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ALGEBRAIC METHODS FOR CONSTRUCTION OF MIXED ORTHOGONAL ARRAYS

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Abstract

Orthogonal arrays (OAs) of strength t (also called t-balanced fractional designs) are difficult to construct, but they have useful properties that can be employed in the theory of experimental design and in practical applications to statistical quality management.

Specifically, strength 3 OAs permit estimation of all the main effects of the experimental factors, without confounding them with the two-factor interactions. Strength 4 OAs allow us to also separately estimate all two-factor interactions. These arrays are in great demand not only in well-known areas like statistical quality control of industries and services [12], software engineering [13], but also in emerging and fast-developed areas such as computational biology, drug designs and/or medical sciences, in particular DNA micro-array experiments [6, 21].

In this paper, we introduce some new methods for constructing mixed orthogonal arrays of strength t, with a given parameter set of run-size and factor levels. A few new arrays with run size up to 100 have been found with the proposed methods.

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1 Introduction

Orthogonal arrays (OAs) with strength $t > 1$ (also called t-balanced fractional designs) are difficult to construct, but they have good features which can be employed in the theory of experimental design, algebraic coding theory, and in practical applications to statistical quality management [22].

In this paper, we introduce new methods that employ algebraic formulations to construct mixed OAs with strength $t > 1$. We recall some recent relevant works, as well as introduce our theoretic problems in Section 2. In Section 3, we review the arithmetic formulation and then discuss its modification that results in an optimal runsize OA. Section 4 recalls some concepts from the algebraic geometry method for solving our second problem. Next we present our new method using linear algebra and algebraic geometry in Section 5; this method results in a necessary condition for constructing mixed orthogonal arrays (OAs) of arbitrary strength t. Section 6 finally concludes the paper with few comments.

2 Background and problems

2.1 Background

The following concepts will be used throughout the paper.

Definition 1.

- *For a natural number $d > 1$, we fix d finite sets $Q_1, Q_2, \ldots, Q_d$ called* factors*. In this paper, each Q_i is taken to be a subset of the complex numbers. The elements of a factor are called its* levels*. The* (full) factorial design *with respect to these factors is the Cartesian product $D = Q_1 \times Q_2 \times \ldots \times Q_d$.*

- *A* fractional design *or* fraction *F of D is a subset of D (possibly with multiplicities). We frequently consider F to be a matrix whose rows are elements of D. Take $r_i := |Q_i|$ to be the number of levels of the ith factor. We say that F is* symmetric *if $r_1 = r_2 = \cdots = r_d$, otherwise F is* mixed.

- *F is said to be a* strength t orthogonal array (OA) *or* t-balanced *if, for each choice of t coordinates (columns) from F, every combination of coordinate values from those columns occurs equally often; here t is a natural number.*

Some standard constructions from the theory of orthogonal arrays are reviewed in [7] and [9, Section 3.3, pp 28–31].

Let $s_1 > s_2 > \cdots > s_m$ be the distinct factor sizes of F, and suppose that F has exactly a_i factors with s_i levels. We call the partition

$$r_1 \cdot r_2 \cdots r_d = s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}$$

the *design type* of F. We usually take the r_i in non increasing order, so that they are related to the s_k by

$$\begin{aligned} s_1 = r_1 = \cdots = r_{a_1}, s_2 = r_{a_1+1} = \cdots = r_{a_1+a_2}, \ldots, \\ s_m = r_{a_1+a_2+\cdots+a_{m-1}+1} = \cdots = r_{a_1+a_2+\cdots+a_m} = r_d. \end{aligned}$$

If F has N rows, we say F has run size N and write

$$F = \mathrm{OA}(N; s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}; t).$$

For example

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

is a $4 \cdot 2^3$ mixed orthogonal array of strength 3. We use the following lemma on run sizes of OAs to narrow down the set of candidate arrays given their parameters.

Lemma 1 (Divisibility condition). *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* $|I| = t$*.*

The most efficient way to construct strength t arrays is by starting with a full array with t factors, then extending it column by column. So our first problem is:

Problem 1 (Orthogonal Array Column Extension). *Given a strength* t *orthogonal array* F_0 *with* N *runs and* d *factors, extend it to a strength* t *orthogonal array* $F = [F_0|X]$ *with* $d+1$ *factors, where* X *is a new factor (or column).*

Section 3 presents a modification of our arithmetic method [11] for constructing $\mathrm{OA}(64; 4^4 \cdot 2^6; 3)$, an array achieving its optimal run size with respect to the Rao bound [7].

