq 2$ by (IS) and (O).
OA$(72; 6 \cdot 3 \cdot 2^a; 3)$ exists for $a \leq 4$ by (IS) and (O').
OA$(72; 4 \cdot 3^2 \cdot 2^a; 3)$ exists for $a \leq 1$ by (T), but not for $a = 2$ by Div.
OA$(72; 3^2 \cdot 2^a; 3)$: See a construction of the case $a = 12$, $b = 2$ at Brouwer [2004]. When $b = 1$, $a \leq 20$; an OA$(72; 3 \cdot 2^a; 3)$ exists obviously. The open cases are $13 \leq a \leq 20$.

(ii) $N = 80$: OA$(80; 5 \cdot 4^b \cdot 2^a; 3)$ with $a \geq 1$: For $b = 1$, $a \leq 12$, we get $a = 5$ by juxtaposing two arrays OA$(40; 2 \cdot 5 \cdot 2^5; 3)$; and $a = 6$ by the arithmetic method below. If we take the derived designs at the 4-factor, then $a \leq 8$ [Wu et al., 1992]. For $b = 0$, $a \leq 15$, we obtain $a = 9$ by juxtaposing an array OA$(32; 2^{16}; 3)$ and OA$(48; 3 \cdot 2^9; 3)$. Hence, the open cases are $7 \leq a \leq 8$ for $b = 1$; and are $10 \leq a \leq 15$ for $b = 0$.

(iii) $N = 81$: OA$(81; 9 \cdot 3^b; 3)$, $b \leq 4$: by (B) and (***).
OA$(81; 3^b; 3)$: $3 \leq b \leq 10$: by (L); see Hedayat et al. [1999, Section 5.9] for nonexistence of $b = 11$.

(iv) $N = 88$: OA$(88; 11 \cdot 2^a; 3)$ with $2 \leq a \leq 6$: $a = 6$ is obtained similarly as in the case OA$(72; 9 \cdot 2^6; 3)$).

(v) $N = 96$: OA$(96; 6 \cdot 4^b \cdot 2^a; 3)$: For $b = 2$, $a \leq 9$. We get $a = 3$ by juxtaposing an OA$(32; 2 \cdot 4^2 \cdot 2^3; 3)$ and an OA$(64; 4 \cdot 4^2 \cdot 2^8)$. Furthermore, an OA$(96; 6 \cdot 4^2 \cdot 2^4; 3)$ will be made by Construction (Q) below. We make an OA$(96; 6 \cdot 4^2 \cdot 2^5; 3)$ by (La). An OA$(96; 6 \cdot 4^2 \cdot 2^6; 3)$ is found by (IS). For $b = 1$, $a \leq 12$. We get $a = 8$ from splitting a 4-level factor in OA$(96; 6 \cdot 4^2 \cdot 2^6; 3)$. Hence, for $b = 2$, the open cases are $7 \leq a \leq 9$; and for $b = 1$, $a \leq 12$, the open case is OA$(96; 6 \cdot 4 \cdot 2^9; 3)$.
OA$(96; 4^c \cdot 3^b \cdot 2^a; 3)$:

> The case $b = 0$. We use Construction (Q).
> The case $b = 1$. For $c = 2$, we consider OA$(96; 4^2 \cdot 3 \cdot 2^a; 3)$, a is bounded above by 13 [Wang and Wu, 1991]. We employ Construction (A) below for the case $a = 5$, and we split the 6-level factor in OA$(96; 6 \cdot 4^2 \cdot 2^6; 3)$ to get $a = 7$. For $c = 1$, then $a \leq 20$ (by Del) in OA$(96; 4 \cdot 3 \cdot 2^a; 3)$. Splitting the 6-level factor in OA$(96; 6 \cdot 4 \cdot 2^8; 3)$ gives OA$(96; 4 \cdot 3 \cdot 2^9; 3)$. For $c = 0$, then $a \leq 31$ in OA$(96; 3 \cdot 2^a; 3)$. Juxtaposing three OA$(32; 2^{16}; 3)$ gives OA$(96; 3 \cdot 2^{16}; 3)$.

So the open cases are OA$(96; 4^2 \cdot 3 \cdot 2^8; 3)$, OA$(96; 4 \cdot 3 \cdot 2^{10}; 3)$, and OA$(96; 3 \cdot 2^{17}; 3)$.

Quasi-multiplication construction (Q). We construct OA$(96; 4^c \cdot 2^a; 3)$. The generalized Rao bound of a is reached for all $c = 0, 1, 2$. If $c = 2$, $a \leq 20$, and $a = 20$ is constructed in several steps in the following construction,

We use the difference scheme construction [Wang and Wu, 1991] to make an array $f_0 :=$ OA$(24; 4 \cdot 2^{20}; 2) = [A|B]$, where A is the 4-column, **0**, **1**, **2**, **3** are constant vectors of appropriate length, and $B = \mathrm{OA}(24; 2^{20}; 2)$:

$$f_0 := \left[\begin{array}{c|c} A & B \\ \mathbf{0} & \ldots \\ \mathbf{1} & \ldots \\ \mathbf{2} & \ldots \\ \mathbf{3} & \ldots \end{array}\right].$$

Next we make three arrays $\mathrm{OA}(24; 4 \cdot 2^{20}; 2)$ by cyclically taking modulo 4 for the 4-column, and modulo 2 for the binary part, i.e.:

$$f_i = [\,(A+i) \mod 4 \quad | \quad (B+i) \mod 2\,], \qquad \text{for } i \ge 1.$$

Lastly, the desired array is formed by first, concatenating f_0, f_1, f_2, f_3, to form $f = \mathrm{OA}(96; 4 \cdot 2^{20}; 3)$, then adding the second 4-level column to f, we get:

$$\mathrm{OA}(96, 4^2 \cdot 2^{20}, 3) := \left[\begin{array}{c|c} \mathbf{0} & f_0 \\ \mathbf{1} & f_1 \\ \mathbf{2} & f_2 \\ \mathbf{3} & f_3 \end{array}\right]$$

If $c = 1$, $a \le 23$. $a = 23$ is made by (M). If $c = 0$, $a \le 48$, $a = 48$ is made by (H).

Arithmetic construction of $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^3; 3)$. We use the method of Section 3.5. Let S_1 denote for the 6-level column, S_2 and S_3 the two 4-level columns, and X_1, X_2, X_3 the three 2-level columns of the array. Here $n = \mathrm{lcm}(6, 4, 4) = 12$, so $A = A_0 = \{0, 1, 2, 3, 4, 5\}$, and $B = \mathbb{Z}_{12} \setminus A = \{6, 7, 8, 9, 10, 11\}$. Columns S_1, S_2, S_3 form a full design $D = \mathbb{Z}_6 \times \mathbb{Z}_4 \times \mathbb{Z}_4$ of 96 runs, so any binary column X is a function of $[S_1, S_2, S_3]$. Using (3.5.1), there is a 3-to-1 mapping between the column S_1 with X, and 2-to-1 mappings between the columns S_2, S_3 with S. Therefore, columns X_1, X_2, X_3, X_4 can be defined respectively by the linear functionals $h_i : D \to \mathbb{Z}_{12}$:

$$\begin{aligned} h_1 &= (a_0 x + a_1 y + a_2 z) \bmod 12, \quad h_2 = (b_0 x + b_1 y + b_2 z) \mod 12, \\ h_3 &= (c_0 x + c_1 y + c_2 z) \bmod 12, \quad h_4 = (d_0 x + d_1 y + d_2 z) \mod 12, \end{aligned}$$

where $a_i, b_i, c_i, d_i \in \mathbb{Z}_{12} \quad (i = 0, 1, 2)$ are unknown coefficients. We start with column X_1. Note that any constraint found for X_1's coefficients also hold for those of X_2, X_3, X_4. Firstly, X_1 is orthogonal to $[S_2, S_3]$, denoted by $X_1 \perp [S_2, S_3]$, only if for every fixed pair $(y, z) \in \mathbb{Z}_4 \times \mathbb{Z}_4$, the scattering coefficient of the columns $[S_2, S_3]$ in $\mathbb{Z}_{12}$ is $c_{2,3} = q_{2,3} = \frac{N}{4.4.2} = 3$. Recall from (3.5.3) that values of a binary column X (being determined by a function $f : D \to \mathbb{Z}_{12} \to \mathbb{Z}_2$) are computed by using the partition function $g : \mathbb{Z}_{12} \to \mathbb{Z}_2$

$$X := 0 \quad \text{if} \quad h \in A; \quad \text{and} \quad X := 1 \quad \text{if} \quad h \in B.$$

So half of the six values $a_0 x + a_1 y + a_2 z \pmod{12}$ are in A, and half are not. Taking $(y, z) = (0, 0)$ implies that $a_0 \in \{2, 6, 7, 9, 10, -10, -6, -5, -3, -2\} =: L_1$. Similarly, $X_1 \perp [S_1, S_2], [S_1, S_3]$ implies $a_1, a_2 \in \{3, 6, 7, 9, -9, -6, -5, -3\} =: L_2$.

Hence we have proved the following lemma.

Lemma 61. *If the binary columns X_1, X_2, X_3 are orthogonal to D then*

$$a_0, b_0, c_0, d_0 \in L_1, \quad a_1, a_2, b_1, b_2, c_1, c_2, d_1, d_2 \in L_2.$$

Checking all possibilities of the vector $\boldsymbol{a} = [a_0, a_1, a_2]$ shows that there are only two binary columns X orthogonal to Q with $a_0 = 7, 9$. They are given by vectors $\boldsymbol{a} = [7, 6, 6], [9, 6, 6]$. Next, we find the maximum number of binary columns with the same coefficient $a_0 \neq 7, 9$ for variable x (in functions $h_1, \dots, h_4$). The first three columns X_1, X_2, X_3 in this series are given by $h_1 = a_0x + a_1y + a_2z \bmod 12$, $h_2 = a_0x + b_1y + b_2z \bmod 12$, and $h_3 = a_0x + c_1y + c_2z \bmod 12$, resulting in:

$$\begin{aligned} h_2 &= h_1 + (b_1 - a_1)y + (b_2 - a_2)z \mod 12\\ h_3 &= h_1 + (c_1 - a_1)y + (c_2 - a_2)z \mod 12\\ h_3 &= h_2 + (c_1 - b_1)y + (c_2 - b_2)z \mod 12. \end{aligned} \tag{6.3.1}$$

LEMMA 62. *If* $X_2 \perp [X_1, S_3]$, $X_2 \perp [X_1, S_2]$, $X_3 \perp [X_1, S_3]$, $X_3 \perp [X_1, S_2]$, $X_3 \perp [X_2, S_3]$, $X_3 \perp [X_2, S_2]$, *then* $\{b_1 - a_1, b_2 - a_2, c_1 - a_1, c_2 - a_2, c_1 - b_1, c_2 - b_2\}$ *is a sub set of* L_2.

PROOF. The functions (6.3.1) are degree 1 polynomials. □

Due to this lemma, the set L_2 is updated to $L_2 := \{3, 6, 9, -9, -6, -3\}$. There are 10 solutions (triples of binary columns), which have the same coefficient a_0, for example $[10, 3, 9], [10, 6, 6], [10, 9, 3]$. If only two binary columns have the same coefficient a_0, we get 32 solutions, for instance $[[2, 3, 3], [2, 9, 9], [6, 6, 6]]$. (Distinct coefficients a_0 give no result). Remark that, trying combine the above solutions to form the fourth column gives no answer. By splitting the 6-column, we get an $\mathrm{OA}(96; 3 \cdot 4^2 \cdot 2^4; 3)$. How about $\mathrm{OA}(96; 3 \cdot 4^2 \cdot 2^a; 3)$ for $a \geq 5$?

Arithmetic construction of $\mathrm{OA}(96; 3 \cdot 4^2 \cdot 2^a; 3)$. From Lemma 60, we know a is bounded above by 18. By juxtaposing three arrays $\mathrm{OA}(32; 4^2 \cdot 2^4; 3)$ we obtain an $\mathrm{OA}(96; 3 \cdot 4^2 \cdot 2^4; 3)$. By the arithmetic construction, we find an $\mathrm{OA}(96; 3 \cdot 4^2 \cdot 2^5; 3) = \mathrm{OA}(96; 3 \cdot 4^2 \cdot 2 \cdot 2^4; 3)$, in which the last four binary columns are determined by the vectors $[3, 3, 2, 6]$, $[3, 6, 8, 2]$, $[6, 9, 4, 2]$, and $[9, 9, 8, 6]$. To conclude, using the arithmetic method, we have

PROPOSITION 63. $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^3; 3)$ *and* $\mathrm{OA}(96; 3 \cdot 4^2 \cdot 2^5, 3)$ *exist.*

6.4. Enumerating isomorphism classes

Notice that the methods of ILP and automorphism groups in Chapter 4 now are implemented for extension of binary columns only. We have

THEOREM 64. *The numbers of isomorphism classes of strength 3 orthogonal arrays with run size* $8 \leq N \leq 100$ *are as indicated in Table 6.4.*

In the table, we use multiplicity notation for automorphism group orders. We abbreviate n^1 to n, where n is a group size. In the third column of the table, number 0 indicates that there is no array. This conclusion is based on the Rao bound, the Delsarte bound, the divisibility condition (on the run size) or by explicit nonexistence proofs. In these cases, a particular name of lower bound or an explicit nonexistence proof is indicated. Open cases are indicated by '≥ 0', ie, we do not know whether an array exists or not with the parameters given in the first and second column. That means exhaustive computing (Constructions (B) and (IS)) fails to construct those arrays, or no proof of nonexistence has been found yet for the time being. For series having more than 5000 non-isomorphic arrays, we only list the number of arrays, not giving the automorphism group size. The actual OAs will be put at Nguyen [2005].

