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PERMUTATION GROUPS AND INTEGER LINEAR ALGEBRA FOR ENUMERATION OF ORTHOGONAL ARRAYS

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Abstract

We introduce new group theoretic methods for constructing mixed orthogonal arrays (OAs). In brief, we employ combinatorics, graph and permutation group theory, together with integer linear formulation as major engines to provide a framework for constructing and enumerating mixed OAs of any strength with all feasible factor levels and with run sizes satisfying the Rao bound. The proposed methods are validated by constructing a few new strength 3 mixed OAs with run sizes at most 100.

1 Introduction

A comprehensive reference on the use of OAs as factorial design in diverse problems of Statistical Parameter Optimization was provided by Wu and Hamada (2000) [27]. Furthermore, Glonek (2004) [23] discussed usages of OAs in fast developing areas as biostatistics, and Sudhir (2006) [22] proposed new applications of balanced factorial design in newly emerging areas as bio-informatics.

From the purely mathematical statistics point of view, Bulutoglu and Margot (2006) [4] fully enumerated binary OAs of strength 4 with run size at most 144. Stufken and Tang (2007) [21], more recently provided a complete solution to enumerating non-isomorphic two-level OAs of strength t with $t+2$ constraints

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for any t and any run size $N = \lambda\, 2^t$. Gupta (2007) [24] listed Hadamard designs with run-size at most 1000, and most recently, mixed-level OAs of strength 3 with run-size at most 100 together with most Hadamard matrices with run-size at most 1500 are both online reported at [13].

1.1 Recent relevant works on the Construction of OAs

Algebraic View for computing fractional designs. Following terminologies of [5, 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 a field $\mathbb{F}$. Given a finite set of polynomials $f_1, f_2, \ldots, f_s$, an ideal

$$J = \langle f_1, f_2, \ldots, f_s \rangle := \left\{ \sum_{i=1}^{s} h_i f_i \text{ where } h_i \in \mathbb{F}[\boldsymbol{x}] \right\}$$

being generated by the $\{f_i\}$, is called zero-dimensional if its set $\mathrm{Z}(J)$ of solutions is finite. Now let J be an ideal of $\mathbb{F}[\boldsymbol{x}]$, written $J \trianglelefteq \mathbb{F}[\boldsymbol{x}]$ and be zero-dimensional, and denote by $\pi : \mathbb{F}[\boldsymbol{x}] \to \mathbb{F}[\boldsymbol{x}]/J$ the canonical surjection. We have a standard result as follows.

Fact 1. $|\,\mathrm{Z}(J)| = \dim_{\mathbb{F}}(\mathbb{F}[\boldsymbol{x}]/J) < \infty$. If, moreover G is a Groebner basis of J with respect to (w.r.t.) a given ordering $\preceq$, we know that $\big\langle\, \mathrm{LT}(J) \big\rangle = \big\langle\, \mathrm{LT}(G) \big\rangle$, and more importantly $\mathrm{Z}(J) = \mathrm{Z}(G)$, where $\mathrm{LT}(J)$ is the set of all leading terms of polynomials in J w.r.t $\preceq$.

Concept 1. The followings are crucial for algebraically formulating our problems.

- 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.
- The term $\boldsymbol{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d}$ 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. An one-factor effect is just a power of a single factor, called the main effect of that factor; while the term factor interaction is used frequently for at least two factors.
- A full factorial design D, composed by finite factor sets $Q_1, Q_2, \ldots, Q_d$, where factor Q_i has r_i levels, is considered as a finite subset of $\mathbb{F}^d$.
- Fix a subset F of D. The vanishing ideal $\mathrm{I}(F)$ consists of precisely all polynomials of the ring $\mathbb{F}[\boldsymbol{x}]$ that vanish on F. Denote by

  $$\mathrm{Est}(F) = \{\boldsymbol{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_d^{\alpha_d} : \boldsymbol{x}^{\boldsymbol{\alpha}} \notin \big\langle\, \mathrm{LT}(\mathrm{I}(F)) \big\rangle\}$$

  the set of estimable terms being associated with the fraction F. The set

  $$\mathrm{O}(D) := \mathrm{Est}(D) = \{\boldsymbol{x}^{\boldsymbol{\alpha}} : \alpha_i = 0, 1, \ldots, r_i - 1, i = 1, \ldots, d\}$$

  is called the complete set of estimable terms of D.

For instance, if $D = \{-1, 1\}^3$, then

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

Definition 1. A fraction F is said to be a strength t orthogonal array (OA) or t-balanced fraction 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.

Write $F = \mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; t)$ if F has N rows, d factors, the ith factor has r_i levels, and strength t. In [16], we raised the following two problems:

Fundamental Problem 1. Constructing a fraction with given estimable terms.

Input: Given $E = \{t_1, \ldots, t_\mu\} \subset \mathrm{O}(D)$, a fixed order ideal.

The aim: compute a fraction F of D, such that $E = \mathrm{Est}(F)$, that is, $\overline{E}$ is a basis of the quotient ring $R = \mathbb{F}[\boldsymbol{x}]/\,\mathrm{I}(F)$ as a $\mathbb{F}$-vector space.

Here $\mathrm{Est}(F) = \{\boldsymbol{x}^{\boldsymbol{\alpha}} : \boldsymbol{x}^{\boldsymbol{\alpha}} \notin \big\langle \mathrm{LT}(\mathrm{I}(F)) \big\rangle\}$ can be interpreted as a set of the factor interactions that could affect the product quality when we conduct the experiments of F in engineering and technological practices.

Fundamental Problem 2. Constructing strength t orthogonal arrays.

Input: Given a set of factors, take $E = \{t_1, \ldots, t_\mu\} \subset \mathrm{O}(D)$ be a fixed order ideal, consisting of the main effects and some factor interactions of interest.

The aim: compute a balanced fraction F of strength t, such that $E = \mathrm{Est}(F)$, that is, $\overline{E}$ is a basis of $R = \mathbb{F}[\boldsymbol{x}]/\,\mathrm{I}(F)$ as a $\mathbb{F}$-vector space.

The first problem was solved by L. Robbiano et al. from 2001, see more details in Chapter 4, Dickenstein-Emiris (2005) [19]. Based on L. Robbiano' work, the second problem has been algebraically solved in [16], and for consistency, we recall our key results here.

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 R. 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. We see, by the standard algebraic Fact 1, if F exists and is finite, then $\mathbb{F}[\boldsymbol{x}]/\,\mathrm{I}(F)$ has finite dimension and the multiplication matrices commute pairwise. So they generate a commutative sub-algebra of the non-commutative ring of all square matrices.

Theorem 1. Suppose that F has no repeated runs. The characteristic polynomial of L_M is

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

Observation 1. From this theorem, observe that 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 the following facts.

- 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 (i.e. strength 2 OA), then the size of F must be a multiple of the products of each pair of levels, and so on.

Corollary 2. (Necessary conditions for the existence of OA)

Let F be a t-balanced fraction of a full factorial 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 $\alpha_j \in \{0, 1, \ldots, r_j - 1\}$, $L_{{x_i}^{\alpha_i}{x_j}^{\alpha_j}}$ has trace
$$\frac{N}{r_i\ r_j} \sum_{l=0}^{r_i-1} l^{\alpha_i} \sum_{m=0}^{r_j-1} m^{\alpha_j}.$$

1.2 Enumeration of orthogonal arrays: Literature and our work

After the work of Bulutoglu and Margot (2006) [4], Angelopoulos, Evangelaras, Koukouvinos and Lappas (2007) [1] proposed a construction and identification of non-isomorphic binary orthogonal arrays using frequency counting, Hamming distance distribution and D-efciency criteria in a column extension algorithm. Recently Schoen, Eendebak and Nguyen (2009) [7] reported a complete enumeration of pure-level and mixed-level OAs using backtrack search.

So far we have been mostly focusing on the construction problem. We now propose new ways of enumerating balanced and mixed fractional factorial designs in Sections 2, 3, and 4 possibly provide a complete answer for the construction and enumeration of mixed OAs. Precisely, we solve the following.

Fundamental Problem 3. Enumerating strength t orthogonal arrays (OAs).

Input: $F = \mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; t)$, a strength t orthogonal arrays

The aim: combine, in several ways distinct computer-algebraic flavor methods to provide a complete answer for the enumeration of strength t mixed OAs of the form $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d \cdot s; t)$, i.e. we find all non-isomorphic column vectors X of s levels that makes the extension $[F|X]$ an $\mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d \cdot s; t)$.