2.2 Recent progress

The main aim of experimental design is to identify an unknown function $\phi : D \to \mathbb{R}$ on the full design D, which is a mathematical model of some quantity of interest (favor, usefulness, best-buy, quality, ...) that is be computed or optimized. OAs can provide smaller (and so more economic) fractional designs, which still allow us to identify the most important features of ϕ.

A comprehensive reference on the use of orthogonal arrays (OAs) as factorial design in diverse problems of statistical parameter optimization is provided by Wu and Hamada [22]. Stufken and Tang [20] provided a complete solution to enumerating non-isomorphic two-level OAs of strength t with $t+2$ constraints for any t and any run size $N = \lambda\, 2^t$. More recently, Bulutoglu and Margot [2] formulated an integer linear programming (ILP) method for classifying OAs of strength 3 and 4 with run size at most 162. A few specific construction methods of OAs have been proposed in Brouwer et al. [1] and Nguyen [11]. Mixed-level OAs of strength 3 with run-size at most 100 are online at [10], and strength at least 2 at [19].

In this work, we consider computer-algebraic methods, combined in several ways to construct mixed OAs.

2.3 Overview of algebraic geometry for computing fractional factorial designs

We follow the terminology of [4, 17]. Recall that the ring $\mathbb{F}[\boldsymbol{x}] := \mathbb{F}[x_1, x_2, x_3, \ldots, x_d]$ consists of multivariate polynomials over some subfield $\mathbb{F}$ of the complex field $\mathbb{C}$. An ideal

$$J = \langle f_1, \ldots, f_s \rangle := \left\{ \sum_{i=1}^{s} h_i f_i \text{ where } h_i \in \mathbb{F}[\boldsymbol{x}] \right\}$$

is called *zero-dimensional* if its root set $\mathrm{Z}(J)$ has a finite number of elements. Now let J be an ideal of $\mathbb{F}[\boldsymbol{x}]$, written $J \trianglelefteq \mathbb{F}[\boldsymbol{x}]$ and be zero-dimensional. Let

$$\pi : \mathbb{F}[\boldsymbol{x}] \to \mathbb{F}[\boldsymbol{x}]/J$$

be the canonical surjection, we know $|\,\mathrm{Z}(J)| = \dim_{\mathbb{F}}(\mathbb{F}[\boldsymbol{x}]/J) < \infty$. Fix a monomial ordering $\preceq$ on terms $\boldsymbol{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d} \in \mathbb{F}[\boldsymbol{x}]$, where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_d) \in \mathbb{N}^d$ is a multi-index vector. We write $\mathrm{LT}(J)$ for the set of all leading terms (with respect to that ordering) of polynomials in J. If G is a *Groebner basis* of J with respect to the given ordering $\preceq$, we know that $\big\langle \mathrm{LT}(J) \big\rangle = \big\langle \mathrm{LT}(G) \big\rangle$, and more importantly $\mathrm{Z}(J) = \mathrm{Z}(G)$. A set O of monomials is called an *order ideal* with respect to the ordering $\preceq$ if whenever $u \in O$, every monomial $v \preceq u$ is also in O.

Let $D = Q_1 \times \ldots \times Q_d$ be a full factorial design as in Definition 1. Let $C = \{f_1, \ldots, f_d\}$ be the set of canonical polynomials of the factors of D, where the canonical polynomial associated with a factor Q_i is $\prod_{j \in Q_i}(x_i - j)$. For example, if there are $d = 2$ factors with level sets $Q_1 = \{0, 1, 2\}$, $Q_2 = \{0, 1\}$ then $f_1(x_1) = x_1(x_1 - 1)(x_1 - 2)$, $f_2(x_2) = x_2(x_2 - 1)$. For a fraction F of D, define the vanishing ideal $\mathbb{I}(F)$ consisting of all polynomials of $\mathbb{F}[\boldsymbol{x}]$ that vanish on F. Note that $\mathbb{I}(D) = \langle C \rangle$, and since $F \subseteq D$, we get $\mathbb{I}(F) \supseteq \mathbb{I}(D)$. Call

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

the set of *estimable terms* associated with the fraction F and order $\preceq$. The set $\mathrm{Est}(F)$ is always an order ideal. In particular, the complete set of *estimable terms*

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

depends only on the type of D (not on the ordering).