Table 6.4: Non-isomorphic OAs of strength 3 with $8 \leq N \leq 100$

N	Type	#	Size of the automorphism group	Methods
8	2^4	1	192	(I)
16	$4 \cdot 2^3$	1	192	(I)
16	$4 \cdot 2^4$	0		(Rao)
24	$6 \cdot 2^3$	1	1728	(IS)
24	$6 \cdot 2^4$	0		(Rao)
24	$3 \cdot 2^3$	2	288^1, 12288^2	(IS)
24	$3 \cdot 2^4$	3	48, 384, 1152	(IS)
24	$3 \cdot 2^5$	0		(5.1)
27	3^4	1	1296	(IS)
27	3^5	0		(Rao)
32	$4^2 \cdot 2^2$	2	128, 512	(IS)
32	$4^2 \cdot 2^3$	2	128, 384	(IS)
32	$4^2 \cdot 2^4$	2	512, 1536	(IS)
32	$4^2 \cdot 2^5$	0		(Rao)
32	$4 \cdot 2^3$	3	1152, 24576, 12582912	(IS)
32	$4 \cdot 2^4$	7	64, 96^2, 384, 1152, 1536, 4608	(IS)
32	$4 \cdot 2^5$	7	16, 32, 64, 128^2, 256, 512	(IS)
32	$4 \cdot 2^6$	11	24^2, 64^4, 128, 256^2, 768, 1536	(IS)
32	$4 \cdot 2^7$	8	84, 96^2, 128, 384, 768^2, 10752	(IS)
32	$4 \cdot 2^8$	0		(Rao)
36	$3^2 \cdot 2^2$	3	576, 8192, 196608	(IS)
36	$3^2 \cdot 2^3$	0		(Div)
40	$10 \cdot 2^3$	1	691200	(IS)
40	$10 \cdot 2^4$	0		(Rao)
40	$5 \cdot 2^3$	9	5760, 73728^4, 12582912^4	(B)
40	$5 \cdot 2^4$	28	32^4, 96^8, 192^4, 288^4, 2304^4, 4608^3, 23040	(B)
40	$5 \cdot 2^5$	2	1^2	(IS)
40	$5 \cdot 2^6$	1	60	(IS)
40	$5 \cdot 2^7$	0		(X)
48	$12 \cdot 2^3$	1	24883200	(IS)
48	$12 \cdot 2^4$	0		(Rao)
48	$6 \cdot 4 \cdot 2^2$	3	128, 192, 2304	(IS)
48	$6 \cdot 4 \cdot 2^3$	0		(O)
48	$6 \cdot 2^3$	24	34560^1, 294912^7, 25165824^{12}, 28991029248^3	(B)
48	$6 \cdot 2^4$	122	64^{24}, 96^4, 128^{12}, 288^{19}, 384^{36}, 1152^7, 3456^4, 9216^7, 13824^4, 23040^4, 138240	(B)
48	$6 \cdot 2^5$	578	8^{264}, 16^{66}, 24^{20}, 32^{117}, 48^{10}, 64^{45}, 128^{12}, 256^{24}, 384^4, 512^{12}, 4608^4	(B)
48	$6 \cdot 2^6$	1879	2^{120}, 4^{606}, 8^{192}, 12^{56}, 16^{177}, 24^{28}, 32^{354}, 48^{37}, 64^{126}, 72^{14}, 96^{20}, 128^{105}, 384^4, 512^{24}, 1536^{12}, 13824^4	(B)
48	$6 \cdot 2^7$	1525	2^{120}, 4^{120}, 6^{192}, 8^{150}, 12^{170}, 16^{174}, 24^{30}, 32^{240}, 64^{63}, 96^{10}, 128^{30}, 168^{21}, 192^{42}, 256^{21}, 288^{14}, 384^{82}, 768^{21}, 1536^{21}, 96768^4	(B)
48	$6 \cdot 2^8$	0		(Rao)
48	$4 \cdot 3 \cdot 2^2$	5	1152, 8192, 98304, 1048576, 4194304	(IS)
48	$4 \cdot 3 \cdot 2^3$	35	4^3, 8^7, 16^9, 24, 32^2, 48^4, 64, 96^3, 144, 192, 288, 384, 1152	(IS)
48	$4 \cdot 3 \cdot 2^4$	19	4^8, 8^{10}, 16	(IS)
48	$4 \cdot 3 \cdot 2^5$	0		(O')
48	$3 \cdot 2^a$, $3 \leq a \leq 9$			(Br)
48	$3 \cdot 2^{10}$	0		(IS)
54	$6 \cdot 3^3$	2	216, 2592	(IS)
54	$6 \cdot 3^4$	0		(IS)

continued on next page

Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
54	$3^5 \cdot 2$	4	6, 12, 18, 72	(IS)
54	$3^5 \cdot 2^2$	0		(Div)
54	3^5	4	36, 40, 144, 960	(3^5)
54	3^6	0		(Del)
56	$14 \cdot 2^3$	1	1219276800	(IS)
56	$14 \cdot 2^4$	0		(Rao)
56	$7 \cdot 2^3$	66	241920, 1474560^{11}, 75497472^{31}, 28991029248^{23}	(B)
56	$7 \cdot 2^4$	479	48^{25}, 64^{150}, 192^{31}, 384^{75}, 576^{62}, 1152^{70}, 1728^{23}, 5760^{11}, 27648^{15}, 46080^{11}, 138240^5, 967680	(B)
56	$7 \cdot 2^5$	2760	2^{2520}, 4^{240}	(IS)
56	$7 \cdot 2^6$	2950	1^{840}, 2^{1260}, 4^{420}, 6^{296}, 12^{86}, 24^{48}	(IS)
56	$7 \cdot 2^7$	0		(Rao)
60	$5 \cdot 3 \cdot 2^2$	6	5760, 24576, 196608, 1048576, 4194304, 16777216	(IS)
60	$5 \cdot 3 \cdot 2^3$	0		(Div)
64	$16 \cdot 2^3$	1	78033715200	(IS)
64	$16 \cdot 2^4$	0		(Rao)
64	$8 \cdot 4 \cdot 2^2$	4	256, 1024, 1152, 36864	(IS)
64	$8 \cdot 4 \cdot 2^3$	11	12, 16, 32^3, 96, 128^2, 192, 1024, 3072	(IS)
64	$8 \cdot 4 \cdot 2^4$	20	48, 64^3, 128^6, 256, 384, 512^3, 768^2, 1536, 4096, 12288	(IS)
64	$8 \cdot 4 \cdot 2^5$	0		(Rao)
64	$8 \cdot 2^3$	187	1935360, 8847360^{16}, 301989888^{70}, 57982058496^{85}, 118747255799808^{15}	(B)
64	$8 \cdot 2^4$	2576	96^{200}, 128^{750}, 192^{220}, 256^{150}, 384^{25}, 768^{70}, 1024^{75}, 1152^{305}, 1536^{150}, 2304^{140}, 3456^{255}, 4608^{70}, 5760^{71}, 34560^{16}, 55296^{15}, 138240^{26}, 221184^{15}, 276480^{16}, 967680^6, 7741440, 2304, 3456^3, 4608, 5760, 34560, 55296	(B)
64	$8 \cdot 2^5$	≥ 20489		(B)
64	$8 \cdot 2^6$	≥ 19217		(B)
64	$8 \cdot 2^7$	≥ 23159		(B)
64	$8 \cdot 2^8$	0		(Rao)
64	4^6	1	48	(B)
64	4^7	0		(Rao)
64	$4^5 \cdot 2$	1	68	(B)
64	$4^5 \cdot 2^2$	1	8	(B)
64	$4^5 \cdot 2^3$	0		
64	4^5	1	144	(B)
64	$4^4 \cdot 2$	3	256, 512, 1536	(B)
64	$4^4 \cdot 2^2$	5	256, 512, 1024^2, 1536	(B)
64	$4^4 \cdot 2^3$	3	256, 384, 512	(IS)
64	$4^4 \cdot 2^4$	3	256, 1024^2	(IS)
64	$4^4 \cdot 2^5$	1	512	(IS)
64	$4^4 \cdot 2^6$	1	3072	(IS)
64	$4^4 \cdot 2^7$	0		(Rao)
64	4^4	19	384^8, 512^6, 3072^3, 9216^2	(B)
64	$4^3 \cdot 2$	10	8, 16, 24, 32, 48, 64, 128, 256, 384, 3072	(IS)
64	$4^3 \cdot 2^2$	107	2^3, 4^9, 6, 8^{24}, 16^{20}, 24, 32^{19}, 48, 64^{12}, 96, 128^6, 256^5, 384, 512^2, 768^2	(IS)
64	$4^3 \cdot 2^3$	237	2^6, 4^{30}, 6, 8^{42}, 16^{51}, 32^{46}, 48^2, 64^{30}, 96^3, 128^{18}, 256^4, 384^2,512, 1536	(IS)

continued on next page

Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
64	$4^3 \cdot 2^4$	255	2^4, 4^{27}, 6^3, 8^{34}, 16^{61}, 24, 32^{46}, 48^4, 64^{36}, 96^3, 128^{19}, 192, 256^{10}, 384^2, 512^2, 1536^2	(B)
64	$4^3 \cdot 2^5$	126	4^7, 6, 8^{14}, 16^{22}, 24, 32^{25}, 48^2, 64^{19}, 96^2, 128^{18}, 192, 256^{10}, 512^2, 1536^2	(B)
64	$4^3 \cdot 2^6$	35	16^4, 32^6, 48^4, 64^6, 96^3, 128^7, 256, 384, 768^3	(B)
64	$4^3 \cdot 2^7$	12	48^2, 64^3, 128, 384^4, 768^2	(B)
64	$4^3 \cdot 2^8$	2	$6, 28$	(B)
64	$4^3 \cdot 2^9$	0		(5.10)
64	$4^2 \cdot 2^2$	34		(B)
64	$4^2 \cdot 2^3$	1740	1^{32}, 2^{92}, 4^{375}, 8^{376}, 16^{220}, 24^{16}, 32^{121}, 48^{34}, 64^{71}, 96^{67}, 128^{126}, 192^9, 256^{21}, 288^4, 384^7, 512^7, 768, 1024^{19}, 1152^2, 2048^{14}, 3072, 4096^{44}, 4608, 8192^{16}, 12288^2, 16384^8, 24576^4, 32768^{16}, 65536^5, 196608^5, 393216^4, 2097152^9, 4194304^4, 8388608^2, 536870912^3, 549755813888, 1649267441664	(B)
64	$4^2 \cdot 2^4$	≥ 5500		,,
64	$4^2 \cdot 2^5$	≥ 5630		,,
64	$4^2 \cdot 2^6$	≥ 1885		,,
64	$4^2 \cdot 2^7$	≥ 6673		,,
64	$4^2 \cdot 2^8$	≥ 953		,,
64	$4^2 \cdot 2^9$	≥ 146		,,
64	$4^2 \cdot 2^{10}$	≥ 4	32, 64^2, 256	,,
64	$4^2 \cdot 2^{11}$	≥ 1		,,
64	$4^2 \cdot 2^{12}$	≥ 1		,,
64	$4^2 \cdot 2^{13}$	0		(Rao)
64	$4 \cdot 2^3$	12	4947802324992, 10567230160896^2, 541653102231552, 6847565144260608^3, 692533995824480256^2, $887444442696174796 8^2$, 232638235986146045932 3392	(B)
64	$4 \cdot 2^4$	163	9216, 16384^2, 24576^4, 32768^6, 49152^2, 131072^4, 294912^2, 524288^{13}, 1048576^{12}, 1572864^4, 2097152^3, 3145728^{15}, 4194304^{16}, 6291456^3, 8388608^7, 12582912^4, 50331648^4, 134217728^3, 268435456^8, 402653184^4, 536870912^6, 805306368^{21}, 1610612736^4, 6442450944^3, 19327352832^2, 274877906944, 412316860416^4, 1649267441664, 4947802324992^2, 6597069766656, 19791209299968	,,
64	$4 \cdot 2^5$	12692		,,
64	$4 \cdot 2^6$	≥ 7258		,,
64	$4 \cdot 2^7$	≥ 9570		,,
64	$4 \cdot 2^8$	≥ 1189	1^{100}, 2^{264}, 4^{335}, 8^{169}, 16^{132}, 24^2, 32^{90}, 48^6, 64^{35}, 96^9, 128^{14}, 192^3, 256^7, 384^5, 512^3, 768^5, 1024, 1536^5, 3072, 6144^2, 21504	,,
64	$4 \cdot 2^9$	≥ 13	8^2, 16, 32^2, 64^3, 96^3, 256, 6144	,,
64	$4 \cdot 2^{10}$	≥ 1		,,
64	$4 \cdot 2^{11}$	≥ 1		,,
64	$4 \cdot 2^{12}$	≥ 1		,,
64	$4 \cdot 2^{13}$	≥ 1		,,
64	$4 \cdot 2^{14}$	≥ 1		,,
64	$4 \cdot 2^{15}$	≥ 1		,,
64	$4 \cdot 2^{16}$	0		(Rao)