Our contribution. In this article, we introduce a few new methods using group theoretic computation and integer linear formulation as major engines to resolve the third fundamental problem formulated above. Specifically the methods allow enumerating isomorphism classes of almost all mixed OAs of strength 3 with all feasible factor levels, and computationally with run size at most 100. The proposed methods meaningfully provide a generic framework and could be easily modified for computing any larger strength OAs.
For convenience, we abbreviate methods used for constructing and enumerating OAs, and use abbreviations for specific lower bounds and for particular nonexistence proofs as well; they are listed in Table 1. We could group identical values in the factor levels $T = r_1 \cdot r_2 \cdots r_d$ to get a new design type $T = s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}$; and assume that $\{s_k\}$ is an decreasing sequence.

1.3 Parameter sets of strength 3 OAs with run size $72 \leq N \leq 100$

The divisibility condition for the run size N of a strength t fractional design F requests integrality of the fraction N over any product of t factor levels, while the Rao bound provides a lower bound of N in terms of its parameters. Both give necessary conditions for the existence of F.

Lemma 3 (Divisibility condition-(Div)). 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 $\prod_{i \in I,\, |I|=t} r_i$.

Proof. This says that the t times derived design has an integral run size. $\square$
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 [2], we constructed all orthogonal arrays of strength 3 with run sizes N at most 64. We extend that to the cases $72 \leq N \leq 100$ in this paper.

Proposition 4. The nontrivial design types for OAs of strength 3 and run size at most 100 allowed by (Div) and (Rao) are:

1. run size $8m$, type 2^a for $4 \leq a \leq 4m$, with $1 \leq m \leq 12$;
2. run size $27m$, type 3^a for $4 \leq a \leq 5m$, with $1 \leq m \leq 2$.

Notation	Methods	Reference
(A)	Arithmetic	[14]
(B)	Backtrack search for $s_1^a s_2^b$ OAs	[7]
(C)	Colored graphs	Section 2.2
(Con)	Concatenation	[2]
(La)	Latin squares	[14]
(H)	Hadamard construction	[2]
(I)	Integer linear algebra(ILA)	Section 3
(IS)	ILA with symmetry	Section 4
(J) and (L)	Juxtaposition and Linear code	[2]
(M) and (O)	Multiplication and Even sum	[2]
(O'), (Br)	Brouwer's construction	[3]
(Q)	Quasi-multiplication	[14]
(S) and (T)	Split and Trivial design	[2]
(X), (X_6),		[2]
(X_3), (X_4), (X_5)	explicit constructions	[2]
(X_1), (X_7), (***)	mixed additive codes	[2]
(3^5)	Hedayat, Seiden, and Stufken' construction	[9]
(Rao)	the generalized Rao bound	[18, 9, 2]
(Del)	the Delsarte bound	[6]
(Div)	the divisibility	
(5.1)	$\nexists\, \mathrm{OA}(24; 3 \cdot 2^5; 3)$	Sec. 5.1, [2]
(5.9)	$\nexists\, \mathrm{OA}(64; 4^5 \cdot 2^3; 3)$	Sec. 5.9, [2]
(5.10)	$\nexists\, \mathrm{OA}(64; 4^3 \cdot 2^9; 3)$	Sec. 5.10 [2]

Table 1: An overview of constructions, lower bounds on run sizes

N	Design type $T = s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}$	Parameters
72	$3^b \cdot 2^a$	$1 \leq b \leq 2,\ a + 2b \leq 25$
	$6^2 \cdot 2^a$	$2 \leq a \leq 4$
	$6 \cdot 3^b \cdot 2^a$	$a + b \geq 3,\ a + 2b \leq 11$
	$9 \cdot 2^a$	$3 \leq a \leq 7$
80	$4 \cdot 2^a$	$3 \leq a \leq 19$
	$5 \cdot 4^b \cdot 2^a$	$a + b \geq 3,\ b \leq 1,\ a + 3b \leq 15$
	$10 \cdot 4^b \cdot 2^a$	$a + b \geq 3,\ b \leq 1,\ a + 3b \leq 7$
81	$9 \cdot 3^a$	$3 \leq a \leq 4$
84	$7 \cdot 3 \cdot 2^2$	
88	$11 \cdot 2^a$	$3 \leq a \leq 7$
96	$3 \cdot 2^a$	$a \geq 3$
	$4^c \cdot 3^b \cdot 2^a$	$1 \leq c \leq 2,\ a + b + c \geq 4,$ $b \leq 1,\ a + 2b + 3c \leq 26$
	$6 \cdot 4^b \cdot 2^a$	$a + b \geq 3,\ b \leq 2,\ a + 3b \leq 15$
	$8 \cdot 6^c \cdot 3^b \cdot 2^a$	$b + c \leq 1,\ a + 2b + 5c \leq 11$
	$12 \cdot 4^b \cdot 2^a$	$a + b \geq 3,\ b \leq 1,\ a + 3b \leq 7$

Table 2: Parameters of strength 3 OAs of with $N \leq 100$.

Proof. The nontrivial mixed design types for OAs of strength 3 and run size at most 100 allowed by (Div) and (Rao) are given in Table 2. We show here how to get eligible parameters for some options of the most interesting case $N = 96$, other results can be similarly obtained. For $N = 96$, consider the following options.

- 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 derived designs OA$(12; 6^b \cdot 2^a; 2)$ gives us $a + b \geq 2$, $12 \geq 1 + 5b + a$, or $a + 5b \leq 11$.

  If $b = 0$, $a \leq 11$, and if $b = 1$, $a \leq 6$.

- OA$(96; 4^c \cdot 3^b \cdot 2^a; 3)$ with $b + c > 0$. When $c > 0$, we use (Rao) for the derived OA$(16; 4^{c-1} \cdot 3^b \cdot 2^a; 2)$; when $c = 0$, employ (Rao) for OA$(32; 3^{b-1} \cdot 2^a; 2)$. Then $0 \leq b \leq 1$, $0 \leq c \leq 2$, $a+b+c \geq 4$, and $3(c-1)+2b+a \leq 23$. 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 $b = 0$, $a \leq 20$.

□

The structure of the paper

Firstly in Section 2, we discuss about permutation group and colored graph of an OA. Specifically part 2.1 defines the full group of isomorphisms of OAs, as well as the automorphism group of an OA. We, furthermore associate an OA with a colored graph in part 2.2, that in turn allows us to compute canonical graphs and find isomorphism classes of orthogonal arrays. These mathematical ingredients, in Sections 3 and 4 all together make a solid base for efficiently listing non-isomorphic columns in the column extension problem of a given balanced fractional factorial design.

More precisely, we combine the concepts of group theoretic and graph theory with integer linear modeling to construct all non-isomorphic candidates of a new factor of an OA in Section 3 and 4, the major parts of the article. Section 5 finally lists few newly found arrays and concludes the paper.

2 Permutation group for enumerating of mixed OAs

It is not immediately obvious how to define isomorphisms of a factorial design. In fact, there is more than one sensible definition that could be made. We give the definition that is most useful for our purposes in this section.

Notation. The following notations will be used through out the paper.

- Let N be a positive integer and $T := r_1 \cdot r_2 \cdots r_d$ (equivalently $T := s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}$) be a design type. Denote by $\mathbf{OA}(N;T)$ the set of all OAs with given type T and run size N.
- Set $U := \{(i,j,x) \mid i = 1,\dots,N,\ j = 1,\dots,d,\ x \in Q_j\}$, and call it the underlying set of $\mathbf{OA}(N;T)$. In other words, U consists of all possible triples of a row i, a column j, and an entry F_{ij} for any matrix $F \in \mathbf{OA}(N;T)$.
- The k-th column index set $J_k \subseteq \mathbb{N}_d := \{1, 2, \cdots, d\}$ precisely consists of column indices of factors having s_k levels, for each $k = 1, ..., m$.