For instance, if $F = D = \{-1, 1\}^3$, we get $\mathbb{I}(D) = \langle x_1^2 - 1, x_2^2 - 1, x_3^2 - 1 \rangle$, leading terms $\mathrm{LT}(\mathbb{I}(D)) = \{x_1^2, x_2^2, x_3^2\}$, and $\mathrm{Est}(D) = \{1, x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2x_3\}$ for any monomial ordering. We can now state our second problem:

Problem 2 (Constructing a fraction with given estimable terms).
Given an order ideal $E \subseteq \mathrm{Est}(D)$, compute a fraction $F \subseteq D$ such that $E = \mathrm{Est}(F)$.

Note that this is equivalent to the condition that $\overline{E} := \pi(E)$ is a basis of the quotient ring $\mathbb{F}[\boldsymbol{x}]/\mathbb{I}(F)$ as a $\mathbb{F}$-vector space.

2.4 Relationship with experimental design and industry

Using the polynomial model for $\phi : D \to \mathbb{R}$, we want to estimate the coefficients of the main effects (corresponding to linear terms) and interaction effects (corresponding to higher degree monomials). In their pioneering work [16, 17], Pistone, Riccomagno and Wynn showed that a fraction F could be used to estimate all the effects corresponding to monomials in $\mathrm{Est}(F)$. Problem 2 above, is essentially the reverse of this procedure. In applications to statistical quality control, we would take E to be the factor interactions that we think will effect the product quality. Then we use a fractional factorial design F with $\mathrm{Est}(F) = E$ to conduct the experiments in practice.

In addition to specifying the estimable terms, we often want to impose orthogonality conditions so that the fractions have desirable statistical properties. So we can now formulate our third problem:

Problem 3 (Constructing a balanced fraction with given estimable terms).
Given an order ideal $E \subseteq \mathrm{Est}(D)$ and integer $t > 1$, compute a strength t orthogonal array $F \subseteq D$ such that $E \subseteq \mathrm{Est}(F)$.

A specific approach for Problem 1 will be described in Section 3, due to which many OAs at most 100 runs was listed, including an optimal OA$(64; 4^4 \cdot 2^6; 3)$. The second problem was solved by Caboara and Robbiano [3], (see Chapter 4, Dickenstein-Emiris [5]). In Section 4 we briefly review their method, then in Section 5 a new method for solving the third problem will be introduced.

3 An arithmetic approach for solving Problem 1

In [1], we listed mixed OAs with at most 64 runs, together with constructions, but without showing all of the proofs. In Section 2 of Nguyen [11], we formulated an arithmetic method that was used to find arrays OA$(96; 6 \cdot 4^2 \cdot 2^3; 3)$ and OA$(96; 3 \cdot 4^2 \cdot 2^5; 3)$, but this method could not construct the OA$(64; 4^4 \cdot 2^6; 3)$. In this section, we give the proof of the construction of the array OA$(64; 4^4 \cdot 2^6; 3)$, listed in [1], using a variation of the arithmetic approach in [11]. First we review the arithmetic approach.

3.1 Description of the arithmetic method

This method constructs extensions of a full factorial design. Let column S_i correspond to factor Q_i, we could rewrite our full design as $D = [S_1|\dots|S_d]$, an unreplicated full factorial design of type $r_1 \cdots r_d$ with $d \geq 3$, $r_1 \geq r_2 \geq \dots \geq r_d \geq 2$. Choose $s \geq 2$ such that s divides $\frac{N}{r_i r_j}$ for every pair of distinct indices $i, j = 1, \dots, d$. We find a column X that makes the extension $[S_1|\dots|S_d|X]$ an OA$(N; r_1 \cdot r_2 \cdots r_d \cdot s; 3)$. As a results, we can find an OA$(N; r_1 \cdot r_2 \cdots r_d \cdot s^m; 3)$ for $m > 1$. Denote an arbitrary run of D by $\boldsymbol{u} := (u_1, u_2, \dots, u_d)$. Since D is a full design, the column X is determined 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. We now characterize the f_X such that $[D|X]$ has strength 3. Fix $K = \{1, 2, 3, \dots, d\}$, for $1 \leq i < j \leq d$, we let

$$Q_{ij} := \prod_{l \in K \setminus \{i,j\}} Q_l, \qquad n_{ij} := \frac{N}{r_i r_j}, \qquad q_{ij} := \frac{n_{ij}}{s}. \tag{1}$$