continued on next page

Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
72	$18 \cdot 2^3$	1	6320730931200	(IS)
72	$18 \cdot 2^4$	0		(Rao)
72	$9 \cdot 2^3$	5	17418240, 61931520, 1509949440, 173946175488, 118747255799808	(B)
72	$9 \cdot 2^4$	26	64, 96, 128, 192, 288, 384^2, 512, 576, 768, 2304, 3456, 3840, 4608, 6912, 10368, 11520, 23040, 27648, 34560, 241920, 552960, 829440, 1935360, 7741440, 69672960	,,
72	$9 \cdot 2^5$	≥ 27349		,,
72	$9 \cdot 2^6$	≥ 14484		,,
72	$9 \cdot 2^7$	0		(X)
72	$6^2 \cdot 2^2$	2394	64^{930}, 96^{720}, 192^{320}, 384^{183}, 512^{231}, 41472^{10}	(B)
72	$6^2 \cdot 2^3$	0		(O)
72	$6 \cdot 3 \cdot 2^2$	9	98304, 589824, 2097152, 8388608, 16777216, 536870912, 805306368, 3221225472, 9663676416	
72	$6 \cdot 3 \cdot 2^3$	231	1^5, 2^{28}, 4^{47}, 6, 8^{68}, 12^2, 16^{47}, 24^2, 32^{14}, 48^9, 64^6, 96, 576	(IS)
72	$6 \cdot 3 \cdot 2^4$	289	1^{215}, 2^{33}, 3^3, 4^{22}, 8^9, 12^1, 16^4, 48^2	(IS)
72	$6 \cdot 3 \cdot 2^5$	0		(O')
72	$6 \cdot 2^3$	82	28991029248^4, 782757789696^{13}, 21134460321792^{21} 2567836929097728^{19}, 138663194171277312^{21}, 8187922952619753996288^4	(B)
72	$6 \cdot 2^4$	156	256^{36}, 512^{72}, 3072^{32}, 4096^{12}, 110592^4	,,
72	$6 \cdot 2^5$	64296		,,
72	$6 \cdot 2^6$	≥ 34719		,,
72	$6 \cdot 2^7$	≥ 50906		,,
72	$6 \cdot 2^8$	≥ 3978		,,
72	$6 \cdot 2^9$	≥ 388	1^{80}, 2^{219}, 4^{34}, 8^{21}, 16^{21}, 24, 32^8, 128^3, 10368	,,
72	$6 \cdot 2^{10}$	≥ 31	4^7, 8^5, 16, 64^2, 144^9, 288^3, 576^3, 51840	,,
72	$6 \cdot 2^{11}$	≥ 3	1440^2, 110880	,,
72	$6 \cdot 2^{12}$	0		(Rao)
72	$4 \cdot 3^2 \cdot 2$	17	8192, 49152, 65536, 196608, 524288^4, 4194304^4, 8388608, 9437184, 268435456, 402653184, 1610612736	(IS)
72	$4 \cdot 3^2 \cdot 2^2$	0		(Div)
72	$3^2 \cdot 2^2$	9	3693514644397228032, 657366253849018368, 2154057740612463382624, 36520347436056576, 19967499960663932928, 5135673858195456, 56358560858112, 427972821516288, 39582418599936	(B)
72	$3^2 \cdot 2^3$	465	3456, 4096, 8192^2, 16384^7, 24576^2, 32768^5, 49152, 65536^{11}, 98304,131072^2, 196608^{11}, 262144^{27}, 393216^3, 524288^{23},786432^5, 1048576^{23},1179648, 1572864^9, 2097152^{16}, 2359296^3, 3145728^{23}, 4194304^{50},4718592^5, 6291456^8, 8388608^{20}, 9437184^{10}, 12582912^2, 14155776, 16777216^5, 18874368^{13}, 25165824^3, 28311552, 33554432^2, 37748736^8, 42467328, 50331648, 67108864^{24}, 75497472^4, 84934656^2, 113246208, 134217728^{26}, 50994944^4, 169869312,	

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Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
			226492416, 268435456^{9}, 301989888^{3}, 339738624^{4}, 402653184^{9}, 536870912, 679477248^{3}, 805306368^{8}, 1073741824^{10}, 1358954496, 1610612736, 2038431744, 2147483648, 2293235712, 3057647616, 4076863488, 4586471424^{2}, 4831838208^{2}, 5435817984^{2}, 9663676416, 10871635968, 12230590464, 17179869184, 24461180928, 34359738368, 43486543872, 48922361856^{3}, 68719476736^{2}, 97844723712, 103079215104^{2}, 110075314176, 137438953472,146767085568, 206158430208^{4}, 293534171136^{2}, 990677827584, 1761205026816, 3710851743744, 7421703487488, 160489808068608, 213986410758144, 29249267520503808	(B)
72	$3^2 \cdot 2^4$	≥ 50000		(B)
72	$3^2 \cdot 2^5$	≥ 30993		(B)
72	$3^2 \cdot 2^6$	≥ 12167		(B)
72	$3^2 \cdot 2^7$	≥ 1304		(B)
72	$3^2 \cdot 2^8$	≥ 379	1^{36}, 2^{222}, 4^{83}, 8^{20}, 16^{11}, 32^{3}, 64^{2}, 32768, 98304	(B)
72	$3^2 \cdot 2^9$	≥ 157	1^{3}, 2^{109}, 4^{31}, 6^{1}, 8^{9}, 16^{1}, 32^{3}	(I)
72	$3^2 \cdot 2^{10}$	≥ 67	2^{28}, 4^{23}, 8^{5}, 16^{6}, 32^{2}, 64^{3}	(I)
72	$3^2 \cdot 2^{11}$	≥ 14	2^{5}, 4^{4}, 8^{3}, 32^{2}	(I)
72	$3^2 \cdot 2^{12}$	≥ 6	8^{2}, 16, 64, 96, 288	(I)
72	$3^2 \cdot 2^{13}$	≥ 0		
72	$3 \cdot 2^3$	6	24, 48^{4}, 288	(B)
72	$3 \cdot 2^4$	89	805306368, 1207959552, 2717908992, 6442450944, 10871635968, 16307453952, 19327352832, 21743271936^{2}, 24461180928, 32614907904^{2}, 48922361856^{5}, 65229815808, 73383542784, 86973087744, 110075314176, 220150628352^{2}, 440301256704^{3}, 521838526464, 880602513408^{3}, 1043677052928^{2}, 1981355655168, 2348273369088, 2641807540224^{4}, 3962711310336^{3}, 5283615080448^{5}, 7044820107264^{2}, 7421703487488^{2}, 7925422620672^{3}, 21134460321792, 35664401793024^{2}, 42268920643584^{2}, 71328803586048^{2}, 75144747810816, 106993205379072, 142657607172096^{2}, 213986410758144^{4}, 320979616137216, 427972821516288^{2}, 5777633090469888, 17332899271409664^{4}, 34665798542819328^{5}, 48693796581408768^{2}, 138663194171277312, 277326388342554624^{2}, 227442304239437611008, 1819538433915500888064, 5458615301746502664192	,,
72	$3 \cdot 2^5$	≥ 1		,,
72	$3 \cdot 2^6$	≥ 1		,,
72	$3 \cdot 2^7$	≥ 1		,,
72	$3 \cdot 2^8$	≥ 1		,,

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Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
72	$3 \cdot 2^{9}$	≥ 120		,,
72	$3 \cdot 2^{10}$	≥ 1		,,
72	$3 \cdot 2^{11}$	≥ 1		,,
72	$3 \cdot 2^{12}$	≥ 1		,,
72	$3 \cdot 2^{13}$	≥ 0		
80	$20 \cdot 2^{3}$	1	632073093120000	(IS)
80	$20 \cdot 2^{4}$	0		(Rao)
80	$10 \cdot 4 \cdot 2^{2}$	≥ 1		
80	$10 \cdot 4 \cdot 2^{3}$	0		(O)
80	$10 \cdot 2^{3}$	6	174182400, 495452160, 9059696640, 695784701952, 237494511599616, 759982437118771200	(B)
80	$10 \cdot 2^{4}$	≥ 11	1152^{3}, 4608, 10368, 13824, 18432, 41472, 55296^{2}, 1382400	(IS)
80	$10 \cdot 2^{5}$	635	1^{4}, 2^{28}, 4^{97}, 8^{155}, 16^{122}, 24^{6}, 32^{88}, 48^{10}, 64^{31}, 96^{10}, 128^{17}, 144^{4}, 192^{2}, 256^{7}, 288^{16}, 384^{2}, 512^{4}, 576^{7}, 768^{2}, 1024^{3}, 1152^{3}, 2304^{6}, 4608^{3}, 9216^{3}, 18432^{1}, 36864^{2}, 73728^{1}, 1843200^{1}	(B)
80	$10 \cdot 2^{6}$	33071		,,
80	$10 \cdot 2^{7}$	≥ 19204		,,
80	$10 \cdot 2^{8}$	0		(Rao)
80	$5 \cdot 4 \cdot 2^{2}$	25	49152, 196608, 1048576, 2097152^{2}, 4194304, 8388608^{3}, 16777216, 25165824, 134217728^{2}, 268435456^{3}, 536870912^{2}, 2147483648^{2}, 68719476736^{2}, 137438953472, 274877906944, 1099511627776	(IS)
80	$5 \cdot 4 \cdot 2^{3}$	≥ 447		(IS)
80	$5 \cdot 4 \cdot 2^{4}$	≥ 1		,,
80	$5 \cdot 4 \cdot 2^{5}$	≥ 1		,,
80	$5 \cdot 4 \cdot 2^{6}$	≥ 5		,,
80	$5 \cdot 4 \cdot 2^{7}$	≥ 0		
80	$5 \cdot 2^{3}$	50		(B)
80	$5 \cdot 2^{4}$	2174	46080, 49152^{4}, 65536^{16}, 73728^{8}, 98304^{4}, 131072^{20}, 524288^{58}, 1048576^{85}, 1179648^{3} 2097152^{140}, 3145728^{26}, 4194304^{180}, 6291456^{53}, 8388608^{126}, 12582912^{8}, 16777216^{76}, 33554432^{50}, 37748736^{4}, 67108864^{77}, 134217728^{250}, 150994944^{8}, 268435456^{103}, 402653184^{20}, 536870912^{57}, 805306368^{144}, 1073741824^{160}, 1610612736^{32}, 2147483648^{56}, 2415919104^{14}, 3221225472^{20}, 4294967296^{16}, 12884901888^{8}, 34359738368^{39}, 38654705664^{4}, 68719476736^{66}, 103079215104^{20}, 137438953472^{16}, 206158430208^{69}, 274877906944^{4}, 412316860416^{68}, 618475290624^{7}, 1236950581248^{8}, 1649267441664^{4}, 4947802324992^{7}, 6597069766656^{4}, 19791209299968^{3}, 35184372088832^{4}, 105553116266496^{8}, 211106232532992^{4}, 316659348799488^{4}, 2533274790395904^{4}, 5066549580791808^{3}, 25332747903959040^{1}	,,
80	$5 \cdot 2^{5}$	≥ 35137		,,
80	$5 \cdot 2^{6}$	≥ 54859		,,