2.1 Fraction transformations (or isomorphism) of orthogonal arrays

We can now encode any $F \in \mathbf{OA}(N;T)$ by its lookup table

$$Lt(F) := \{(i,j,F_{ij}) \mid i = 1,\dots,N,\ j = 1,\dots,d\} \subseteq U.$$

The encoding map Lt from $\mathbf{OA}(N;T)$ to the power set of U is clearly injective. The image of Lt consists of all sets $S \subseteq U$ with the following property:

$$\#\{x \mid (i,j,x) \in S\} = 1 \text{ for all } i = 1,\dots,N \text{ and } j = 1,\dots,d. \tag{1}$$

We now define three group actions (see Appendix A for more) on the set U:

- The row permutation group is $R := \mathrm{Sym}_N$. It acts via $\phi_R : R \to \mathrm{Sym}(U)$ defined by
$$(i, j, x)^{\phi_R(r)} = (i^r, j, x).$$
- The column permutation group is $C := \prod_{k=1}^{m} C_k$ where $C_k := \mathrm{Sym}(J_k)$. It acts via $\phi_C : C \to \mathrm{Sym}(U)$ defined by
$$(i, j, x)^{\phi_C(c)} = (i, j^c, x).$$
- The level permutation group is $L := \prod_{j=1}^{d} L_j$ where $L_j = \mathrm{Sym}_{r_j}$. This acts via the map $\phi_L : L \to \mathrm{Sym}(U)$ defined by
$$(i, j, x)^{\phi_L(l)} = (i, j, x^{l_j}),$$
where l_j is the projection of l onto L_j.

Definition 2. The full group G of fraction transformations of U is defined as
$$G := \phi_R(R) \quad \phi_C(C) \quad \phi_L(L) \leq \mathrm{Sym}(U). \tag{2}$$

Using (1) we can prove that, for every $F \in \mathbf{OA}(N;T)$ and $g \in G$, there exists a unique $F' \in \mathbf{OA}(N;T)$ with $Lt(F') = Lt(F)^g$. So G acts faithfully on $\mathbf{OA}(N;T)$ via the map $\pi : G \to \mathrm{Sym}(\mathbf{OA}(N;T)) = \mathrm{Sym}(U)$ defined by
$$F^g = F^{\pi(g)} := Lt^{-1}\left(Lt(F)^g\right).$$

The newly defined group G is indeed a permutation group acting on the space $\mathbf{OA}(N;T)$.

Proposition 5. The structure of G is described as follows.

1. $\phi_R(R)$ commutes elementwise with both $\phi_C(C)$ and $\phi_L(L)$.
2. $\phi_C(C_{k_1})$ commutes elementwise with $\phi_C(C_{k_2})$ for $k_1 \neq k_2$.
3. $\phi_C(C_k)$ commutes elementwise with $\phi_L(L_j)$ for $j \notin J_k$.
4. $\phi_L(L_{j_1})$ commutes elementwise with $\phi_L(L_{j_2})$ for $j_1 \neq j_2$.
5. (Column- Level relation.) $\phi_L(\prod_{j\in J_k} L_j)\phi_C(C_k)$ is the wreath product $\mathrm{Sym}_{s_k} \wr C_k$.

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 prove the last item, first of all let column permutation be simply a transposition $c = (i, j)$ 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

$$c.l_i \neq l_i.c \quad \text{and} \quad c.l_j \neq l_j.c, \tag{3}$$

but $c.l_i = l_j.c$ and $c.l_j = l_i.c$. However,

$$c.l_i.l_j = l_j.c.l_j = l_j.l_i.c = l_i.l_j.c, \tag{4}$$

and obviously

$$c.l_p = l_p.c \quad \text{for all } p \neq i, j \tag{5}$$

then

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

Secondly, in generic case, it is well-known that every permutation is a composition of transpositions. Hence, in the case c is a product of transpositions, then these rules are applied consecutively for each cycle existing in c. Precisely, we write $c = (i_1, j_1).(i_2, j_2)\dots(i_q, j_q)$. Put $CI := \{i_1, j_1, i_2, j_2, \dots, i_q, j_q\}$ be the (index) set of columns which are moved by c. Let L_{i_l} be a level permutation on columns i_l, and LI the set of corresponding indexes. Then it is easily seen that

i) if $|CI \cap LI|$ is an even number, Item 5) follows from equations (4) and (5).

ii) if $|CI \cap LI|$ is an odd number, then there exists a cycle (i_p, j_p) in c such that
$i_p \in CI \cap LI$ and $j_p \notin CI \cap LI$, so $j_p \notin LI$. Then Item 5) follows from (3).

□

Hence, we can now identify G with the wreath product $R \times (C \ltimes L)$ where

$$C \ltimes L = \prod_{k=1}^{m} \mathrm{Sym}_{s_k} \wr C_k.$$

Corollary 6. We get the followings.

- The full group or the permutation group acting on the space $\mathbf{OA}(N;T)$ is
$$G = R \times (C \ltimes L). \tag{6}$$
- As a result, the order of G can be calculated from OA parameters, as
$$|G| = N!\, a_1! \cdots a_m!\, (s_1!)^{a_1} \cdots (s_m!)^{a_m}.$$

The next concept plays a crucial role in the remaining parts.

Definition 3. Let F and F' be in $\mathbf{OA}(N;T)$.

- An isomorphism from F to F' is $g \in G$ such that $F^g = F'$.
- The automorphism group of an orthogonal array $F \in \mathbf{OA}(N;T)$ is the normalizer of F in the group G, i.e., $\mathrm{Aut}(F) := \{g \in G \mid F^g = F\}$.
- Any subgroup $A \leq \mathrm{Aut}(F)$ is called a group of automorphisms of F.

See a specific computation of $\mathrm{Aut}(F)$ in Appendix B.

2.2 Orthogonal arrays and colored graphs

Motivation of the approach. It is well known that combinatorial objects can be encoded as colored graphs. For this reason, a great deal of effort has been put into efficient computation of graph automorphisms – the program nauty [15] is extremely effective.

In this section, we show how to encode an array as a colored graph, and how to decode a graph back to an array. We then show how to use nauty to compute the automorphism group and a canonical representative of an isomorphism class of arrays, in particular for OAs having at least three distinct levels. This part provides a fundamental alternative for computing representatives of OA isomorphism classes, in comparison with using lex-least arrays introduced in [7].

2.2.1 Representation of an orthogonal array

Recall that a colored graph is a triple $W = (V, E, \gamma)$, where

- V is a finite set; E is a set of subsets of V of size two; and
- γ is a map from V to a fixed set C.

We call the elements of V vertices (or nodes), the elements of E edges, and the elements of C colors. Denote by $V(x)$ the neighbors of a vertex $x \in V$.

Concept 2. An isomorphism from a colored graph W to another colored graph $W' = (V', E', \gamma')$ is a bijection $s : V \to V'$ such that, for all $v, w \in V$,

- $\{v, w\} \in E$ if, and only if, $\{s(v), s(w)\} \in E'$, and
- $\gamma(v) = \gamma(w)$ if, and only if, $\gamma'(s(v)) = \gamma'(s(w))$.

Let $F = [F_{ij}]$ be an OA with run size N and design type $T = r_1 \cdot r_2 \cdots r_d$.

Definition 4. A colored graph $G_F = (V, E, \gamma)$ associated with F is constructed as follows:

- The vertex set V contains elements ρ_i, for $i = 1, \ldots, N$, corresponding to the rows; γ_j, for $j = 1, \ldots, d$, corresponding to the columns; and σ_{jv}, for $j = 1, \ldots, d$ and $v \in Q_j$, corresponding to the levels in each column.
- E contains edges $E_1 = \{\{\rho_i, \sigma_{jv}\}\}$ and $E_2 = \{\{\gamma_j, \sigma_{jv}\}\}$ whenever $F_{ij} = v$.
- The color set is $C = \{\rho, \gamma, \sigma_j\}$. All vertices ρ_i have color ρ; all vertices γ_j have color γ; and all vertices σ_{jv} have color σ_j.

G_F clearly is a tripartite graph w.r.t the partition of V into row, column and level nodes:

$$V = R \cup S \cup C; \text{ where } R = \{\rho_i\}, C = \{\gamma_j\}, \text{ and } S = \{\sigma_{jv}\}. \tag{7}$$

Obviously the edge set $E = E_1 \cup E_2 \subseteq (R \times S) \cup (S \times C)$, and respectively

$$|V| = N + \sum_{i}^{d} r_i + d \text{ and } \quad |E| = dN + \sum_{i}^{d} r_i.$$

Now call $\mathbf{OA}(N; T; t)$ be the class of all mixed OAs of strength $t \geq 1$, of type T and run size N; we fix a fraction $F \in \mathbf{OA}(N; T; t)$.

Concept 3. With $n_S = |S|$, we denote the color partition of F (or better of G_F) by

$$f := \Big[[1, \dots, N], [N+1, \dots, N+n_S], \tag{8}$$
$$[N+n_S+1, \dots, N+n_S+a_1], \dots, [N+n_S+1+\sum_{i=1}^{m-1} a_i, \dots, |V|] \Big].$$

f determines row, symbol and column-vertices in the graph G_F, respectively. Precisely, in G_F, the set of column-vertices C is a disjoint union of color classes $C_1, \dots, C_m$, called the column-color classes, and the total number of colors 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 $d = \sum_{i=1}^{m} |C_i|$, however the partition (R, S, C) is not a color partition.