Note that our assumptions (due to the Rao bound and the divisibility condition) on s ensure that every q_{ij} is integral. For each $(a, b) \in [S_i|S_j]$, let

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

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

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

Lemma 2. *If f_{ij}^{ab} is a q_{ij}-to-one mapping for all $1 \le i < j \le d$, $a \in \mathbb{Z}_{r_i}$, $b \in \mathbb{Z}_{r_j}$, then $[D|X]$ is a strength 3 orthogonal array.*

This simple but useful observation results in few new OAs with run size between 64 and 100. Among those, $\mathrm{OA}(64; 4^4 \cdot 2^6; 3)$ is the most interesting case, since it is optimal with respect to the Rao bound [1, Section 2].

3.2 Construction of the $\mathrm{OA}(64; 4^4 \cdot 2^6; 3)$

This design is unique up to isomorphism, given the parameter set of runsize and factor levels. The next theorem presents a detailed construction of this array, which was listed as (X_5) in [1]. The idea for this construction is due to Andries Brouwer.

Theorem 1. *Let A and B be the subsets $\{0,1\}$ and $\{2,3\}$ of the cyclic group $\mathbb{Z}_4$ of residues mod 4. An $\mathrm{OA}(64; 4^4 \cdot 2^6; 3)$ can be obtained by taking all row vectors*

$$(x_1, x_2, x_3, x_4, S_1, S_2, S_3, S_4, S_5, S_6) \in \mathbb{Z}_4^4 \times \mathbb{Z}_2^6$$

satisfying

$$x_1 + x_2 + x_3 + x_4 = 0 \pmod 4 \quad \textit{and} \quad S_i = \sum_{j=1}^{4} a_j^{(i)} x_j \pmod 2$$

where the six vectors $a^{(i)}$ for $1 \le i \le 6$ are $(0,1,2,3)$, $(0,1,3,2)$, $(0,2,1,3)$, $(0,2,3,1)$, $(0,3,1,2)$, $(0,3,2,1)$.

Proof . Suppose D is an $\mathrm{OA}(64; 4^4 \cdot 2^6; 3)$. Let X, Y, Z, W be the four quaternary columns, $S_1, \ldots, S_6$ the six binary columns of D. Let x, y, z, w denote the coordinates of a run r corresponding to X, Y, Z, W, and let s_i be the coordinate of r corresponding to column S_i, $\quad i = 1, \ldots, 6$.

First of all, since any three from four columns X, Y, Z, W suffice to determine 64 runs, the 4-level part of D can be viewed as a "quasi" regular design (since 4 is not a prime) 4^{4-1} determined by a defining relation

$$x + y + z + w = c \pmod 4, \qquad \text{for some constant} \quad 0 \le c \le 3. \tag{2}$$

For instance the first column is a function of the next three columns,

$$x = 3y + 3z + 3w + c \pmod 4.$$

Similarly, any binary column S of D must be a function of three columns Y, Z, W, so be determined by a function

$$f(y, z, w) = c_1 y + c_2 z + c_3 w, \tag{3}$$

where distinct coefficients $c_j \in \mathbb{Z}_4^*$ for $j = 1, 2, 3$. These coefficients c_j must be nonzero since column S depends on three independent columns Y, Z, W (in fact on any three from the four 4-level columns). Furthermore they must be distinct, this fact will be justified in the proof of the following lemma. □

Recall that $A = \{0, 1\}$, $\quad B = \{2, 3\}$, we put $s := f(y, z, w) \bmod 4$, write XY for the pair of columns (X, Y), write $S \perp XY$ for the fact that a column S is orthogonal to XY, and write $[F|S]$ for the extended array from an array F by a column S. We have

Lemma 3.

1. *The four quaternary columns defined by* (2) *gives rise an orthogonal array* $F := OA(64; 4^4; 3)$.
2. *Any binary column S defined by the rule:*

$$S := 0 \quad if \quad s \in A; \quad and \quad S := 1 \quad if \quad s \in B, \tag{4}$$

is orthogonal to F, i.e. the extended array $[F|S]$ is an $OA(64; 4^4 \cdot 2; 3)$.