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Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
80	$5 \cdot 2^7$	≥ 6536		,,
80	$5 \cdot 2^8$	≥ 2172		,,
80	$5 \cdot 2^9$	≥ 70		,,
80	$5 \cdot 2^{10}$	≥ 0		
80	$4 \cdot 2^3$	17		(B)
80	$4 \cdot 2^4$	303	16777216, 25165824^5, 33554432, 50331648^3, 75497472^6, 100663296^3, 150994944^3, 201326592, 301989888^19, 603979776^21, 905969664^4, 1207959552^6, 1811939328^35, 2415919104^2, 3623878656^61, 7247757312^8, 10871635968^20, 14495514624^5, 21743271936^15, 43486543872^31, 86973087744^25, 130459631616, 173946175488^10, 260919263232^9, 347892350976, 521838526464^4, 695784701952, 1043677052928, 4174708211712	(B)
80	$4 \cdot 2^5$	≥ 16608		,,
80	$4 \cdot 2^6$	≥ 15082		,,
80	$4 \cdot 2^7$	≥ 54785		,,
80	$4 \cdot 2^8$	≥ 1855		,,
80	$4 \cdot 2^9$	≥ 406		,,
80	$4 \cdot 2^{10}$	≥ 7	1^6, 2	,,
80	$4 \cdot 2^{11}$	≥ 1		,,
80	$4 \cdot 2^{12}$	≥ 1		,,
80	$4 \cdot 2^{13}$	≥ 1		,,
80	$4 \cdot 2^{14}$	≥ 1		,,
80	$4 \cdot 2^{15}$	≥ 1		,,
80	$4 \cdot 2^{16}$	≥ 1		,,
80	$4 \cdot 2^{17}$	≥ 1		,,
80	$4 \cdot 2^{18}$	≥ 1		,,
80	$4 \cdot 2^{19}$	≥ 1		,,
80	$4 \cdot 2^{20}$	0		(Rao)
81	$9 \cdot 3^3$	3	324, 864, 69984	(B), (L)
81	$9 \cdot 3^4$	2	$324, 3888$	(B)
81	$9 \cdot 3^5$	0		(Rao)
81	3^4	32	31104, 49152, 196608^2, 786432, 1048576^2, 1572864, 3145728, 4718592, 6291456^2, 8388608, 25165824^2, 28311552, 37748736^2, 100663296, 301989888^2, 603979776, 1207959552, 1358954496, 1811939328, 5435817984, 8153726976, 86973087744, 3522410053632, 285315214344192, 380420285792256, 1326443518324400147398656	(B)
81	3^5	≥ 9906		(B)
81	3^6	≥ 229	1^{23}, 2^{67}, 3, 4^{37}, 6^{23}, 8^9, 12^{29}, 16^2, 24^{14}, 36^{11}, 48, 72^7, 144^2, 216, 2592, 7776	,,
81	3^7	≥ 478		,,
81	3^8	≥ 78		,,
81	3^9	≥ 1	23328	(L)
81	3^{10}	≥ 1		(L)
81	3^{11}	0		
84	$7 \cdot 3 \cdot 2^2$	≥ 1		
84	$7 \cdot 3 \cdot 2^3$	0		(Div)
88	$22 \cdot 2^3$	1	76480844267520000	(IS)

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Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
88	$22 \cdot 2^4$	0		(Rao)
88	$11 \cdot 2^3$	4428	1916006400, 4459069440^{37}, 63417876480^{442}, 3478923509760^{1554}, 712483534798848^{1855}, 759982437118771200^{539}	(B)
88	$11 \cdot 2^4$	≥ 5000		,,
88	$11 \cdot 2^5$	≥ 87585		,,
88	$11 \cdot 2^6$	≥ 16147		,,
88	$11 \cdot 2^7$	0		(X)
90	$5 \cdot 3^2 \cdot 2$	≥ 1	17280	(IS)
90	$5 \cdot 3^2 \cdot 2^2$	0		(Div)
96	$24 \cdot 2^3$	≥ 1		(IS)
96	$24 \cdot 2^4$	0		(Rao)
96	$12 \cdot 4 \cdot 2^2$	≥ 1		(IS)
96	$12 \cdot 4 \cdot 2^3$	≥ 6	4608, 82944, 1024, 1024, 4608, 248832	
96	$12 \cdot 4 \cdot 2^4$	≥ 16	256^3, 512^2, 2048^3, 4096^3, 12288, 18432^2, 331776, 995328	
96	$12 \cdot 4 \cdot 2^5$	0		(Rao)
96	$8 \cdot 6 \cdot 2^2$	≥ 1		
96	$8 \cdot 3 \cdot 2^2$	≥ 1		
96	$8 \cdot 3 \cdot 2^3$	≥ 1		
96	$8 \cdot 3 \cdot 2^4$	≥ 1		
96	$8 \cdot 3 \cdot 2^5$	0		(O')
96	$8 \cdot 2^3$	1172	118747255799808^{15}, 2003859941621760^{71}, 48693796581408768^{160}, 973875931628175360^{16},$2629465015396073472^{265}$, $14199111083138796748 8^{300}$, $25877879949020457074688^{170}$, $20961082758706570230 49728^{160}$, $2200410623677980916516 68246528^{15}$	(B)
96	$8 \cdot 2^4$	≥ 14500		,,
96	$8 \cdot 2^5$	≥ 23352		,,
96	$8 \cdot 2^6$	≥ 36943		,,
96	$8 \cdot 2^7$	≥ 7600		,,
96	$8 \cdot 2^8$	≥ 971	2^{240}, 4^{240}, 8^{72}, 12^{16}, 16^{318}, 24^{36}, 128^{18}, 144^{16}, 384^6, 432^8, 55296	,,
96	$8 \cdot 2^9$	≥ 193	8^{36}, 16^{10}, 32^{66}, 64^{30}, 96^{16}, 128^3, 256^6, 288^8, 512^3, 1024^6, 1152^8, 165888	,,
96	$8 \cdot 2^{10}$	≥ 3	720^2, 14400	,,
96	$8 \cdot 2^{11}$	≥ 0		
96	$8 \cdot 2^{12}$	0		(Rao)
96	$6 \cdot 4^2 \cdot 2$	≥ 4	32, 64, 256, 9216	(IS)
96	$6 \cdot 4^2 \cdot 2^2$	≥ 249	2^{58}, 4^{65}, 8^{56}, 16^{42}, 32^{19}, 64^7, 128, 256	(IS)
96	$6 \cdot 4^2 \cdot 2^3$	≥ 29987		,,
96	$6 \cdot 4^2 \cdot 2^4$	≥ 7895	1^{1520}, 2^{3649}, 4^{2265}, 8^{403}, 16^{52}, 24, 32^5	,,
96	$6 \cdot 4^2 \cdot 2^5$	≥ 1199	1^{411}, 2^{370}, 4^{250}, 8^{137}, 12, 16^{29}, 48	,,
96	$6 \cdot 4^2 \cdot 2^6$	≥ 8	2^2, 4^2, 8^4	,,
96	$6 \cdot 4^2 \cdot 2^7$	≥ 0		
96	$6 \cdot 4 \cdot 2^2$	≥ 1	648518346341351424	(IS)
96	$6 \cdot 4 \cdot 2^3$	≥ 4		(IS)
96	$6 \cdot 4 \cdot 2^4$	≥ 249		,,
96	$6 \cdot 4 \cdot 2^5$	≥ 29987		,,
96	$6 \cdot 4 \cdot 2^6$	≥ 7895		,,
96	$6 \cdot 4 \cdot 2^7$	≥ 1199	1^{462}, 2^{372}, 4^{290}, 8^{75}	,,
96	$6 \cdot 4 \cdot 2^8$	≥ 8	2^2, 4^4, 8^2	,,
96	$6 \cdot 4 \cdot 2^9$	≥ 0		

continued on next page

Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
96	$4^2 \cdot 3 \cdot 2$	≥ 1	134217728	(IS)
96	$4^2 \cdot 3 \cdot 2^2$	≥ 4		(IS)
96	$4^2 \cdot 3 \cdot 2^3$	≥ 249		,,
96	$4^2 \cdot 3 \cdot 2^4$	≥ 29987		,,
96	$4^2 \cdot 3 \cdot 2^5$	≥ 7895		,,
96	$4^2 \cdot 3 \cdot 2^6$	≥ 1199	1^{696}, 2^{320}, 4^{145}, 8^{38}	,,
96	$4^2 \cdot 3 \cdot 2^7$	≥ 8	2^2, 4^4, 8^2	,,
96	$4^2 \cdot 3 \cdot 2^8$	≥ 0		
96	$4^2 \cdot 2^2$	247	549755813888, 1855425871872^{3}, 2199023255552, 5566277615616^{6}, 7421703487488, 22265110462464^{3}, 25048249270272^{10}, 200385994162176, 225434243432448^{18}, 450868486864896^{4}, 901736973729792^{9}, 2028908190892032^{20}, 4057816381784064^{7}, 5410421842378752^{4}, 18260173718028288^{34}, 36520347436056576^{12}, 73040694872113152, 82170781731127296^{16}, 164341563462254592^{10}, 493024690386763776^{4}, 1479074071160291328^{16}, 1972098761547055104, 2958148142320582656^{8}, 5916296284641165312^{2}, 11832592569282330624^{8}, $13311666640442621952^{10}$, 23665185138564661248, 26623333280885243904^{5}, 53246666561770487808, 79869999842655731712, $119804999763983597568^{10}$, $239609999527967195136^{6}$, 1703893329976655609856, $1940840996176534280601 6^{4}$, $3881681992353068561203 2^{6}$, 1018708622073139313202167808, 4074834488292557252808671232	(B)
96	$4^2 \cdot 2^3$	≥ 1		,,
96	$4^2 \cdot 2^4$	≥ 1		,,
96	$4^2 \cdot 2^5$	≥ 10595		,,
96	$4^2 \cdot 2^6$	≥ 231		,,
96	$4^2 \cdot 2^7$	≥ 8		,,
96	$4^2 \cdot 2^8$	≥ 1		,,
96	$4^2 \cdot 2^9$	≥ 1		,,
96	$4^2 \cdot 2^{10}$	≥ 1		,,
96	$4^2 \cdot 2^{11}$	≥ 1		,,
96	$4^2 \cdot 2^{12}$	≥ 1		,,
96	$4^2 \cdot 2^{13}$	≥ 1		,,
96	$4^2 \cdot 2^{14}$	≥ 1		,,
96	$4^2 \cdot 2^{15}$	≥ 1		,,
96	$4^2 \cdot 2^{16}$	≥ 1		,,
96	$4^2 \cdot 2^{17}$	≥ 1		,,
96	$4^2 \cdot 2^{18}$	≥ 1		,,
96	$4^2 \cdot 2^{19}$	≥ 1		,,
96	$4^2 \cdot 2^{20}$	≥ 1		(Q)
96	$4^2 \cdot 2^{21}$	0		(Rao)

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Table 6.4 (continued)

N	Type	#	Size of the automorphism groups	Methods
96	$4 \cdot 3 \cdot 2^2$	≥ 1		(IS)
96	$4 \cdot 3 \cdot 2^3$	≥ 1		(IS)
96	$4 \cdot 3 \cdot 2^4$	≥ 1	2251799813685248	,,
96	$4 \cdot 3 \cdot 2^5$	≥ 1	64	,,
96	$4 \cdot 3 \cdot 2^6$	≥ 1	2	,,
96	$4 \cdot 3 \cdot 2^7$	≥ 1	2	,,
96	$4 \cdot 3 \cdot 2^8$	≥ 1	2	,,
96	$4 \cdot 3 \cdot 2^9$	≥ 8		(S)
96	$4 \cdot 3 \cdot 2^{10}$	≥ 0		
96	$3 \cdot 2^a$, $3 \leq a \leq 16$	≥ 1		(B)
100	$5^2 \cdot 2^2$	8198		(B)
100	$5^2 \cdot 2^3$	0		(Div)

The method used to obtain the four non-isomorphic arrays $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2; 3)$ differed from the one used for the other series. The first array was obtained by Construction (La), using Latin squares in Section 3.6. By extending this array, we get the $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^a; 3)$s listed for $a = 2, 3, 4, 5, 6$. From the $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^a; 3)$s, with $2 \leq a \leq 6$, we delete the first binary column, and check whether the arrays obtained are among the $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^{a-1}; 3)$s that we already found. Whenever we find a new $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^{a-1}; 3)$, we try extend it. By repeatedly deleting binary columns from the extended OAs, we found three more $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2; 3)$s.

Essentially this method is backtrack with a slightly variation, when we do not know all non-isomorphic arrays with 4 columns. I apply this construction to the series $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2; 3)$, in particular, since Construction (IS) fails (get out of memory) to find all extensions of $\mathrm{OA}(96; 6 \cdot 4^2; 3)$.

6.5. Conclusion

This chapter presented results which are computed by combining methods formulated in Chapters 3 and 4. Specifically, we obtained many orthogonal arrays of strength 3 with run size between 8 and 100.