Example 1. Let $F = \mathrm{OA}(4; 2^3; 2)$, then $N = 4$, $n_S = 6$, $d = 3$, $m = 1$.

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

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 2. Let $F = \mathrm{OA}(6; 3^1 \cdot 2^2; 1)$, so $N = 6$, $n_S = 7$, $d = 3$, $m = 2$.

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

$V = R \cup S \cup C = \{1, 2, \dots, 6, 7, \dots 13, 14, 15, 16\}$. 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 F is performed by its corresponding permutation $p_S = (10, 11)$ on symbol-vertices 10, 11 of the colored graph G_F. Switching columns 2 and 3 of F has counterpart $p_C = (15, 16)$ on column-vertices. And permuting rows 1 and 2 can be done by the permutations on row-vertices $p_R = (1, 2)$.

2.2.2 Properties of colored graphs

Let $\mathcal{G}$ be the set of all colored graphs, and let $\Phi : \mathbf{OA}(N;T;t) \to \mathcal{G}, \quad F \mapsto \Phi(F) = G_F$ be the map that takes a design F to the corresponding colored graph G_F (Definition 4).

Lemma 7. The map Φ is an injection.

To characterize clearly the image $\Phi(\mathbf{OA}(N;T;t)) \subseteq \mathcal{G}$, we write $v(u)$ for the valency of a vertex $u \in V$. Remind 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 $k = 1, \ldots, m$.

Proposition 8. Let F be an OA of strength $t \geq 1$ with factors Q_i and run size N.

1. Then G_F is tripartite with the vertex partition (R, S, C) given by (7) 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.

Proof. Use the OA definition and properties of its corresponding colored graph. □

Definition 5. [The set of colored graphs $\mathcal{G}_{N;T;t}$ associated with $\mathbf{OA}(N;T;t)$]

(i) Given parameters T, N, the set of colored graphs satisfying properties (1) − (5) of Proposition 8 are called the colored graphs associated with $\mathbf{OA}(N;T;t)$ of type T, N . They form a subset of $\mathcal{G}$, denoted by $\mathcal{G}_{N;T;t}$.

(ii) By Proposition 8(1.), vertices of R, S, C of a graph in $\mathcal{G}_{N;T;t}$ are called the row-vertices, the symbol-vertices and the column-vertices respectively.

2.2.3 Demerging a colored graph back to orthogonal array

Let $g \in \mathcal{G}_{N;T;t}$ (the set of colored graphs associated with $\mathbf{OA}(N;T;t)$). 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.

Lemma 9. 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 $\mathcal{G}_{N;T;t}$ 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 $s \in S$; Proposition 8(4.) implies a contradiction.

Next, let us 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. □

Main Theorem 1. Given parameters T and N, such that $\frac{N}{s_k} \in \mathbb{N}$ for all $k \in \{1,\dots,m\}$. Suppose further that there is at least one k for which $\frac{N}{s_k} > 1$, then $\Phi(\mathbf{OA}(N;T;t)) = \mathcal{G}_{N;T;t}$.

Proof. $\Phi(\mathbf{OA}(N;T;t)) \subseteq \mathcal{G}_{N;T;t}$? It is obvious, by Definition 5(i).

$\mathcal{G}_{N;T;t} \subseteq \Phi(\mathbf{OA}(N;T;t))$? Pick a colored graph $g \in \mathcal{G}_{N;T;t}$, then g fulfills properties $(1)-(5)$ of Proposition 8. We construct an array $F_g \in \mathbf{OA}(N;T)$ such that $\Phi(F_g) = g$. 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, ..., s_m such that their neighbors are mutually disjoint subsets of V. From Lemma 9, these vertices are uniquely determined and they form column vertices of g.

Let C be the set of these column-vertices. For each $c \in C$, using Proposition 8(3.) we track its neighbors: 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 Proposition 8. 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 Proposition 8. Besides, each of those row-vertices consists 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, $g = \Phi(F_g) \in \Phi(\mathbf{OA}(N;T;t))$, and so $\mathcal{G}_{N;T;t} \subseteq \Phi(\mathbf{OA}(N;T;t))$. Therefore, $\Phi(\mathbf{OA}(N;T;t)) = \mathcal{G}_{N;T;t}$. □

Corollary 10. 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 $\frac{N}{s_k} > 1$. The mapping Φ then is a bijection between the set $\mathbf{OA}(N;T;t)$ of strength t arrays with type T, N and the set $\mathcal{G}_{N;T;t}$ of colored graphs of type T, N.

Proof. Resulting from Lemma 7 and Main Theorem 1. □

Concept 4. The inverse mapping

$$\Phi^{-1} : \mathcal{G}_{N;T;t} \to \mathbf{OA}(N;T), \quad g \mapsto \Phi^{-1}(g) = F_g$$

is called the demerging mapping of $\mathcal{G}_{N;T;t}$.

This inverse mapping returns a unique array F_g from a colored graph $g \in \mathcal{G}_{N;T;t}$. Any array $F \in \mathbf{OA}(N;T)$ of strength $t \geq 2$ is, moreover determined uniquely by its companion graph $G_F \in \mathcal{G}_{N;T;t}$, by Corollary 10. 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 $k = 1,\dots,m$.

Theorem 11. Let G_F, G_K be the two colored graphs which are formed by two orthogonal arrays $F, K \in \mathbf{OA}(N;T)$. Then F and K are isomorphic arrays if and only if G_F and G_K are isomorphic graphs.

Proof. Consider both ways.

- The only if part: If F and K are isomorphic arrays then $K = F^p$ 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 of the corresponding graph G_F. Putting $p^* = p_R\ p_S\ p_C$, we have $G_F^{p^*} = \Phi(F^p) = \Phi(K) = G_K$. It follows that G_F, and G_K are two isomorphic graphs. The 'only if' part can be seen as follows.

- The if part: If G_F and G_K are isomorphic graphs, we can find a permutation q on vertices (of G_F) such that $G_K = G_F^q$. Since $G_F, G_K \in \mathcal{G}_{N;T;t}$, the graphs G_F, G_K satisfy all the conditions in Proposition 8. 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_K 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 K.

□

Example 3. We construct an OA($6; 3{\cdot}2^2; 1$) from the colored graph given in Figure 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 $1, 2, \ldots 6$, for instance, also have valency 3, but they cannot represent the first column-vertex (3-level column) since their neighbors are not disjoint. 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 obtained is

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

2.2.4 Finding the canonical graph and canonical orthogonal array

For any colored graph W, denote by canon(W) the canonical labeling graph computed using nauty with the color partition f (as in Formula (8)). It consists of a vertex relabeling permutation, p, say and new adjacencies. Hence, canon(W) is fully determined 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. But how to compute non-isomorphic arrays? Theorem 11 gives us a clue, as follows.

Corollary 12. Let $G_F := \Phi(F)$ and $G_K := \Phi(K)$ be the colored graphs of arrays F and K respectively. Then F and K are isomorphic arrays if and only if $\mathrm{canon}(G_F) = \mathrm{canon}(G_K)$.

SUMMARY. The following observations are useful later on.

- If $W \in \mathcal{G}_{N;T;t}$ then $\mathrm{canon}(W) \in \mathcal{G}_{N;T;t}$.
- Let F^* be the canonical labeled orthogonal array of an orthogonal array F. Then $G_F \in \mathcal{G}_{N;T;t}$, and $G_{F^*} \in \mathcal{G}_{N;T;t}$. If F has strength $t \geq 2$, the canonical array F^* is uniquely determined by canon(G_F). Indeed, F^* can be constructed using the scheme $F \to G_F \to \mathrm{canon}(G_F) \to F^*$, in which the first arrow represents the mapping Φ; the second by nauty; while the third arrow computing F^*, is done by the demerging map Φ^{-1}.