3. *There are totally six distinct functions of the form* (4). *The binary columns of D built from these functions form an orthogonal array of strength 5.*

Proof.

1. For $t = 3$, it follows that any three from four columns X, Y, Z, W, say Y, Z, W, form a full design and X is orthogonal to pairs of columns YZ, YW, ZW. The latter statement follows from the equation $x = 3y + 3z + 3w + c \pmod 4$, and from the fact that $W \perp YZ$, $Z \perp YW$, and $Y \perp ZW$ (i.e. fixing (y, z), there is one-to-one correspondence between w and x).
2. We show that column S built by the function

$$f(y, z, w) = c_1 y + c_2 z + c_3 w \quad \text{for any } c_1 \neq c_2 \neq c_3 \in \mathbb{Z}_4^* = \mathbb{Z} \setminus \{0\}$$

is orthogonal to pairs YZ, YW, ZW, then it is also orthogonal with XY, XZ, XW of fraction F. Indeed, orthogonality between S and YZ is satisfied since the sub-design taken from columns Y, Z, W has 64 runs and strength 3. So for each fixed pair (y, z) appearing 4 times in F, four values of w results in four values

$$s = f(y, z, w) \pmod 4 \in \{0, 1, 2, 3\},$$

the first half (0 and 1) is replaced by 0, and the second (2 and 3) by 1 from Rule (4). Therefore there are precisely two runs $(., y, z, ., 0)$ and two runs $(., y, z, ., 1)$ in the extended array $[F|S]$. The orthogonality between S and pairs YW, ZW is obtained similarly. Replacing $z = -x - y - w + c$ to $f(y, z, w)$ gives

$$f(y, z, w) = -c_2 x + (c_1 - c_2) y + (c_3 - c_2) w + c c_2.$$

This expression tells us that if $c_2 \neq c_3$ then $S \perp XY$, and if $c_1 \neq c_2$ then $S \perp XW$. Rewriting $y = -x - z - w + c$, then

$$f(y, z, w) = -c_1 x + (c_2 - c_1)z + (c_3 - c_1)w + cc_1.$$

It shows that $S \perp XZ$ if $c_1 \neq c_3$. Therefore S is orthogonal to any pair of columns of fraction F if nonzero coefficients c_1, c_2, c_3 are pairwise distinct. Remark that if the case like $c_1 = c_2$ occurs, then S is orthogonal only to column X, W, not to Y, Z.

3. From the above proof, there are six functions f_i defined by six coefficient vectors s_i, $(i = 1, \ldots 6)$ which are formed by taking all permutations of 1,2,3. Each function determines a binary column. We make design $D = OA(64; 4^4 \cdot 2^6; 3)$ by appending six binary columns S_i consecutively to fraction F. It is a right time to prove that the sub-design extracted from six binary columns $S_1, \ldots, S_6$ of D actually has strength 3 (or higher). Let look at six factors $S_1, \ldots, S_6$ built up from six vectors s_i or from functions

$$f_1(y, z, w) = y + 2z + 3w, \quad f_2(y, z, w) = y + 3z + 2w,$$

$$f_3(y, z, w) = 2y + z + 3w, \quad f_4(y, z, w) = 2y + 3z + w,$$

$$f_5(y, z, w) = 3y + z + 2w, \quad f_6(y, z, w) = 3y + 2z + w.$$

Summing them up and taking modulo 2 give us

$$f_1 + f_2 + f_3 + f_4 + f_5 + f_6 = 0 \pmod 2. \tag{5}$$

This equation is indeed the defining relation of a regular design 2^{6-1} of strength 5 with 32 runs. Hence our binary part $\mathrm{OA}(64; 2^6; 3)$ of D is a replicate (twice) of this regular design 2^{6-1}, and so the binary part $\mathrm{OA}(64; 2^6; 3)$ has strength 5. We can also show that, for instance, $S_3 \perp S_1 S_2$ by using equation $f_3 = f_1 + f_2 + 2w$. $\square$