APPENDIX A

Selected orthogonal arrays

Table A.1: The set of OA$(48; 3 \cdot 2^9; 3)$s

48.1.9.1	48.1.9.2	48.1.9.3
0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 1 1 1 1	0 0 0 0 0 0 1 1 1 1	0 0 0 0 0 0 1 1 1 1
0 0 0 0 1 1 0 0 1 1	0 0 0 0 1 1 0 0 1 1	0 0 0 0 1 1 0 0 1 1
0 0 0 0 1 1 1 1 0 0	0 0 0 0 1 1 1 1 0 0	0 0 0 0 1 1 1 1 0 0
0 0 1 1 0 0 0 0 1 1	0 0 1 1 0 0 0 0 1 1	0 0 1 1 0 0 0 1 0 0
0 0 1 1 0 0 1 1 0 0	0 0 1 1 0 0 1 1 0 0	0 0 1 1 0 1 0 0 1 1
0 0 1 1 1 1 0 0 0 0	0 0 1 1 1 1 0 0 0 0	0 0 1 1 1 0 1 0 0 1
0 0 1 1 1 1 1 1 1 1	0 0 1 1 1 1 1 1 1 1	0 0 1 1 1 1 1 1 1 0
0 1 0 1 0 1 0 1 0 1	0 1 0 1 0 1 0 1 0 1	0 1 0 1 0 0 1 0 1 0
0 1 0 1 0 1 1 0 1 0	0 1 0 1 0 1 1 0 1 0	0 1 0 1 0 1 1 1 0 1
0 1 0 1 1 0 0 1 1 0	0 1 0 1 1 0 0 1 1 0	0 1 0 1 1 0 0 1 1 1
0 1 0 1 1 0 1 0 0 1	0 1 0 1 1 0 1 0 0 1	0 1 0 1 1 1 0 0 0 0
0 1 1 0 0 1 0 1 1 0	0 1 1 0 0 1 0 1 1 0	0 1 1 0 0 1 0 1 1 0
0 1 1 0 0 1 1 0 0 1	0 1 1 0 0 1 1 0 0 1	0 1 1 0 0 1 1 0 0 1
0 1 1 0 1 0 0 1 0 1	0 1 1 0 1 0 0 1 0 1	0 1 1 0 1 0 0 1 0 1
0 1 1 0 1 0 1 0 1 0	0 1 1 0 1 0 1 0 1 0	0 1 1 0 1 0 1 0 1 0
1 0 0 0 0 1 0 1 0 1	1 0 0 0 0 1 0 1 0 1	1 0 0 0 0 1 0 1 1 0
1 0 0 1 0 0 0 1 1 0	1 0 0 1 0 0 0 1 1 0	1 0 0 1 0 0 0 1 0 1
1 0 0 1 0 1 1 0 0 0	1 0 0 1 0 1 1 0 1 1	1 0 0 1 0 1 1 0 1 1
1 0 0 1 1 0 0 0 0 1	1 0 0 1 1 0 0 0 0 1	1 0 0 1 1 0 1 1 1 0
1 0 1 0 0 1 1 1 1 0	1 0 1 0 0 1 1 1 1 0	1 0 1 0 0 0 1 0 0 0
1 0 1 0 1 0 0 1 1 1	1 0 1 0 1 0 0 1 0 0	1 0 1 0 1 0 0 0 1 1
1 0 1 0 1 1 1 0 0 1	1 0 1 0 1 1 1 0 0 1	1 0 1 0 1 1 1 1 0 1
1 0 1 1 1 0 1 0 1 0	1 0 1 1 1 0 1 0 1 0	1 0 1 1 1 1 0 0 0 0
1 1 0 0 0 0 1 0 1 1	1 1 0 0 0 0 1 0 0 0	1 1 0 0 0 1 0 0 0 1
1 1 0 0 1 0 1 1 0 0	1 1 0 0 1 0 1 1 1 1	1 1 0 0 1 0 0 1 0 0
1 1 0 0 1 1 0 0 1 0	1 1 0 0 1 1 0 0 1 0	1 1 0 0 1 1 1 0 1 0
1 1 0 1 1 1 1 1 1 1	1 1 0 1 1 1 1 1 0 0	1 1 0 1 1 0 1 0 0 1
1 1 1 0 0 0 0 0 0 0	1 1 1 0 0 0 0 0 1 1	1 1 1 0 0 0 1 1 1 1
1 1 1 1 0 0 1 1 0 1	1 1 1 1 0 0 1 1 0 1	1 1 1 1 0 0 0 0 1 0
1 1 1 1 0 1 0 0 1 1	1 1 1 1 0 1 0 0 0 0	1 1 1 1 0 1 1 1 0 0
1 1 1 1 1 1 0 1 0 0	1 1 1 1 1 1 0 1 1 1	1 1 1 1 1 1 0 1 1 1
2 0 0 0 1 0 1 0 1 0	2 0 0 0 1 0 1 0 1 0	2 0 0 0 1 0 1 0 0 1
2 0 0 1 0 1 1 0 1 1	2 0 0 1 0 1 1 0 0 0	2 0 0 1 0 1 1 0 0 0
2 0 0 1 1 0 1 1 0 1	2 0 0 1 1 0 1 1 0 1	2 0 0 1 1 0 0 0 1 0
2 0 0 1 1 1 0 1 1 0	2 0 0 1 1 1 0 1 1 0	2 0 0 1 1 1 0 1 0 1
2 0 1 0 0 0 1 0 0 1	2 0 1 0 0 0 1 0 0 1	2 0 1 0 0 1 0 1 0 1
2 0 1 0 0 1 0 0 1 0	2 0 1 0 0 1 0 0 1 0	2 0 1 0 0 1 1 0 1 0
2 0 1 0 1 0 0 1 0 0	2 0 1 0 1 0 0 1 1 1	2 0 1 0 1 0 0 1 1 0
2 0 1 1 0 1 0 1 0 1	2 0 1 1 0 1 0 1 0 1	2 0 1 1 0 0 1 1 1 1
2 1 0 0 0 0 0 1 1 1	2 1 0 0 0 0 0 1 0 0	2 1 0 0 0 0 0 0 1 1
2 1 0 0 0 1 1 1 0 0	2 1 0 0 0 1 1 1 1 1	2 1 0 0 0 0 1 1 0 0

continued on next page

Table A.1 (continued)

48.1.9.1	48.1.9.2	48.1.9.3
2 1 0 0 1 1 0 0 0 1	2 1 0 0 1 1 0 0 0 1	2 1 0 0 1 1 1 1 1 1
2 1 0 1 0 0 0 0 0 0	2 1 0 1 0 0 0 0 1 1	2 1 0 1 0 1 0 1 1 0
2 1 1 0 1 1 1 1 1 1	2 1 1 0 1 1 1 1 0 0	2 1 1 0 1 1 0 0 0 0
2 1 1 1 0 0 1 1 1 0	2 1 1 1 0 0 1 1 1 0	2 1 1 1 0 0 0 0 0 1
2 1 1 1 1 0 0 0 1 1	2 1 1 1 1 0 0 0 0 0	2 1 1 1 1 0 1 1 0 0
2 1 1 1 1 1 1 0 0 0	2 1 1 1 1 1 1 0 1 1	2 1 1 1 1 1 1 0 1 1

Table A.2: The set of OA($54; 3^5 \cdot 2; 3$)s

54.5.1.1	54.5.1.2	54.5.1.3	54.5.1.4
0 0 0 0 0 0	0 0 0 0 0 0	0 0 0 0 0 0	0 0 0 0 0 0
0 0 0 0 1 1	0 0 0 0 1 1	0 0 0 0 1 1	0 0 0 0 1 1
0 0 1 1 0 1	0 0 1 1 0 1	0 0 1 1 0 1	0 0 1 1 0 1
0 0 1 1 2 0	0 0 1 1 2 0	0 0 1 1 2 0	0 0 1 1 2 0
0 0 2 2 1 0	0 0 2 2 1 0	0 0 2 2 1 0	0 0 2 2 1 0
0 0 2 2 2 1	0 0 2 2 2 1	0 0 2 2 2 1	0 0 2 2 2 1
0 1 0 1 1 0	0 1 0 1 1 0	0 1 0 1 1 0	0 1 0 1 1 0
0 1 0 2 2 0	0 1 0 2 2 1	0 1 0 2 2 1	0 1 0 2 2 1
0 1 1 0 1 1	0 1 1 0 1 1	0 1 1 0 1 1	0 1 1 0 1 1
0 1 1 2 0 0	0 1 1 2 0 0	0 1 1 2 0 0	0 1 1 2 0 0
0 1 2 0 2 1	0 1 2 0 2 0	0 1 2 0 2 0	0 1 2 0 2 0
0 1 2 1 0 1	0 1 2 1 0 1	0 1 2 1 0 1	0 1 2 1 0 1
0 2 0 1 2 1	0 2 0 1 2 1	0 2 0 1 2 0	0 2 0 1 2 1
0 2 0 2 0 1	0 2 0 2 0 0	0 2 0 2 0 1	0 2 0 2 0 0
0 2 1 0 2 0	0 2 1 0 2 0	0 2 1 0 2 1	0 2 1 0 2 0
0 2 1 2 1 1	0 2 1 2 1 1	0 2 1 2 1 0	0 2 1 2 1 1
0 2 2 0 0 0	0 2 2 0 0 1	0 2 2 0 0 0	0 2 2 0 0 1
0 2 2 1 1 0	0 2 2 1 1 0	0 2 2 1 1 1	0 2 2 1 1 0
1 0 0 1 1 1	1 0 0 1 1 1	1 0 0 1 1 1	1 0 0 1 1 1
1 0 0 2 2 1	1 0 0 2 2 0	1 0 0 2 2 0	1 0 0 2 2 0
1 0 1 0 1 0	1 0 1 0 1 0	1 0 1 0 1 0	1 0 1 0 1 0
1 0 1 2 0 1	1 0 1 2 0 1	1 0 1 2 0 1	1 0 1 2 0 1
1 0 2 0 2 0	1 0 2 0 2 1	1 0 2 0 2 1	1 0 2 0 2 1
1 0 2 1 0 0	1 0 2 1 0 0	1 0 2 1 0 0	1 0 2 1 0 0
1 1 0 0 0 1	1 1 0 0 0 1	1 1 0 0 0 1	1 1 0 0 0 1
1 1 0 0 2 0	1 1 0 0 2 0	1 1 0 1 0 0	1 1 0 1 0 0
1 1 1 1 1 0	1 1 1 1 1 0	1 1 1 1 2 1	1 1 1 1 2 1
1 1 1 1 2 1	1 1 1 1 2 1	1 1 1 2 2 0	1 1 1 2 2 0
1 1 2 2 0 0	1 1 2 2 0 0	1 1 2 0 1 0	1 1 2 0 1 0
1 1 2 2 1 1	1 1 2 2 1 1	1 1 2 2 1 1	1 1 2 2 1 1
1 2 0 1 0 0	1 2 0 1 0 0	1 2 0 0 2 0	1 2 0 0 2 1
1 2 0 2 1 0	1 2 0 2 1 1	1 2 0 2 1 1	1 2 0 2 1 0
1 2 1 0 0 1	1 2 1 0 0 1	1 2 1 0 0 1	1 2 1 0 0 0
1 2 1 2 2 0	1 2 1 2 2 0	1 2 1 1 1 0	1 2 1 1 1 1
1 2 2 0 1 1	1 2 2 0 1 0	1 2 2 1 2 1	1 2 2 1 2 0
1 2 2 1 2 1	1 2 2 1 2 1	1 2 2 2 0 0	1 2 2 2 0 1
2 0 0 1 2 0	2 0 0 1 2 0	2 0 0 1 2 1	2 0 0 1 2 0
2 0 0 2 0 0	2 0 0 2 0 1	2 0 0 2 0 0	2 0 0 2 0 1
2 0 1 0 2 1	2 0 1 0 2 1	2 0 1 0 2 0	2 0 1 0 2 1
2 0 1 2 1 0	2 0 1 2 1 0	2 0 1 2 1 1	2 0 1 2 1 0
2 0 2 0 0 1	2 0 2 0 0 0	2 0 2 0 0 1	2 0 2 0 0 0
2 0 2 1 1 1	2 0 2 1 1 1	2 0 2 1 1 0	2 0 2 1 1 1
2 1 0 1 0 1	2 1 0 1 0 1	2 1 0 0 2 1	2 1 0 0 2 0
2 1 0 2 1 1	2 1 0 2 1 0	2 1 0 2 1 0	2 1 0 2 1 1
2 1 1 0 0 0	2 1 1 0 0 0	2 1 1 0 0 0	2 1 1 0 0 1

continued on next page

Table A.2 (continued)

54.5.1I.1	54.5.1.2	54.5.1.3	54.5.1.4
2 1 1 2 2 1	2 1 1 2 2 1	2 1 1 1 1 1	2 1 1 1 1 0
2 1 2 0 1 0	2 1 2 0 1 1	2 1 2 1 2 0	2 1 2 1 2 1
2 1 2 1 2 0	2 1 2 1 2 0	2 1 2 2 0 1	2 1 2 2 0 0
2 2 0 0 1 0	2 2 0 0 1 0	2 2 0 0 1 0	2 2 0 0 1 0
2 2 0 0 2 1	2 2 0 0 2 1	2 2 0 1 0 1	2 2 0 1 0 1
2 2 1 1 0 0	2 2 1 1 0 0	2 2 1 1 0 0	2 2 1 1 0 0
2 2 1 1 1 1	2 2 1 1 1 1	2 2 1 2 2 1	2 2 1 2 2 1
2 2 2 2 0 1	2 2 2 2 0 1	2 2 2 0 1 1	2 2 2 0 1 1
2 2 2 2 2 0	2 2 2 2 2 0	2 2 2 2 2 0	2 2 2 2 2 0