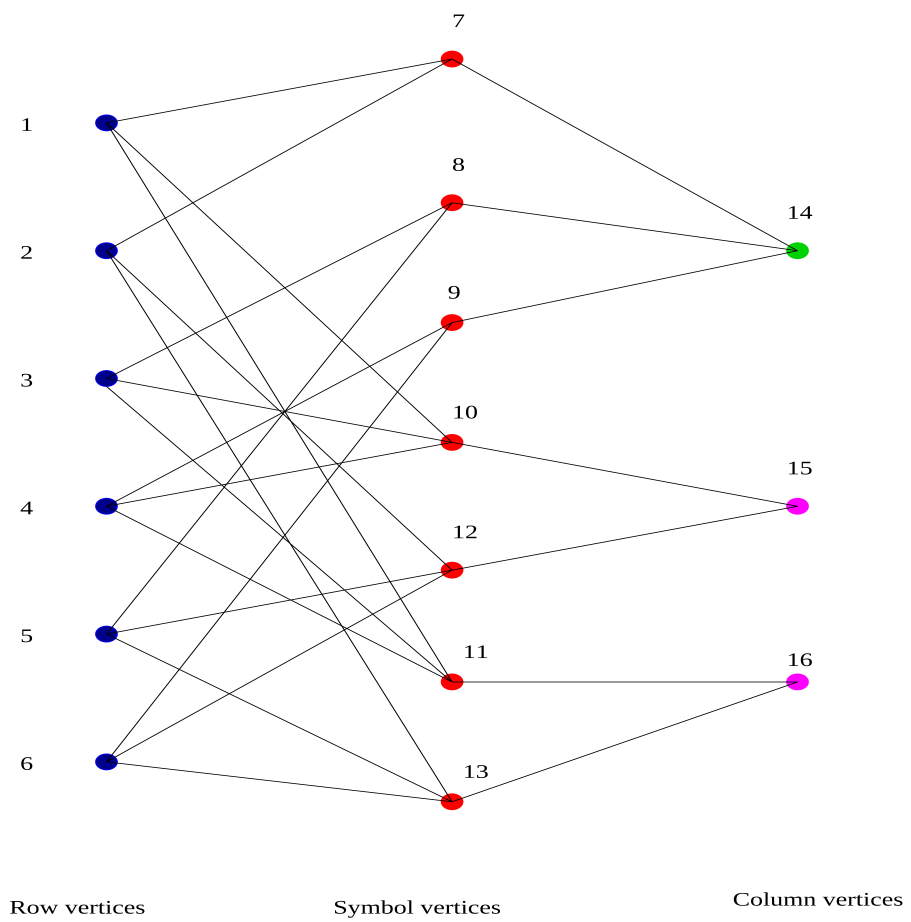

Figure 1: The colored graph of a 6 runs OA

New approaches using integer linear algebra and permutation groups to find new factor of a known factorial design will be described in next parts, Sections 3 and 4.

3 Integer linear formulation for OA enumeration

In this section, we formulate necessary algebraic conditions for the existence of a new factor X in Problem 3, the column extension of orthogonal arrays of strength t. In Section 3.2 we specifically employ the automorphism of each design to prune solution space.

3.1 An integer linear approach solves the extension problem

3.1.1 Transforming the factor extension to a linear system of equations

Assume that $t = 3$. Let $F = \mathrm{OA}(N; r_1 \cdots r_d; 3)$ 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 pair of 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 OAs, $[F|X]$ exists if and only if X is orthogonal to any pair of columns of F. We can find a set P of necessary constraints for the existence of array $[F|X]$ in terms of polynomials in the coordinate indeterminates of X, by the following rules.

Observation 2 (Transformation rules).

(a) Calculate frequencies of 3-tuples, and locate positions of symbol pairs of (S_i, S_j).

(b) Set the sums of coordinate indeterminates of X (corresponding to these positions) equal 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. 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 P of constraints 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 $\sum_{i\neq j}^{3} r_i r_j = 20$ 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 ...

By transformation rule (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:

$$X \perp [S_1, S_2] \Leftrightarrow X \perp Y \Leftrightarrow x_1 + x_2 = x_3 + x_4 = \ldots = x_{15} + x_{16} = \lambda \cdot (0+1) = 1, \ldots,$$

and

$$X \perp [S_2, S_3] \Leftrightarrow X \perp Z \Leftrightarrow x_1 + x_5 + x_9 + x_{13} = \ldots = x_4 + x_8 + x_{12} + x_{16} = \mu \cdot (0+1) = 2.$$

One solution of P is given in the last row of the matrix below:

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

Observe that, although the frequency invariant is a necessary and sufficient condition for X's existence, for $s > 2$, the linear constraints P found using the rules of Observation 2 form a set of necessary conditions only.

We now consider extending strength 3 OAs. The set P of linear constraints with integer coefficients is described by the matrix equation $AX = b$, in which $A \in \mathrm{Mat}_{\mathrm{m_1,N}}(\mathbb{N})$,

$$X = (x_1, \ldots, x_N) \in \{0, 1, \ldots, s-1\}^N \subseteq \mathbb{N}^N \tag{9}$$

is a vector of unknowns, $b \in \mathbb{N}^{m_1}$, and $m_1 := \sum_{i\neq j}^{d} r_i r_j = |P|$. The vector b is formed by counting frequencies of triples involving two known columns in F and the unknown column X as in Observation 2. 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

$$M\,X = c, \tag{10}$$

where $M \in \mathrm{Mat}_{m,N}(\mathbb{Z})$, the set of all $m \times N$ $(m \leq m_1)$ matrices with integral entries, $c \in \mathbb{Z}^m$, and the vector of unknowns $X = (0, x_2, \ldots, x_N) \in \mathbb{Z}^N$.

3.1.2 Solving the obtained integer linear system

We solve the factor extension problem by the following 3-step approach.

1. Build the system (10) using rules (a) and (b) of Observation 2.
2. Find all solutions $X = (x_1, \ldots, x_N)$ in the product set $\{0, 1, 2, \ldots, s - 1\}^N$.
3. Collect non-isomorphic, canonical OAs of the set of all arrays of the form $[F|X]$ into a set L. There are two possibilities: a) if L is empty, conclude F has no extension; and otherwise b) go back to Step 1 for each OA in L until the number of factors meets the number of columns required.

Observation 3.

a/ The first step is already done. The method to solve the last step was given in Section 2.2. 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, then discuss how to combine the automorphism group $\mathrm{Aut}(F)$ of F (Definition 3) for finding non-isomorphic vectors X. Observe that, when extending OAs, the group size tends to grow proportionally with the number of solutions.

b/ The system P described by (10) can be solved over the naturals $\mathbb{N}_{\geq 0}$ 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, set $P = \{f_1, f_2, f_3, \ldots\}$, in which the f_i are linear polynomials in the indeterminates $x_2, \ldots, x_N$. Particularly, when the x_is are binary, we use the following fact.

Proposition 13 (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

$$C = V_f \setminus V_p,\ n_f = |V_f|,\ n_p = |V_p|,\ n_C = |C|.$$

Let S_f be the set of solutions of the equation $f = 0$, and S_p the set of solutions of the equation $p = 0 \mod 2$. Let S_p^i be the solution set of the equation $p = i$ for each $i = 0, \ldots, n_p$.

- 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 equation $f = 0$ 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 $H(n_p, 2)$. $\square$

Therefore, enumerating of strength 3 OAs of the form $[F|X]$ can be solved if there are few arrays F 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 so many isomorphic vector solutions X in each extension. Pruning techniques using the automorphism group associated with F will be exploited to deal with these difficulties in the next part.

3.2 The row permutation group for efficiently computing X in $[F|X]$

The extension $K := [F|X] = \mathrm{OA}(N; r_1 \cdots r_d \cdot s; t)$ depends on solving the integer linear system (10) $M.X = c$ in terms of $X = (x_j) \in \{0, 1, \ldots, s-1\}^N$ for $j = 1, \ldots, N$. This approach is useful if a few constraints, structures or pruning techniques would be found and used to delete out some (not all) isomorphic vectors in each isomorphic class, and we then retain isomorph-free vectors. From that point, the search for all isomorph-free designs becomes feasible. We show how to reduce calculating $(x_j) \in \{0, 1, \ldots, s-1\}^N$ to finding all integral (pivotal) tuples $(y_i) \in \mathbb{Z}^n$ or better $(y_i) \in \mathbb{Z}^{n_0}$, for $n_0 \leq n$ as being described by Eq. (16) in section 3.2.2. Fix an array $F \in \mathbf{OA}(N; T; t)$, recall that $\mathrm{Aut}(F) := \{g \in G \mid F^g = F\}$, with G is the full group of isomorphisms, see Eq. (2).