4 Robbiano's Method for solving Problem 2

We now discuss the idea of the border basis of an order ideal. As in Problem 2, suppose that $E = \{t_1, \ldots, t_\mu\} \subset \mathrm{Est}(D)$ is an order ideal, i.e. it is closed under forming divisors. Define

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

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

Proposition 1. *[5, Proposition 4.3.2, p. 186]. Let I be a proper ideal in $P = \mathbb{F}[\boldsymbol{x}]$, 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 $\mathbb{F}$-vector space, and let $E^+ = \{b_1, \ldots, b_v\}$. Denote by $V(E)$ the $\mathbb{F}$-vector space of $\mathbb{F}[\boldsymbol{x}]$ generated by E. Then there exists unique scalar $a_{jl} \in \mathbb{F} \quad (l = 1, \ldots, \mu)$ with*

$$g_j = b_j - \sum_{l=1}^{\mu} a_{jl} t_l \in I, \text{ for each } j = 1, \ldots, v. \tag{6}$$

Moreover, the ideal I is generated by $g_1, \ldots, g_v$. Hence $b_j = \sum_{l=1}^{\mu} a_{jl} t_l \pmod{I}$, and so $E^+ \subset V(E) \pmod{I}$.

The following concepts are used in a proof of this proposition [see for example, p 186, [5]].

Definition 2.

- *A pair (g, t) is a* marked polynomial *if g is a non-zero polynomial and the monomial t is in the support* $\mathrm{Supp}(g)$ *of 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 $\preceq$. Then the pair (G, E^+) is called the* border basis *of I with respect to E.*

Caboara and Robbiano ([3] and [5, Chapter 4]) used this concept of a *border basis* G of an ideal E and related it to the matrices associated with the left multiplication by x_i, for $i = 1, \ldots, d$. Then the ideal I generated by G is zero dimensional (ie, the zero set $\mathrm{Z}(I)$ is finite or $\dim_{\mathbb{F}}(\mathbb{F}[\boldsymbol{x}]/I) < \infty$) if, and only if, the left multiplication matrices are pairwise commuting. Finally, $\mathrm{Z}(I)$ is the set of runs of a fraction F such that $\mathrm{Est}(F) = E$. More concretely, the relationship of border bases and commuting matrices is stated in [5, Theorem 4.3.17], and an algorithm to obtain a fraction F solving Problem 2 is given in [5, Theorem 4.4.4].

5 Our linear algebra method for Problem 3

We now give a new technique for handling the third fundamental problem: computing balanced fractional designs with given estimable terms. The idea is to represent the strength of a balanced fractional design by linear algebraic conditions.

Suppose $F \subseteq D$ is a fraction with d factors, considered as a finite subset of $\mathbb{F}^d$. In this section, we represent the factors $Q_1, \ldots, Q_d$ by variables $x_1, \ldots, x_d$. Let $J = \mathbb{I}(F)$ and let $V = P/J$. Then $E = \mathrm{Est}(F) = \{h_1, \ldots, h_\mu\}$ is a set of monomials such that $\overline{E} = \{\overline{h}_1, \ldots, \overline{h}_d\}$ is a basis for P/J as a $\mathbb{F}$-vector space

Let $M = \boldsymbol{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_d^{\alpha_d}$ be a monomial. The left action of M induces an endomorphism of V. Let L_M be the matrix of this action with respect to the basis $\overline{E}$. The matrices $L_{x_1}, \ldots, L_{x_d}$ are called the *elementary multiplication matrices*.

5.1 Key result

The following result combines the Gröbner basis method with multiplication matrices (for instance, see [5, Definition 4.1.1, page 172]) to make balanced fractions with given estimable terms.

We see, by standard algebraic facts, if F exists and is finite, then $P/\mathbb{I}(F)$ has finite dimension and the multiplication matrices commute pairwise. So they generate a commutative subalgebra of the non-commutative ring of all square matrices.

Our main result is the following.