Table A.3: Four good OA($72; 3^2 \cdot 2^7; 3$)s

72.2.7.552	72.2.7.1081	72.2.8.280	72.2.8.379
0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 1 1	0 0 0 0 0 0 0 1 1	0 0 0 0 0 0 1 1 1	0 0 0 0 0 1 1 1 1
0 0 0 0 0 1 1 0 1	0 0 0 0 0 1 1 0 1	0 0 0 0 1 1 0 0 1	0 0 0 0 1 0 0 1 1
0 0 0 0 1 0 1 1 0	0 0 0 0 1 0 1 1 0	0 0 0 1 0 1 1 1 0	0 0 0 1 0 1 1 0 0
0 0 1 1 0 1 0 0 1	0 0 1 1 0 1 0 0 1	0 0 1 0 1 0 0 0 1	0 0 1 0 1 1 1 0 0
0 0 1 1 1 0 0 1 0	0 0 1 1 1 0 0 1 0	0 0 1 1 0 0 1 1 0	0 0 1 1 0 0 0 1 1
0 0 1 1 1 1 1 0 0	0 0 1 1 1 1 1 0 0	0 0 1 1 1 1 0 0 0	0 0 1 1 1 0 1 0 1
0 0 1 1 1 1 1 1 1	0 0 1 1 1 1 1 1 1	0 0 1 1 1 1 1 1 1	0 0 1 1 1 1 0 1 0
0 1 0 0 1 1 0 0 0	0 1 0 0 1 1 0 0 0	0 1 0 1 1 0 0 1 1	0 1 0 1 1 0 0 0 1
0 1 0 0 1 1 1 1 1	0 1 0 0 1 1 1 1 1	0 1 0 1 1 1 1 0 0	0 1 0 1 1 1 1 1 0
0 1 0 1 0 0 1 0 1	0 1 0 1 0 1 0 1 0	0 1 1 0 0 1 0 1 0	0 1 1 0 1 0 1 1 0
0 1 0 1 0 1 0 1 0	0 1 0 1 1 0 1 0 1	0 1 1 0 1 0 1 0 0	0 1 1 1 0 1 0 0 1
0 1 1 0 1 0 1 0 1	0 1 1 0 0 1 1 0 0	0 1 0 1 0 1 0 1 1	0 1 0 0 1 1 0 0 1
0 1 1 0 1 1 0 1 0	0 1 1 0 1 0 0 1 1	0 1 0 1 1 0 1 0 1	0 1 0 1 0 0 1 1 0
0 1 1 1 0 0 0 0 0	0 1 1 1 0 0 0 0 0	0 1 1 0 0 0 0 1 1	0 1 1 0 0 0 1 0 0
0 1 1 1 0 0 1 1 1	0 1 1 1 0 0 1 1 1	0 1 1 0 0 1 1 0 0	0 1 1 0 0 1 0 1 1
0 2 0 1 0 1 1 1 0	0 2 0 1 0 0 1 0 1	0 2 1 0 1 1 1 1 1	0 2 1 0 0 0 0 1 0
0 2 0 1 1 0 0 1 1	0 2 0 1 0 0 1 1 0	0 2 1 1 0 0 1 0 1	0 2 1 0 1 0 1 0 1
0 2 0 1 1 0 1 0 0	0 2 0 1 1 1 0 0 1	0 2 1 1 0 1 0 0 1	0 2 1 1 0 1 1 1 1
0 2 0 1 1 1 0 0 1	0 2 0 1 1 1 0 1 0	0 2 1 1 1 0 0 1 0	0 2 1 1 1 1 0 0 0
0 2 1 0 0 0 1 1 0	0 2 1 0 0 1 0 1 1	0 2 0 0 0 1 1 0 1	0 2 0 0 0 1 1 0 1
0 2 1 0 0 1 0 1 1	0 2 1 0 0 1 1 1 0	0 2 0 0 1 0 1 1 0	0 2 0 0 1 1 0 1 0
0 2 1 0 0 1 1 0 0	0 2 1 0 1 0 0 0 1	0 2 0 0 1 1 0 1 0	0 2 0 1 0 0 0 0 0
0 2 1 0 1 0 0 0 1	0 2 1 0 1 0 1 0 0	0 2 0 1 0 0 0 0 0	0 2 0 1 1 0 1 1 1
1 0 0 0 1 1 0 1 1	1 0 0 0 1 1 0 1 1	1 0 0 1 1 0 0 1 1	1 0 0 1 1 0 0 1 0
1 0 0 0 1 1 1 0 0	1 0 0 0 1 1 1 0 0	1 0 0 1 1 1 1 0 0	1 0 0 1 1 1 1 0 1
1 0 0 1 0 1 1 1 0	1 0 0 1 0 1 1 1 1	1 0 1 0 1 1 1 1 1	1 0 1 0 1 1 0 0 1
1 0 0 1 1 0 0 0 0	1 0 0 1 1 0 0 0 0	1 0 1 1 0 0 1 0 1	1 0 1 1 0 0 1 1 0
1 0 1 0 0 1 1 1 1	1 0 1 0 0 1 0 1 0	1 0 0 0 1 1 0 1 0	1 0 0 0 1 0 1 1 0
1 0 1 0 1 0 0 0 1	1 0 1 0 1 0 1 0 1	1 0 0 1 0 0 0 0 0	1 0 0 1 0 1 0 0 1
1 0 1 1 0 0 0 1 1	1 0 1 1 0 0 0 1 1	1 0 1 0 0 0 0 1 1	1 0 1 0 0 0 1 1 1
1 0 1 1 0 0 1 0 0	1 0 1 1 0 0 1 0 0	1 0 1 0 0 1 1 0 0	1 0 1 0 0 1 0 0 0
1 1 0 0 0 1 0 0 1	1 1 0 0 0 0 0 0 1	1 1 0 0 0 0 0 0 0	1 1 0 0 0 0 1 0 1
1 1 0 0 1 0 1 1 0	1 1 0 0 0 0 1 1 0	1 1 0 1 0 1 1 1 0	1 1 0 0 0 1 0 1 0
1 1 0 1 1 0 0 1 1	1 1 0 1 0 1 1 0 0	1 1 1 1 0 1 0 0 1	1 1 1 0 0 1 1 0 0
1 1 0 1 1 1 1 0 1	1 1 0 1 1 0 0 1 1	1 1 1 1 1 0 0 1 0	1 1 1 1 1 0 0 1 1
1 1 1 0 0 0 0 1 0	1 1 1 0 0 1 1 1 1	1 1 0 0 0 1 1 0 1	1 1 0 0 0 0 0 1 1
1 1 1 0 0 1 1 0 0	1 1 1 0 1 0 0 0 0	1 1 0 0 1 0 1 1 0	1 1 0 1 1 1 1 0 0
1 1 1 1 0 1 0 0 1	1 1 1 1 1 1 0 0 1	1 1 1 0 1 0 0 0 1	1 1 1 1 1 0 0 0 0
1 1 1 1 1 0 1 1 0	1 1 1 1 1 1 1 1 0	1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1
1 2 0 0 0 0 0 0 0	1 2 0 0 0 0 0 1 0	1 2 0 0 0 1 0 1 1	1 2 0 0 1 0 1 0 0
1 2 0 0 0 0 1 1 1	1 2 0 0 1 1 1 0 1	1 2 0 0 1 0 1 0 1	1 2 0 1 0 1 0 1 1

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Table A.3 (continued)

72.2.7.552	72.2.7.1081	72.2.8.280	72.2.8.379
1 2 0 1 0 0 1 0 1	1 2 0 1 0 1 0 0 0	1 2 1 0 0 0 1 1 0	1 2 1 0 1 1 0 1 0
1 2 0 1 0 1 0 1 0	1 2 0 1 1 0 1 1 1	1 2 1 0 1 1 0 0 0	1 2 1 1 0 0 1 0 1
1 2 1 0 1 0 1 0 1	1 2 1 0 0 0 1 0 1	1 2 0 1 0 0 1 1 1	1 2 0 0 1 1 1 1 1
1 2 1 0 1 1 0 1 0	1 2 1 0 1 1 0 1 0	1 2 0 1 1 1 0 0 1	1 2 0 1 0 0 0 0 0
1 2 1 1 1 1 0 0 0	1 2 1 1 0 1 0 0 1	1 2 1 1 0 1 0 1 0	1 2 1 0 1 0 0 0 1
1 2 1 1 1 1 1 1 1	1 2 1 1 1 0 1 1 0	1 2 1 1 1 0 1 0 0	1 2 1 1 0 1 1 1 0
2 0 0 1 0 0 1 0 1	2 0 0 1 0 0 1 0 1	2 0 1 0 0 1 0 1 0	2 0 1 0 0 0 0 0 1
2 0 0 1 0 1 0 1 0	2 0 0 1 0 1 1 1 0	2 0 1 0 1 0 1 0 0	2 0 1 0 1 1 1 1 1
2 0 0 1 1 0 1 1 1	2 0 0 1 1 0 0 0 1	2 0 1 1 0 1 0 0 1	2 0 1 1 0 1 0 1 0
2 0 0 1 1 1 0 0 1	2 0 0 1 1 1 0 1 0	2 0 1 1 1 0 0 1 0	2 0 1 1 1 0 1 0 0
2 0 1 0 0 0 1 1 0	2 0 1 0 0 0 1 1 0	2 0 0 0 0 1 1 0 1	2 0 0 0 0 1 1 1 0
2 0 1 0 0 1 0 0 0	2 0 1 0 0 1 0 0 0	2 0 0 0 1 0 1 1 0	2 0 0 0 1 0 0 0 0
2 0 1 0 1 0 1 0 1	2 0 1 0 1 0 1 1 1	2 0 0 1 0 1 0 1 1	2 0 0 1 0 0 1 0 1
2 0 1 0 1 1 0 1 0	2 0 1 0 1 1 0 0 1	2 0 0 1 1 0 1 0 1	2 0 0 1 1 1 0 1 1
2 1 0 0 0 0 0 1 1	2 1 0 0 0 1 0 0 1	2 1 0 0 0 0 1 1 1	2 1 0 0 1 1 0 0 0
2 1 0 0 0 0 1 0 0	2 1 0 0 1 0 1 1 0	2 1 0 0 1 1 0 0 1	2 1 0 1 0 0 1 1 1
2 1 0 1 0 1 1 1 0	2 1 0 1 0 1 0 1 1	2 1 1 0 1 1 1 1 1	2 1 1 0 1 1 1 1 1
2 1 0 1 1 0 0 0 0	2 1 0 1 1 0 1 0 0	2 1 1 1 0 0 1 0 1	2 1 1 1 0 0 0 0 0
2 1 1 0 0 1 1 1 1	2 1 1 0 0 0 1 0 1	2 1 0 0 1 1 0 1 0	2 1 0 0 1 0 1 0 1
2 1 1 0 1 0 0 0 1	2 1 1 0 1 1 0 1 0	2 1 0 1 0 0 0 0 0	2 1 0 1 0 1 0 1 0
2 1 1 1 1 1 0 1 1	2 1 1 1 0 0 0 1 0	2 1 1 1 0 0 1 1 0	2 1 1 0 1 0 0 1 0
2 1 1 1 1 1 1 0 0	2 1 1 1 1 1 1 0 1	2 1 1 1 1 1 0 0 0	2 1 1 1 0 1 1 0 1
2 2 0 0 0 1 0 0 1	2 2 0 0 0 0 0 1 1	2 2 0 0 0 0 0 0 0	2 2 0 0 0 0 0 1 1
2 2 0 0 1 0 0 1 0	2 2 0 0 0 1 1 0 0	2 2 0 1 0 1 1 1 0	2 2 0 0 0 1 1 0 0
2 2 0 0 1 1 1 0 0	2 2 0 0 1 0 0 0 0	2 2 0 1 1 0 0 1 1	2 2 0 1 1 0 1 1 0
2 2 0 0 1 1 1 1 1	2 2 0 0 1 1 1 1 1	2 2 0 1 1 1 1 0 0	2 2 0 1 1 1 0 0 1
2 2 1 1 0 0 0 0 0	2 2 1 1 0 0 0 0 0	2 2 1 0 0 0 0 1 1	2 2 1 0 0 0 1 1 0
2 2 1 1 0 0 0 1 1	2 2 1 1 0 1 1 1 1	2 2 1 0 0 1 1 0 0	2 2 1 0 0 1 0 0 1
2 2 1 1 0 1 1 0 1	2 2 1 1 1 0 0 1 1	2 2 1 0 1 0 0 0 1	2 2 1 1 1 0 0 1 1
2 2 1 1 1 0 1 1 0	2 2 1 1 1 1 1 0 0	2 2 1 1 1 1 1 1 1	2 2 1 1 1 1 1 0 0

NOTES: 6 blocks for 72.2.7.552 (72.2.8.280) generated by PQ and FG (PQ^2 and BG); additional generator for 12 blocks: CG (EG).

APPENDIX B

Notation

We use the following basic notation and terminology throughout the thesis.

Common notation. As a rule-of-thumb, writing $A := B$ or $B =: A$ means that we define a set (a group, a structure ...) A with the value B, that was well-determined. We write $(a_1, \ldots, a_i, \ldots, a_d)$ for a vector, write $[a_1, \ldots, a_i, \ldots, a_d]$ for a list of d entries, and $\{a_1, \ldots, a_i, \ldots, a_d\}$ for a set of d elements.