3.2.1 The row permutation group acting on an orthogonal array

We first define the row permutation group of F. Let $g \in \mathrm{Aut}(F)$. Then g induces a permutation g_1 in the full group G_K of K, see Formula (6). Let g_R be the row permutation component of g, then g_R is also the row permutation component of g_1. Due to Definition 3, we have

Theorem 14. For $g \in \mathrm{Aut}(F)$, g induces $g_1 \in G_K$ and generates the image K^{g_1} which is isomorphic to K.

Proof. Formula (2) says 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. Besides, the row permutation g_R induces a row permutation $g_1 \in G_K$, we furthermore have

$$K^{g_1} = [F|X]^{g_1} = [F^g|X^{g_R}] = [F|X^{g_R}] \tag{11}$$

since g already fixes F, and only g_R acts on the column X by moving its coordinates. As a result, $K^{g_1} = [F|X^{g_R}]$ is isomorphic to $K := [F|X]$. $\square$

Definition 6. Let $H := \mathrm{Row}(\mathrm{Aut}(F))$ be the group of all row permutations g_R extracted from the group $\mathrm{Aut}(F)$. We call H the row permutation group of F.

The direct product of H and τ is very useful for pruning later on, given by

$$\sigma := H \times \tau, \tag{12}$$

where $\tau := \mathrm{Sym}_s$ is the group of symbol permutations acting on the coordinates of X. We might impose some extra constraints on the system, due to the following.

Observation 4.

For each generator p of $H = \mathrm{Row}(\mathrm{Aut}(F))$ such that at least one of its cycles has even length, we extract those even length cycles into a set Ec. We do not use odd length cycles of p. Then, for each $h \in Ec$, 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 15. If $Ec \neq []$, for each $h \in Ec$ having the form

$$h = \prod_i (i_1, i_2) \quad \prod_j (j_1, j_2, j_3, j_4) \ldots$$

where $1 \leq i_1 \neq i_2 \neq j_1 \neq j_2 \neq j_3 \neq j_4, \ldots \leq N$, we can add the following inequality

$$x_{i_1} + x_{j_1} + x_{j_3} + \ldots \leq x_{i_2} + x_{j_2} + x_{j_4} + \ldots \tag{13}$$

into the original system P without missing any non-isomorphic vector solution X.

Proof. Suppose $h = \prod_i (i_1, i_2) \quad \prod_j (j_1, j_2, j_3, j_4) \ldots \in Ec$, and $Z = [z_1, z_2, z_3, \ldots, z_N]$ 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 $X = [x_1, x_2, x_3, \ldots, x_N]$ 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 (13). □

For example, let $h = (1,2)(7,8,9,10)(13,16) \in Ec$, then $h^{-1} = (1,2)(7,10,9,8)(13,16)$, we can impose the following inequality $x_1 + x_7 + x_9 + x_{13} \leq x_2 + x_8 + x_{10} + x_{16}$ into the original set P. Indeed, suppose $Z = [z_1, z_2, z_3, \ldots, z_{16}]$ is a solution, and

$$(*) \ldots z_1 + z_7 + z_9 + z_{13} \geq z_2 + z_8 + z_{10} + z_{16}.$$

The image

$$X = Z^h = (z_{i^{h^{-1}}}) = (z_2, z_1, z_3, z_4, z_5, z_6, z_{10}, z_7, z_8, z_9, z_{11}, z_{12}, z_{16}, z_{14}, z_{15}, z_{13})$$

satisfies (13), since (*) means $x_2 + x_8 + x_{10} + x_{16} \geq x_1 + x_9 + x_7 + x_{13}$.

3.2.2 Combining linear spaces with symmetries

Now we 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 Eq. (10) over $\mathbb{Q}$. The set S in fact is an affine space in $\mathbb{Q}^N$; and obviously

$$\mathrm{Z}(P) = S \cap \{0, 1, \ldots, s-1\}^N.$$

Moreover, $\mathrm{Z}(P)$ is a subset of $\bigcap_{h \in H} S^h$, with $S^h := \{X^h : h \in H\}$. Indeed, because $\mathrm{Z}(P)^h = \mathrm{Z}(P)$ for all $h \in H$, we have $\mathrm{Z}(P) \subseteq S^h$, for all $h \in H$.

Definition 7. We call the intersection $\bigcap_{h \in H} S^h$ the H-invariant core of $\mathrm{Z}(P)$.

By definition it is the maximal H-invariant subset of S. The H-invariant core $\bigcap_{h \in H} S^h$ of $\mathrm{Z}(P)$ is still an affine space since the image S^h 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 H-invariant core of $\mathrm{Z}(P)$ could have smaller dimension.

Example 5. 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 H we can reduce it to dimension 20.

How to compute the H-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 the field $\mathbb{Q}$). Let $n := N - \mathrm{rank}(M)$ be the dimension of S, then $|B| = n$, and

$$S = v + \langle B \rangle = v + \sum_{i=1..n} b_i B_i, \text{ where indeterminates } b_i \in \mathbb{Q}. \tag{14}$$

Observation 5. Let $p \in H$, 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,

$$S^p = v^p + \langle B^p \rangle = v^p + \sum_{i=1..n} c_i B_i^p, \text{ where } c_i \in \mathbb{Q}. \tag{15}$$

Furthermore, $S \cap S^p \neq \emptyset$ if and only if the system

$$v^p - v = \sum_{i=1..n} b_i B_i - \sum_{i=1..n} c_i B_i^p, \text{ or equivalently}$$
$$v^p - v = \left[B_1 | B_2 | \ldots | B_n | - B_1^p | - B_2^p | \ldots | - B_n^p\right] [b_1, \ldots, b_n, c_1, \ldots, c_n]^T$$

has solution $b_1, \ldots, b_n, c_1, \ldots, c_n$. Hence, if $S \cap S^p \neq \emptyset$, its basis and the specific vector v can be found by substituting $b_1, \ldots, b_n$ back into (14), (or $c_1, \ldots, c_n$ into (15)). We may prune the integral solution set $\mathrm{Z}(P)$ by computing its H-invariant core.

Let H_G be a set of generators of H, we compute $\bigcap_{h \in H} S^h$ using the following procedure.

Algorithm 1 Computing H-invariant core

Find-H-invariant-core(S, H_G)

Input the affine solution space S of (10), and the generators H_G;

Output the affine space $\bigcap_{h\in H} S^h$.

Set $Y := S$;
`Repeat`

- $W := Y$;
- Update $Y := (\bigcap_{p\in H_G} Y^p) \cap Y$;

`Until` $Y = W$;
Return Y.

Proof. Let Y_0 be the output of the procedure, we show that $Y_0 = \bigcap_{h\in H} S^h$. The space Y_0 has property that $Y_0 = \bigcap_{p\in H_G} Y_0^p \cap Y_0$. Therefore, $Y_0 = Y_0^p$ for all $p \in H_G$. Since any permutation $h \in H$ is a product of $p \in H_G$, we get $Y_0 = Y_0^h$. □

SUMMARY.

Having obtained the H-invariant core $Y_0 =: [u, C]$ of $\mathrm{Z}(P)$, we update $S := Y_0$, and update the dimension n to a possibly smaller dimension $n_0 = \dim(Y_0)$. The integral vector solution X (viewed as column vector) then is computed by:

$$X^T = (0, x_2, x_3, \ldots, x_N)^T = u + \sum_{i=1..n_0} y_i\, C[i], \tag{16}$$

where pivotal variables $y_i \in \mathbb{Z}$. In brief, solving the linear system P in terms of natural vector $(x_j) \in \{0, 1, \ldots, s-1\}^N$ $(j = 1, \ldots, N)$ therefore is reduced to finding all integral pivotal tuples $(y_i) \in \mathbb{Z}^n$ for $i = 1, \ldots, n$, or better, to finding shorter integral pivotal tuples $(y_i) \in \mathbb{Z}^{n_0}$ for $i = 1, \ldots, n_0$ (if there exists the H-invariant core).