Theorem 2. *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. Suppose the fraction F have N runs, and denote $\boldsymbol{p} = (p_1, \ldots, p_d)$ for a run in F. The vanishing ideal of $\boldsymbol{p}$ is

$$\mathbb{I}(\boldsymbol{p}) = \big\langle \{x_1 - p_1, \ldots, x_d - p_d\} \big\rangle. \tag{7}$$

The vanishing ideal of the fraction F is

$$\mathbb{I}(F) = \bigcap_{\boldsymbol{p}\in F} \mathbb{I}(\boldsymbol{p}). \tag{8}$$

The Chinese Remainder Theorem for ideals (see, for example, [8, Corollary 2.2]) gives us the decomposition:

$$P/\mathbb{I}(F) = \bigoplus_{\boldsymbol{p}\in F} P/\mathbb{I}(\boldsymbol{p}). \tag{9}$$

Consider a run $\boldsymbol{p} = (p_1, \ldots, p_d)$ as a variety. Each $P/\mathbb{I}(\boldsymbol{p})$ is isomorphic to $\mathbb{F}[\boldsymbol{p}] = \mathbb{F}$ (see [17, Definition 19], e.g. for the definition of $\mathbb{F}[\boldsymbol{p}]$), so $P/\mathbb{I}(\boldsymbol{p})$ is a 1-dimensional sub-algebra of the quotient algebra $P/\mathbb{I}(F)$. Hence, $P/\mathbb{I}(F)$ is isomorphic to the algebra $\mathbb{F}^d$.

From Equation (7), since $x_i - p_i \in \mathbb{I}(\boldsymbol{p})$, so we have $x_i^{\alpha_i} = p_i^{\alpha_i}$ in $P/\mathbb{I}(\boldsymbol{p})$, for all $i = 1, \ldots, d$. As a result, for each $v \in P/\mathbb{I}(\boldsymbol{p})$:

$$(x_i^{\alpha_i} - p_i^{\alpha_i})\, v = 0, \text{ so } \quad L_{x_i}^{\alpha_i}(v) = L_{x_i{}^{\alpha_i}}(v) = x_i^{\alpha_i}.v = p_i^{\alpha_i} v, \text{ for } i = 1, \ldots, d,$$

that means v is an eigenvector of the matrix $L_{x_i}^{\alpha_i} = (L_{x_i})^{\alpha_i}$ with eigenvalue $p_i^{\alpha_i}$. Hence p_i is an eigenvalue of the matrix L_{x_i} $(i = 1, 2, \cdots, d)$. 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

$$L_M = L_{x_1{}^{\alpha_1} \ldots x_d^{\alpha_d}} = L_{x_1}^{\alpha_1} \ldots L_{x_d}^{\alpha_d}, \text{ and } \quad L_M(v) = p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_d^{\alpha_d} v.$$

Therefore, F consists of all vectors $\boldsymbol{p} = (p_1, \ldots, p_d)$ where v is some common eigenvector with eigenvalue p_i with respect to the matrix L_{x_i}. We conclude that 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 $P/\mathbb{I}(\boldsymbol{p})$ are N eigenspaces for L_M, with corresponding eigenvalues $p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_d^{\alpha_d}$ for each run $\boldsymbol{p} = (p_1, \ldots, p_d)$. As a result, since L_M is an $N \times N$ matrix, the theorem is now proved. □

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 for balanced fractions F, using to the following observation.

- 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.

5.2 A necessary condition for the existence of balanced fractions

Corollary 1. *Let F be a t-balanced fraction of a design D in $\mathbb{F}^d$. Assume that factor x_i has levels $0, 1, \ldots, r_i - 1$.*

(a) If $t \geq 1$ and $\alpha_i \in \{0, 1, \ldots, r_i - 1\}$, then the left multiplication matrix $L_{x_i{}^{\alpha_i}}$ has trace

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

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

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

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

Proof. For each factor i, the number $\lambda_i = |F|/r_i$ must be a positive integer. The fraction F can be decomposed into λ_i blocks $F_1, \ldots, F_{\lambda_i}$, each block has r_i runs such that their ith coordinates are $0, 1, \ldots r_i - 1$. Hence, Item (a) is proved, due to the fact

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

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

We have employed these results to find extra constraints for computing any factorial fractions using L. Robbiano's method, with intensively use of computer algebra systems. Due to the prohibitively high computational complexity of computing Gröbner bases, however, this method is useful in theory, but in practice it only constructs designs having very moderate run sizes. See Chapter 2 of [9] for computational experiments.

6 Closing comments and future work

We have discussed mathematical and computational aspects of a few factorial design construction problems. Specifically, in Section 5 we stated a necessary condition for the existence of balanced fractional factorial designs provided the design defining parameters. An arithmetic formulation, in addition resolves the factor (column) enlarging problem of mixed balanced fractions with strength at least 2, provided a fix number of experiments.