Factorial designs and fractional factorial designs. Suppose that we have d finite sets $Q_1, Q_2, \ldots, Q_d$ contained in a field k, called the *factor sets* or *factors*. Note that the Q_i are only taken as subsets of a field for convenience. The *(full) factorial design* with respect to these d factors is the Cartesian product $D = Q_1 \times \ldots \times Q_d \subset k^d$. Moreover, $r_i := |Q_i|$ is the number of *levels* of the factor i. We say that D is *symmetric* if $r_i = r$ for all i; otherwise, D is *mixed*, that is $r_i \neq r_j$ for some $i \neq j$. Let $s_1, s_2, \ldots, s_m$ be the distinct levels of D, and suppose that D has exactly a_i factors with s_i levels. We call $s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}$ the *design type* of D. For example, if $Q_1 = \{0, 1, 2, 3\}$, $Q_2 = Q_3 = Q_4 = \{0, 1\}$, then

$$D = \{(0,0,0,0), (0,0,0,1), (0,0,1,0), (0,0,1,1), \ldots, (3,1,1,0), (3,1,1,1)\}$$

is the $4 \cdot 2^3$ mixed factorial design.

Suppose D is a $s_1^{a_1} \cdots s_m^{a_m}$ mixed factorial design. A *fraction* F of D is a subset consisting of elements of D. If F has an element with multiplicity greater than one, we say F has *replications*. This is also called an $s_1^{a_1} \cdots s_m^{a_m}$ *fractional design*. For example

$$\begin{aligned} F = \{\ & (0,0,0,0), (0,1,0,1), (0,0,1,1), (0,1,1,0), (1,0,0,0), (1,1,0,1), \\ & (1,0,1,1), (1,1,1,0), (2,1,1,1), (2,0,1,0), (2,1,0,0), (2,0,0,1), \\ & (3,1,0,0), (3,1,0,1), (3,1,1,0), (3,1,1,1)\ \} \end{aligned}$$

is a $4 \cdot 2^3$ mixed fractional design. We usually consider a fractional design as a matrix whose rows correspond to the elements of the multiset, in any order, and whose columns correspond to the factors. So the example above becomes

$$F = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \end{bmatrix}^T,$$

where T denotes transpose.

Let t be a natural number. A fraction F of D is called t-*balanced* if, for each choice of t columns from F, every possible combination of coordinate values from those columns occurs equally often. In other words, for every index set $I \subseteq \{1, \ldots, d\}$ of size t, each row of $\prod_{i \in I} Q_i$ occurs equally often in the projection of

F onto the coordinates indexed by I. Note that a fraction with strength t also has strength s for all $1 \le s \le t$. The example above has strength 3 but not strength 4. A t-balanced fraction F is also called a *mixed orthogonal array of strength t* of strength t. If F has N rows, we write $F = \mathrm{OA}(N; s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}; t)$. We also refer to the rows of F as *runs*, so N is the *run size*.

An orthogonal array is called *trivial* if it contains each element of $Q_1 \times Q_2 \times \cdots \times Q_d$ the same number of times. We say that a triple of column vectors X, Y, Z are *orthogonal* if each possible value (x, y, z) appears in $[X|Y|Z]$ with the same frequency. So an array has strength three if, and only if, every triple of columns in the array is orthogonal.

In some circumstances, we also use the notation $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; t)$ where we allow some $r_i = r_j$ for $i \neq j$. Of course the existence of $\mathrm{OA}(N; r_1 \cdot r_2 \cdots, r_d; t)$ does not depend on the ordering of the parameters r_j, and we can take them in non-increasing order if we wish. The relation between the s_k and and r_j then is:

$$s_1 = r_1 = \ldots = r_{a_1}, s_2 = r_{a_1+1} = \ldots = r_{a_1+a_2}, \ldots,$$
$$s_m = r_{a_1+a_2+\cdots+a_{m-1}+1} = \ldots = r_{a_1+a_2+\cdots+a_m} = r_d.$$

Sometimes we find it useful to consider arrays with $r_i = 1$ for some i. An $\mathrm{OA}(N; 1 \cdot r_1 \cdot r_2 \cdots r_d; t)$ is equivalent to an $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; t)$, provided $t \le d$.

Permutations. If X is a set, a permutation on X is a *bijection* from X to itself. We write $\mathrm{Sym}(X)$ for the *symmetric group* on X, ie, the group of all permutations on X. Moreover, if N is a positive integer, we write Sym_N instead of $\mathrm{Sym}(\{1, 2, \ldots, N\})$. We usually write elements of Sym_N in *cycle notation*, so the permutation $p = (1, 2, 3)(4, 5)$ is defined by $1^p = 2,\ 2^p = 3,\ 3^p = 1,\ 4^p = 5,\ 5^p = 4$. We denote the collection of all k-subsets of X by $\binom{X}{k}$, and the *power set* (set of all subsets) of X by $\mathcal{P}(X) = \bigcup_k \binom{X}{k}$. We say a group K *acts* on a set X if we can define a group homomorphism $\phi : K \longrightarrow \mathrm{Sym}(X)$ such that for $x \in X$ and $g, h \in K$ we have:

$$x^{\phi(gh)} = (x^{\phi(g)})^{\phi(h)}.$$

We abbreviate $x^{\phi(g)}$ by x^g. In general, we write permutation action on the right. Let $p \in \mathrm{Sym}_N$. The *action of p on a subset* $B := \{x_1, x_2, \ldots, x_k\}$ of $\{1, 2, \ldots, N\}$ is given by:

$$B^p := \{x_1^p, x_2^p, \ldots, x_k^p\}. \tag{B.0.1}$$

With this action, the group Sym_N acts naturally on the set $\binom{\{1,2,\ldots,N\}}{k}$ of all subsets of $\{1, 2, \ldots, N\}$ of size k. The *action of p on a list* $Y := [y_1, y_2, \ldots, y_N]$ of length N is given by

$$[y_1, y_2, \ldots, y_N]^p := [y_{1^{p^{-1}}}, y_{2^{p^{-1}}}, \ldots, y_{N^{p^{-1}}}]$$

where $y_1, y_2, \ldots, y_N$ are arbitrary objects. In other words, we compute the ith position of Y^p by $Y^p[i] = y_{i^{p^{-1}}} = Y[i^{p^{-1}}]$. The group Sym_N also acts on the set of length N lists since for every $i = 1 \ldots N$ and $p, q \in \mathrm{Sym}_N$ we have

$$Y^{pq}[i] = y_{i^{q^{-1}p^{-1}}} = y_{(i^{q^{-1}})^{p^{-1}}} = Y^p[i^{q^{-1}}] = (Y^p)^q[i].$$

For instance, $k = 8$, $p = (2, 4) \in \mathrm{Sym}(\{2, 3, \ldots, 8\})$ gives

$$\{1, 3, 4, 5, 8\}^{(2,4)} = \{1, 2, 3, 5, 8\}.$$

If $p = (2, 4, 8, 3)$, then $p^{-1} = (2, 3, 8, 4)$, and

$$[1, 3, 5, 8, -100, 2, A, B]^{(2,4,8,3)} = [1, 5, B, 3, -100, 2, A, 8].$$

APPENDIX C

Glossary

Table C.1: Common notation and algebraic notation

Notation	Meaning
$\mathbb{N}$	natural numbers
$\mathbb{Z}$, $\mathbb{Z}_n = \{0, 1, 2, \ldots, n-1\}$	integers and the ring of integers modulo n
$\mathbb{Q}$	rationals
$\mathbb{R}$	real numbers
k, $\overline{k}$	field of coefficients and its algebraic closure
$\lvert A \rvert$, A^c	number of elements and complement of a set A
A^T	transpose of A when A is a matrix or a vector
$A \times B$	Cartesian product of two sets A, B
d	number of factors, variables, indeterminates,
N	run size of an orthogonal array
$\boldsymbol{x} = (x_1, \ldots, x_d)$	vector of factors, variables or indeterminates
$k[\boldsymbol{x}]$	$k[x_1, \ldots, x_d]$, the ring of polynomials with coefficients in k
	over the indeterminates $x_1, \ldots, x_d$
X	a finite set, a factor or a vector of length N
$\mathrm{Z}(J)$	the zero set of an ideal J over a filed k
V	an algebraic variety, a vector space
(G)	an ideal generated by a generating set G
$\langle B \rangle$	a k-vector space generated by a basis B
$\boldsymbol{\alpha} = (\alpha_1, \alpha_2 \ldots, \alpha_d)$	a d-tuple of nonnegative integers
$\boldsymbol{x}^{\boldsymbol{\alpha}}$	a term $x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_d^{\alpha_d}$
$\boldsymbol{x}^* = \{x_1, \ldots, x_d\}^*$	the set of terms in $x_1, \ldots, x_d$
$\mathrm{I}(V)$	vanishing ideal of a variety V
$\mathrm{I}(F)$	defining ideal or design ideal of a fraction F

Table C.2: Notation of construction and enumeration methods

Notation	Meaning
$\mathbb{X}$	set of all t-(v,k,λ) block designs, or
	set of all combinatorial structures of given type
$\mathrm{Aut}(F)$	automorphism group of a fraction
$\mathrm{Sym}(X)$	full symmetric group on a finite set X
Sym_N	$\mathrm{Sym}(\{1,2,\dots,N\})$
$Q_1, Q_2, \dots, Q_d$	factor sets or factors
$r_i = \lvert Q_i \rvert$	number of levels of factor i
$Q = Q_1 \times \ldots \times Q_d$	full factorial design in d factors Q_i
$\boldsymbol{p} \in Q$	a design point, an experimental run
m	number of distinct levels in a fractional factorial design
$s_1, \dots, s_m$	distinct levels of a fractional design having m sections
$s_1^{a_1} \cdots s_m^{a_m}$	design type of a fraction
$\mathrm{OA}(N; s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}; t)$	a strength t OA with N runs, m distinct sections
F	an orthogonal array of strength t, $t \geq 1$
$\mathcal{F}(U,N)$	set of all OAs having design type U and run size N
T	underlying set (the look-up table) of $\mathcal{F}(U,N)$
	or the search tree in backtrack search
P	a linear system of equations with integer coefficients
$\mathrm{Z}(P)$	set of vector solutions of a linear system P
$\mathrm{Z}(u)$	set of sub-vectors of solutions $X \in \mathrm{Z}(P)$
	without component u
n	dimension of the affine space $\mathrm{Z}(P) \bigcap \mathbb{Q}$
$I_N := [1,2,\dots,N]$	row-index list of a strength 3 orthogonal array F
$\mathrm{RowInd}(F_i)$	row-index set of a strength 2 derived design F_i of F
$L(F_i)$	row permutation subgroup associated with F_i
$F_{i_1,\dots,i_m}$	$\mathrm{OA}((r_1 r_2 \cdots r_m)^{-1}N; r_{m+1} \cdots r_d; t-m)$ the derived
	designs of an OA F taken with respect to an m-tuple of
	symbols $i_1, \dots, i_m$ where $i_j = 1, \dots, r_j$, and $j = 1, \dots, m$
$\mathrm{RowInd}(F_{i_1,\dots,i_m})$	row-index set of $F_{i_1,\dots,i_m}$
$V_{i_1,\dots,i_m}$	set of vector solutions of $F_{i_1,\dots,i_m}$
$L_{i_1,\dots,i_m}$	subgroup associated with $F_{i_1,\dots,i_m}$

Table C.3: Notation of selection methods

Notation	Meaning
n_2	maximum number of estimable components of 2-factor interactions in a model based on an orthogonal array
n_+	additional higher-order interaction components that are estimable
n_{pe}	number of degrees of freedom obtained from duplicate runs
$n_{2(...)}$	rank of the matrix with all components of 2-factor interactions
$n_{2(..0)}$	rank of the interaction matrix excluding components of the 3×3 interaction
$n_{2(.00)}$	rank of the matrix of just the 2×2 interactions
$n_{2(0.0)}$	rank of just the 2×3 interactions
GWLP	generalized word-length pattern $(A_1, A_2, \ldots, A_n)$
A_4	fourth component of GWLP
df_6	minimum decrease in n_2 in case the design was to be blocked in 6 blocks
df_{12}	minimum decrease for the 12 blocks case
EC_v	estimation capacity for v two-factor interactions
$EC_{(...)}$	mean estimation capacity over all models with 0 up to 45 two-factor interactions
$EC_{(..0)}$	mean estimation capacity of the interaction models excluding the components of the 3×3 interaction
$EC_{(.00)}$	mean estimation capacity of models involving just the 2×2 interactions
$EC_{(0.0)}$	mean estimation capacity of just the 2×3 interactions

APPENDIX D

Installed packages

Singular code for computing estimators of a regression model

function COMPUTE-SET-ESTIMABLE-TERMS(F)
  Input: F is a fractional design; and $<$ is a term order.
  Output: Set of estimable terms of a model based on F.
  `int` z, d; `list` X, T; `ideal` b, c, canon y, Est, J, D, Gb; `intvec` V; ▷ Type declaration
  `timer` $= 1$; $z =$ `rtimer`; ▷ computing time of each command will be printed
  $V =$ Get-levels-design(F); ▷ the levels
  $d =$ `ncols`(F); ▷ the number of factors
  $T =$ Gen-lterm1(F, V, d); ▷ main function computes estimators
  $LtI = T[1]$; ▷ leading terms of the vanishing ideal I(F)
  $Gb = T[2]$; ▷ Gröbner basis of I(F)
  $X = T[6]$; ▷ factor indeterminates
  Est = Reverse($T[3]$); Est = `sort`(Est)[1]; ▷ estimable terms
  $b =$ `std`($T[4]$); canon = Form-list(b); ▷ canonical polynomials
  $c =$ Extract-k-interactions(Est, X, 2); ▷ 2-interaction terms
  $y =$ Extract-k-interactions(Est, X, 1); $y = 1, y$; ▷ grand mean and MEs
  if `size`(c) > 0 **then**
    $J = y, c$;
  else
    $J = y$;
  end if ▷ grand mean, MEs and 2-interactions
  $D =$ Differ-ideal(Est, J); ▷ higher-than-2 interactions
  $z =$ `rtimer` $- z$; ▷ computing time
  Return `list`(Est, canon, Gb, LtI , J, c, D)
end function