3.2.3 Solving efficiently the linear system $MX = c$

We show how to find pivotal variables y_i by depth-first and breath-first schemes. Let $ExtraS$ be the set of these extra inequalities found from Lemma 15. Let Y be the set of coordinates of X in terms of $(y_i)_{i=1,\ldots,n}$. We split Y into 3 subsets:

$$\begin{aligned}
Y_1 &:= \{\text{ monomials}\},\\
Y_2 &:= \{\text{ monomials with constant, and be grouped with respect to } y_i\}, \quad (17)\\
Y_3 &:= \{\text{ polynomials with at least two indeterminates } y_i\}.
\end{aligned}$$

For $t = 2$ we cut vector X into r_1 sub-vectors

$$L_X := \Big[\big(x_1, \dots, x_{\frac{N}{r_1}}\big), \dots, \big(x_{\frac{(r_1-1)N}{r_1}}, \dots, x_N\big)\Big],$$

and for $t = 3$ cut X into $r_1 r_2$ sub-vectors

$$L_X := \Big[\big(x_1, \dots, x_{\frac{N}{r_1 r_2}}\big), \dots, \big(x_{\frac{(r_1 r_2-1)N}{r_1 r_2}}, \dots, x_N\big)\Big].$$

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 $ExtraS \le 0$ (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. A combination of depth-first and breath-first schemes to find all solutions $(y_i) \in \mathbb{Z}^n$ is presented in Algorithm 2.

Example 6. Extending $F = \mathrm{OA}(16; 2^3; 3)$ to $[F\ X] = \mathrm{OA}(16; 2^3 \cdot 4; 3)$. The group
$H = \mathrm{Row}(\mathrm{Aut}(F))$ 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 a set $ExtraS$ of 169 extra inequalities by Lemma 15. The solution vector $X \in \{0,1,2,3\}^{16}$ ($N = 16$) in terms of $(y_i) \in \mathbb{Z}^8$ ($n = 8$) is $X = (x_j) =$

$$=(0, y_1+6, y_2+6, -y_1-y_2-6, y_3, -y_1-y_3, y_4, y_1-y_4+6,$$
$$y_5, -y_1-y_5, y_6+6, y_1-y_6, y_7+6, y_1-y_7, y_8, -y_1-y_8)$$

We want to find all $(y_1, \dots, y_8) \in \mathbb{Z}^8$ so that $X \in \{\,0,1,2,3\,\}^{16}$ by splitting

$$Y = \{y_1+2, y_2+2, -y_1-y_2-2, y_3, -y_1-y_3, y_4, y_1-y_4+2,$$
$$y_5, -y_1-y_5, y_6+2, y_1-y_6, y_7+2, y_1-y_7, y_8, -y_1-y_8\}$$

into $Y_1 = \{y_3, y_4, y_5, y_8\}$; $Y_2 = \big\{[y_1+6], [y_6+6, y_2+6], [y_7+6]\big\}$; 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 $ExtraS$, and employing the fact that each of the four vectors having strength 1: $(0, y_1+6, y_2+6, -y_1-y_2-6)$, $(y_3, -y_1-y_3, y_4, y_1-y_4+6)$,

$$(y_5, -y_1-y_5, y_6+6, y_1-y_6),\ (y_7+6, y_1-y_7, y_8, -y_1-y_8).$$

At each iteration, whenever $Y_1 = \emptyset$, 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 $(y_i) \in \mathbb{Z}^8$, of these only one forms an unique $\mathrm{OA}(16; 2^3 \cdot 4; 3)$.

Algorithm 2 Recursive computing of $(y_i) \in \mathbb{Z}^n$

COMPUTE-PIVOTALS(Y, $ExtraS$, L_X)

Input Y; $ExtraS$ and L_X

Output All vectors $(y_i)_{i=1,\dots,n} \in \mathbb{Z}^n$, and all isomorph-free $(x_j) \in \{0, 1, \dots, s-1\}^N$

STEP 1:
`Repeat`

- split $Y = Y_1 \cup Y_2 \cup Y_3$ by (17)
- form all partial vectors by making the hypercube from variables of Y_1
- prune them using $ExtraS \leq 0$, and L_X
- substitute each valid partial vector back to Y

`Until` $Y_1 = \emptyset$
Comment: only keep intermediate valid nodes in the search tree;

$\diamond$ Since $Y = Y_2 \cup Y_3$,
STEP 2: Extend the valid partial vectors made above by all possible vectors of Y_2

STEP 3: Collect the full vector solutions $(y_i)_{i=1,\dots,n} \in \mathbb{Z}^n$, then $(x_j) \in \{0, 1, \dots, s-1\}^N$
Comment: always certificate newly extended nodes using $ExtraS$ and L_X

STEP 4: Return the representatives in the $\sigma := H \times \tau$-orbits [see Eq. (12)] of Z(P).

Comment: The final step can be much efficiently developed in Section 4.

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4 Row permutation subgroups for pruning solution spaces

It is now obvious that, by recursion, the process of building X can be brought back to strength 1 derived designs. We can effectively prune $\mathrm{Z}(P)$ from those smallest sub-designs by finding some subgroups of $H = \mathrm{Row}(\mathrm{Aut}(F))$ acting on strength 1 derived designs. Those subgroups, discussed in next parts, must have the property that they act separately on the row-index sets corresponding to the derived designs.

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 the list I_N with $\{1, 2, \ldots, N\}$ in this section. Then H acts naturally on X' indices. Furthermore, we employ the following.

Concept 5. We say a row permutation $g_R \in H$ acts fixed-point free, or globally on X if it moves every index. Otherwise, if the moved points of g_R form a proper subset J of $\{1, \ldots, N\}$, i.e., it fixes point-wise the complement 'list' of J in I_N, we say g_R acts locally at that subset.

The first step is to localize the formation of a vector X of the form (9) 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 $\frac{N}{r_1}$:

$$X = [u_1; u_2; \ldots; u_{r_1}], \text{ where } u_i = \left(x_{\frac{(i-1)N}{r_1}+1}, \ldots, x_{\frac{iN}{r_1}}\right). \tag{18}$$

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 $V = V_1 \times V_2 \times \ldots \times V_{r_1}$. We propose a simple scheme, Algorithm 3 to find all non isomorphic solution vectors $X \in V$.

4.1 Forming permutation subgroups of the derived designs

Remind that we view $F \in \mathrm{OA}(N; r_1 \cdot r_2 \cdots r_d; 3)$ 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

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

Define the stabilizer in H of F_i by

$$N_H(F_i) := \mathrm{Normalizer}\,\big(H, \mathrm{RowInd}(F_i)\big) = \big\{h \in H : \mathrm{RowInd}(F_i)^h = \mathrm{RowInd}(F_i)\big\}. \tag{19}$$

Algorithm 3 Find all non isomorphic vectors X in $[F|X]$

EXTEND-ONE-FACTOR(F)

Input F is a strength t design;

Output All non-isomorphic extensions of F to $[F|X]$

a/ Find all candidate sub-vectors $u_i \in V_i$, $i = 1, \ldots, r_1$.

b/ Discard (prune) them as many as possible by using subgroups of H.

c/ Plug those u_is together, then compute the representatives of the $\sigma = H \times \tau$-orbits in V, the solution space $\mathrm{Z}(P)$ of P.

In this way, we find r_1 subgroups of H corresponding to the derived designs F_i. But it can happen that $\mathrm{RowInd}(F_l)^h \neq \mathrm{RowInd}(F_l)$ for some $h \in N_H(F_i)$ and $1 \leq l \neq i \leq r_1$.
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:

$$L(F_i) := \mathrm{Centralizer}\,\big(N_H(F_i), J(F_i)\big), \tag{20}$$

where $J(F_i) := I_N \setminus \mathrm{RowInd}(F_i)$ is the sublist of I_N consisting of elements not in $\mathrm{RowInd}(F_i)$. The group $L(F_i)$ acts locally at $\mathrm{RowInd}(F_i)$, i.e. acts on the row-indices of F_i and fixes pointwise any row-index outside F_i.

Definition 8. We call these subgroups L_i (of H) the row permutation subgroups associated with strength 2 derived designs .

These subgroups can be determined further as follows. For an integer $m = 1, 2, \ldots, t-1$ and for $j = 1, 2, \ldots m$, denote by

$$F_{i_1,\ldots,i_m} := \mathrm{OA}\left(\frac{N}{r_1 r_2 \cdots r_m}; r_{m+1} \cdots r_d; t-m\right) \tag{21}$$

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

$$\mathrm{RowInd}(F_{i_1,\ldots,i_m}) := \bigcap_{j=1}^{m} \big\{ l \in \{1, 2, \ldots, N\} : F[l, j] = i_j - 1 \big\}. \tag{22}$$

Let $J(F_{i_1,\ldots,i_m}) := I_N \setminus \mathrm{RowInd}(F_{i_1,\ldots,i_m})$. Generalizing (19) and (20) gives:

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

Definition 9. $L(F_{i_1,\dots,i_m})$ is called the subgroup associated with the derived design $F_{i_1,\dots,i_m}$, for $1 \le i_j \le r_j$, $j = 1, 2, \dots m$. We say $L(F_{i_1,\dots,i_m})$ acts locally on the derived design $F_{i_1,\dots,i_m}$, and write $L_{i_1,\dots i_m} := L(F_{i_1,\dots,i_m})$ 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.