Moreover, a parallel computing approach can return lexicographically minimum in column (LMC) matrices, more details can be found in Schoen, Eendebak and Nguyen [18] and Phan, Soh and Nguyen [14, 15]. A combination of ILP and group computation, in a future paper, could provide a way for completely enumerating mixed OAs.

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References

[1] Brouwer, A. E., Cohen, A. M. and Nguyen, M. V. M, Orthogonal arrays of strength 3 and small run sizes, *Journal of Statistical Planning and Inference*, **136**, 3268-3280 (2006)

[2] Bulutoglu, D.A. and Margot, F. (2008) Classification of orthogonal arrays by integer programming, *Journal of Statistical Planning and Inference*, **138**, 654-666

[3] M. Caboara and L. Robbiano. Families of estimable terms. In *Proceedings of the 2001 International Symposium on Symbolic and Algebraic Computation*, ACM, 56-63, (2001).

[4] David Cox, John Little, Donal O'Shea *Ideals, Varieties, and Algorithms: Introduction to Computational Algebraic Geometry & Commutative Algebra*, Springer (2005)

[5] Alicia Dickenstein, Ioannis Z. Emiris, *Solving Polynomial Equations*, Springer, (2005)

[6] Glonek G.F.V. and Solomon P.J., Factorial and time course designs for cDNA microarray experiments, *Biostatistics* **5**, 89-111 (2004)

[7] Hedayat, A. S. and Sloane, N. J. A. and Stufken, J., Orthogonal Arrays, *Springer-Verlag*, Germany (1999)

[8] Serge Lang, Algebra, Third Edition, *Springer* (2002)

[9] Nguyen, V. M. Man, Computer-Algebraic Methods for the Construction of Designs of Experiments, Ph.D. thesis, `http://alexandria.tue.nl/extra2/200512795.pdf`, *Technische Universiteit Eindhoven*, Netherlands (2005)

[10] Nguyen, V. M. Man, An online service for computing mixed orthogonal arrays, HCMC University of Technology, `http://elearning.cse.hcmut.edu.vn/samgroup/OA.jsp`

[11] Nguyen, V. M. Man Some new constructions of strength 3 mixed orthogonal arrays, *J. Statist. Plann. Inference*, **138/1**, 220-233 (2008)

[12] Madhav Phadke, Quality Engineering using robust design, *Prentice Hall*, USA (1989)

[13] Madhav Phadke, Design Of Experiment For Software Testing, `www.isixsigma.com/`

[14] Hien Phan, Ben Soh and Man Nguyen, A step-by-step extending parallelism approach for Enumeration of Combinatorial Objects, *Springer-Verlag*, Berlin Heidelberg, Part I, LNCS 6081, pp. 463475, (2010)

[15] Hien Phan, Ben Soh and Man Nguyen, A Parallelism Extended Approach for the Enumeration of Orthogonal Arrays, *Springer-Verlag*, Berlin Heidelberg, Part I, LNCS 7016, pp. 482494, (2011)

[16] G. Pistone and H. P. Wynn, *Generalised confounding with Grobner bases*, Biometrika, 83, 653-666 (1996).

[17] G. Pistone, E. Riccomagno and H. P. Wynn, *Algebraic Statistics*, Chapman and Hall, USA (2001)

[18] Eric D. Schoen, Pieter T. Eendebak, and Man V. M. Nguyen, Complete enumeration of pure-level and mixed-level orthogonal array, Journal of Combinatorial Designs, 18(2):123 - 140 (2010)

[19] N. J. A. Sloane `http://www2.research.att.com/~njas/oadir/index.html/`

[20] John Stufken and Boxin Tang, Complete Enumeration of Two-Level Orthogonal Arrays of Strength D With $D+2$ Constraints, *The Annals of Statistics*, **35**, Number 2, pp. 793-814 (2008)

[21] Sudhir Gupta, Balanced Factorial Designs for cDNA Microarray Experiments, *Communications in Statistics: Theory and Methods*, **35**, Number 8 , pp. 1469-1476 (2006)

[22] Wu C. F. J. and Hamada, M., Experiments: Planning, analysis, and parameter design optimization, *A Wiley-Interscience Publication*, MR1780411, USA (2000)