Singular code for constructing 3*-balanced designs*

function INVERSE-PROBLEM(U, c)
  Input: U a design type, and c an index indicating a design being computed.
  Output: Fractions F having given estimable terms E determined by c.
  `int` $ok, d, nu, mu, nm, max1, max2$; `intvec` V; ▷ Type declaration
  `list` $G, H, X, sys, K, A, E, E2, C, M, Est, L, LF$;
  $d =$ Number-factors(U);
  $H =$ Get-levels-from-design-type(U);
  $V = H[1]; K = H[2]$; ▷ the levels and the weight vector of factor indeterminates
  if (`size`(U) $== 1$) **then**
    `ring` $R = 0, x(1..d)$, `dp`;
  else
    if (`size`(U) $== 2$) **then**
      `ring` $R = 0, (x(1..d)), ($`wp`$(K[1], K[2]))$;
    else
      if (`size`(U) $== 3$) **then**
        `ring` $R = 0, (x(1..d)), ($`wp`$(K[1], K[2], K[3]))$;
      end if
    end if
  end if ▷ declare base ring R
  ▷ we use `wp` ordering for mixed design to collect all MEs involving the largest-level factor

X = Form-var(d); A = Initialize-XCE(c, X);
$E = A[1]$; $L = A[2]$; ▷ estimable terms and design type
C = Compute-nu-mu(X, E, L, c);
$nu = C[1]$; $mu = C[2]$; $nm = nu * mu$; ▷ $mu = |\,\mathrm{Est}(F)|$, $nm = |\{a_{jl}\}|$
▷ now extend R to a new ring R_1 that includes new variables a_{jl}
`def` R_1 = `extendring`(nm, "a(", "`dp`(nm)", 0, R);; `setring` R_1;
`ideal` $a, GB, canon, Gb, X, Lv$; ▷ type redeclaration after redefining ring
X = Form-var(d); a = Get-vars-A-from-ring(nm);
sys = Construct-system(d, c, X, a, L);
$GB = sys[1]$; ▷ system of polynomials in terms of a_{jl}
$G = sys[2]$; ▷ border basis
canon = $sys[3]$; ▷ canonical polynomials
$E2 = sys[4]$; ▷ $E2 = G \setminus$ canon, border basis except canonical polynomials
$M = sys[5]$;; ▷ multiplication matrices
$max1 = 25; max2 = 75$;
▷ used to decide computing Grobener basis when reducing system or not
kill sys; ▷ to free memory
Gb = ReduceSystem($1, GB, max1, max2$); ▷ main procedure reduces system GB
LF = Factor-solve0(L, Lv, Gb, G, X, mu);
▷ main procedure compute designs
Return LF;
end function

GAP code for constructing strength 3 OAs: version 1, using local row permutations

function MAKE-COLUMN-X-USE-ROW-SYMBOL-PERMS(Lf, lev, t,d)
Input: Lf a list of OAs, lev the factor's level, t strength, number of factors $d \geq c + b + a$
Output: Strength t OAs having design type $[[s_1, c], [s_2, b], [2, a + 1]]$ if $lev = 2$;
if $Lf = []$ **then**
Return $[[], [], []]$;
end if;
$Ans := []$; $Ans2 := []$; $LSols := []$; $extA := []$;
q := Extend-design-type($Lf[1], s$); $U := q[1]$; ▷ the design type before extending,
$U_1 := q[2]$; ▷ U has the form $[[s_1, c], [s_2, b], [2, a]]$, $U_1 = [[s_1, c], [s_2, b], [2, a + 1]]$
if `Sum`$(U, v \to v[2]) = d$ **then**
$Ans2 := Lf$;
else
$i := 0$;
for f `in` Lf **do**
$i := i + 1$; L := Build-column-X-use-AutF(f, U, lev, t, U_1);
▷ main function finds all extensions of f, using localization at derived designs
if $L \neq []$ **then**
$extA$:= `Concatenation`($extA, [i]$); Ans := `Concatenation`(Ans, L);
▷ $extA$ stores indices of extendable arrays
Y := `List`($Ans, b \to$ Size-autmomorphism-group(b, U_1));
Write-arrays-to-disk(Ans, Y, U_1, $extA$);
end if;
end for;
end if;
if `Sum`$(U, v \to v[2]) = d$ **then**
Ans := The-case-reaching-bound($Ans2$, U, d, lev, t, $extA$);
Return Ans;
else ▷ The current number of factors is $\sum_{v \in U_1} v[2]$;
M := The-case-not-yet-reaching-bound(Ans, U_1, lev, t, $extA$);
Ans :=MAKE-COLUMN-X-USE-ROW-SYMBOL-PERMS(M, lev, t, d);
Return Ans;
end if;
end function

GAP code for constructing strength 3 OAs: version 2, by computing pivotal variables

function MAKE-COLUMN-X-USE-LA-GROUP-METHOD2(Lf, lev, t, d)
  Input: Lf a list of OAs, lev the new level, t the strength, number of factors $d \geq c+b+a$
  Output: Strength t OAs having design type $[[s_1, c], [s_2, b], [2, a+1]]$ if $lev = 2$.

  if $Lf = []$ **then** Return $[[], [], []]$;
  end if;
  $Ans := []$; $Ans2 := []$; $extA := []$; $N :=$ `Length`$(Lf[1])$;
    ▷ N is the run size
  $q :=$ Extend-design-type$(Lf[1], lev)$; $U := q[1]$;
    ▷ U is the design type before extending
  $U_1 := q[2]$;
    ▷ and design type after extending $U_1 = [[s_1, c], [s_2, b], [2, a+1]]$

  if `Sum`$(U, v \rightarrow v[2]) = d$ **then** $Ans2 := Lf$;
  else
    $stringx :=$ Form-name-variables-without-x0(N, 1);;
    $R :=$ `PolynomialRing`(`Rationals`, $stringx$);; $stringx := []$;
    $x :=$ `IndeterminatesOfPolynomialRing`(R); $R :=$ `PolynomialRing`(`Rationals`, x);
    $i := 0$;
    for f `in` Lf **do**
      $i := i + 1$; $L :=$ Extend-one-column (f, lev, t , x);
        ▷ main function finds all extensions of f, using integral pivotal variables
      if $L \neq []$ **then**
        $extA :=$ `Concatenation`$(extA, [i])$; $Ans :=$ `Concatenation`(Ans, L);
        $Y :=$ `List`$(Ans, b \rightarrow$ Size-autmomorphism-group$(b, U_1))$;
        Write-arrays-to-disk(Ans, Y, U_1, $extA$);
      end if;
        ▷ store results accumulated up to the ith array
    end for;
  end if;

  if `Sum`$(U, v \rightarrow v[2]) = d$ **then**
    $Ans :=$ The-case-reaching-bound($Ans2$, U, d, lev, t, $extA$);
    Return Ans;
  else
    $M :=$ The-case-not-yet-reaching-bound(Ans, U_1, lev, t, $extA$);
      ▷ computing non-isomorphic OAs, by employing canonical labeling arrays
    $Ans :=$MAKE-COLUMN-X-USE-LA-GROUP-METHOD2(M, lev, t, d);
    Return Ans;
  end if;
end function

◇ Note that the procedures MAKE-COLUMN-X-USE-ROW-SYMBOL-PERMS(Lf, lev, t, d) and MAKE-COLUMN-X-USE-LA-GROUP-METHOD2(Lf, lev, t, d) are implemented for extending binary columns only.

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Samenvatting

In dit proefschrift bestuderen we de constructie van orthogonale arrays (OAs) van sterkte 3. Elk drietal kolommen uit deze arrays heeft de eigenschap dat elke combinatie van de daarmee corresponderende factorinstellingen even vaak voorkomt. We beschouwen ook de selectie van een OA als proefopzet. We gebruiken algebra, modulaire rekenkunde en meetkunde om afzonderlijke arrays te construeren, en we gebruiken combinatoriek en verzamelingenleer om alle niet-isomorfe OAs op te sommen van sterke 3 en met gegeven aantallen runs, factoren en niveaus van de factoren. We stellen criteria voor om arrays te selecteren die het meest nuttig zijn voor praktijkproblemen.

Eerst beschouwen we het probleem om schatbare termen te vinden van een gegeven design, en het omgekeerde probleem om fractionele designs, inclusief sterkte-t designs, te maken met bepaalde schatbare termen. We tonen aan dat deze problemen aangepakt kunnen worden met methodologie die gebruik maakt van Gröbner bases. Onze praktische implementatie in een computer-algebra pakket laat echter zien dat de constructiemethode alleen voor kleine gevallen werkt.

Ten tweede stellen we enkele specifieke constructiemethoden voor van OAs van sterkte 3. Met behulp van lineaire codes, Hadamard matrices en Latijnse vierkanten maken we verscheidene nieuwe OAs met 80 en 96 runs. De specifieke constructies geven ons inzicht in de wetmatigheden van OAs. Er is echter geen afzonderlijke constructiemethode die alle niet-isomorfe OAs van een bepaald type kan voortbrengen.

Ten derde stellen we een *backtrack* algoritme voor om een reeks OAs van een gegeven type te genereren. Dit algoritme maakt gebruik van de automorfisme groep van een OA. We stellen ook een methode voor om bestaande OAs uit te breiden met behulp van integer linear programming. Een mengeling van deze benaderingen stelt ons in staat om elke reeks OAs van sterkte 3 te construeren, mits het aantal runs niet al te groot is.

Verder behandelen we het probleem om OAs voor praktijksituaties te selecteren. We gebruiken daarbij diverse reeksen $3^a 2^b$ arrays als voorbeelden. We stellen voor om arrays alleen beschikbaar te houden als ze toelaatbaar zijn volgens verscheidene nader uitgewerkte criteria, waaronder het vermogen van een array om de runs orthogonaal op de hoofdeffecten te verblokken.

Tenslotte geven we een verzameling van de meeste niet-isomorfe arrays van sterkte 3 met ten hoogste 100 runs.

Summary

In this thesis, we study the construction of strength-3 orthogonal arrays (OAs). Each triple of columns from these arrays has every combination of the corresponding factor settings occurring equally often. We also consider the selection of an OA as an experimental design. We employ algebra, modular arithmetic, and geometry to construct individual arrays. We use combinatorics and group theory to list all non-isomorphic OAs of strength 3 with a given number of runs, and given numbers and levels of the factors. We propose criteria to select arrays that are most useful for practical problems.

First, we address the problem of finding estimable terms given a design, and the inverse problem of making fractional designs, including strength t designs, with certain estimable terms. We show that these problems can be tackled by Gröbner bases methodology. However, our practical implementation in a computer-algebra package shows that the construction method only works for small cases.

Second, we propose some specific constructions of OAs of strength 3. Using techniques from linear codes, Hadamard matrices, and Latin squares, we produce several new OAs with 80 and 96 runs. The specific constructions give us an insight into the regularity of OAs. However, no single construction method can generate all strength 3 non-isomorphic OAs of certain types.

Third, to generate a series of OAs of a given type, we propose a backtrack search approach using the automorphism group of an OA. We also propose to extend existing OAs with integer linear programming. A mixture of these approaches permit the construction of any series of OAs of strength 3 and moderate run-size.

Further, we address the problem of selecting OAs for practical uses, using several series of $3^a \cdot 2^b$ arrays as examples. We propose to retain arrays only if they are admissible according to several criteria, including the ability of an array to block the runs orthogonally to the main effects.

Finally, we present a collection of most of the non-isomorphic strength 3 OAs with run size at most 100.

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Curriculum Vitae

Born on March 17, 1969 in Mytho, Vietnam, Nguyễn Văn Minh Mẫn studied at the Nguyen Dinh Chieu High School in Mytho during 1983-1986. He studied mathematics at the University of Education, Ho-Chi-Minh City, Vietnam.

From January 1991 to June 1998 he worked as a high-shool teacher in mathematics and computer science. From January 1995 to January 1998, he followed a masters program in computer algebra at the School of Natural Sciences, University of Ho-Chi-Minh City. He graduated with a thesis whose title 'Giả thuyết Jacques Dixmier và giả thuyết Nguyễn Hữu Anh trên đại số Weil', which translates as 'Jacques Dixmier and Nguyen Huu Anh Conjectures on the Weil Algebra'.

During 1999 and 2001, he was a mathematics lecturer in the Department of Information Technology, University of Technology, Ho-Chi-Minh City. From October 2001 to September 2005 he was a Ph.D. student in the Discrete Mathematics Group at the Eindhoven University of Technology, the Netherlands, under the supervision of Prof. Dr. Arjeh M. Cohen.