4.2 Using permutation subgroups of the derived designs

We now show how to use the subgroups $L_{i_1,\dots,i_m}$. Recall that $\mathrm{Z}(P)$ is the set of all natural solutions X. From Eq. (11) in Theorem 14, K^g is an isomorphic array of $K = [F|X]$, hence the vector X^g can be pruned from $\mathrm{Z}(P)$, for any solution X and any permutation $g \in \mathrm{Aut}(F)$.

Notation. These notations will be used for the remaining parts of the paper.

For a fixed m-tuple of symbols $i_1, \dots, i_m$, let $V_{i_1,\dots,i_m}$ be the set of solutions of fraction

$$F_{i_1,\dots,i_m} = \mathrm{OA}((r_1 r_2 \cdots r_m)^{-1} N; r_{m+1} \cdots r_d; t - m), \text{ for } 1 \le m \le t - 1.$$

For any sub-vector $u \in V_{i_1,\dots,i_m}$, from (22) and (18), let

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

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

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

We have

Main Theorem 2. For any pair of sub-vectors $u, v \in V_{i_1,\dots,i_m}$, if $v = u^{g_R}$ for some row permutation $g_R \in L_{i_1,\dots,i_m}$, we have $\mathrm{Z}(u) = \mathrm{Z}(v)$.

We prove this key theorem in the next two claims. In Lemma 16, without loss of generality, it suffices to give the proof for the first strength 2 derived array. Its generalization, i.e. the induction step then will be presented in Theorem 17.

Lemma 16 (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

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

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

As a result, 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 we get $V_1 \neq \emptyset$, 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 $L_1, \ldots, L_{r_1}$.

Concept 6. We call this procedure, that results from Main Theorem 2, the local pruning process using strength 2 derived designs.

Next, if $t \geq 3$ we extend the proof of Lemma 16 to cases $2 \leq m \leq t-1$.

Theorem 17 (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 16, 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 $\mathrm{OA}(r_2^{-1}n; r_3 \cdots r_d; 1)$. Any 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

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

- Known that the subgroup $L(f_j) := \text{Centralizer}\big(N_H(f_j), J(f_j)\big)$ (see from (22) and Definition 9) consists of row permutations acting locally on

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

  Hence the subgroup $L(f_j)$ fixes $J(f_j) = [1, \ldots, N] \backslash \text{RowInd}(f_j)$ pointwise. Since V_1 is the Cartesian product of the subsets $V_{1,j} := \{ u_{1,j} \}$, we prune $V_{1,j}$ using $L(f_j)$, for all $j = 1, \ldots, r_2$.

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

$$\mathrm{Z}_X(u_{1,1}) := \Big\{ \, [\, [u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \,] : \text{ for } X = [u_1; u_2; \ldots; u_{r_1}] \in \mathrm{Z}(P) \Big\},$$

$$\mathrm{Z}_Y(v_{1,1}) := \Big\{ [[v_{1,2}; \ldots; v_{1,r_2}]; v_2; \ldots; v_{r_1}] : \text{ for } Y = [v_1; v_2; \ldots; v_{r_1}] \in \mathrm{Z}(P) \Big\},$$

  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

$$\begin{aligned} K^h &= [F|X]^h = F^h|\, X^h = F|\, X^h \\ &= F|\, [\, u_1^h; u_2; \ldots; u_{r_1} \,] \\ &= F|\, \big[[u_{1,1}^h; u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big] \\ &= F|\, \big[[v_{1,1}; u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big]. \end{aligned}$$

- Hence, $Y = \big[[v_{1,1}; u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big]$ is a solution 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, $j = 1, \ldots, r_2$.

$\square$

4.3 Operations on derived designs- An agent-based localization

The above-proposed localizing idea can be enhanced further when 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. Specifically, notice that strength 1 and strength t designs require special operations. To be precise, at the global scale of strength t design, it suffices to find only the representatives of the $H \times \tau$-orbits [see Formula (12)] in the solution space $\mathrm{Z}(P)$ of P.

We now formalize our new agent-based localization. Recall from (21) that the symbols $i_1, \ldots, i_m$ $(1 \le i_j \le r_j)$ indicate the derived design having symbol i_j in column j, for $j = 1, \ldots, m$. From Definition 9, $L_{i_1,\ldots,i_m}$ are the subgroups associated with the derived designs $F_{i_1,\ldots,i_m}$ having strength $t - m$. When $m = t - 1$, 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.

At initial designs $F_{i_1,\ldots,i_{t-1}}$ (Initial step when $m = t - 1$):

Input: $F_{i_1,\ldots,i_{t-1}}$;

Operation:

- form $V_{i_1,\ldots,i_{t-1}}$, the set of all strength 1 vectors of length $(r_1 r_2 \cdots r_{t-1})^{-1} N)$ being appended to $F_{i_1,\ldots,i_{t-1}}$,
- compute $L_{i_1,\ldots,i_{t-1}}$, and
- find the representatives of $L_{i_1,\ldots,i_{t-1}}$ - orbits in the set $V_{i_1,\ldots,i_{t-1}}$;

Output: these representatives, ie, solutions of $F_{i_1,\ldots,i_{t-1}}$.

At strength k derived designs $(1 < k \le t - 1)$: let $m := t - k$, we have

Input: the vector solutions having length $(r_1 r_2 \cdots r_m \cdot r_{m+1})^{-1} N$ of strength $k - 1$ sub-designs; and the subgroup $L_{i_1,\ldots,i_m}$;

Operation:

- form sub-vector solutions having length $(r_1 r_2 \cdots r_m)^{-1} N)$ of $F_{i_1,\ldots,i_m}$,
- prune these solutions by $L_{i_1,\ldots,i_m}$;

Output: representatives of the $L_{i_1,\ldots,i_m}$- orbits in the set $V_{i_1,\ldots,i_m}$.

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 $(i = 1, 2, \ldots, m)$;

Output: Two steps

a/ (Isomorph-free test 1) returns solution vectors X which are non-isomorphic up to $\sigma = H \times \tau$,

b/ (Isomorph-free test 2) forms orthogonal arrays $K = [F|X]$ of the same strength t, then select only non-isomorphic arrays, by computing their canonical arrays, as suggested in Section 2.2.

We brief ours ideas in Algorithm 4, PRUNING-USES-SYMMETRY(F, d).

Example 7. 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 $H = \mathrm{Row}(\mathrm{Aut}(F))$, and update it by $H = \mathrm{Stabilizer}(H, [1])$, 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
$L_2 = [(), (23,24), (21,22), (21,22)(23,24), (19,20), (19,20)(23,24),$
$(19,20)(21,22), (19,20)(21,22)(23,24), (17,18), (17,18)(23,24),$
$(17,18)(21,22), (17,18)(21,22)(23,24), (17,18)(19,20),$
$(17,18)(19,20)(23,24), (17,18)(19,20)(21,22), (17,18)(19,20)(21,22)(23,24)]$

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.

Observation 6.

Note 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 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 (19) and in (20). But the subgroups found in this way help reducing isomorphic vectors only when the group $H = \mathrm{Row}(\mathrm{Aut}(F))$ has very large size. When array F already has many columns, H's size usually declines.

Algorithm 4 Pruning uses subgroups of derived designs

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 $V_{i_1,\dots,i_{m-1}}$.

Comment: For strength $t = 3$, in Step 1), we form subvectors $u_{i,j} \in V_{i,j}$ simultaneously at the $r_1 r_2$ sets $V_{i,j}$, then 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 $\sigma = H \times \tau$-orbits of V, $V = \{\text{vectors of length } N\}$

Comment: Each vector in V is formed by sub-vectors found from Step 1

2b) append non-isomorphic vectors X to F to get strength t OAs $[F|X]$,

2c) compute and store only their distinct canonical graphs/ arrays, [Section 2.2]

2d) get back non-isomorphic orthogonal arrays into a list Lf, return Lf.

$\diamond$ STEP 3: Repeating step.

`If` # current columns $< d$ Call PRUNING-USES-SYMMETRY(f, d) for each $f \in Lf$
`Else` Return Lf `EndIf`

---

5 Summary and conclusion

New 3-balanced fractions obtained by using the combined approach

Some new and very difficult-to-construct arrays that previous well-known methods failed to compute, found by our approach, are listed in Table 3. In the table we have used multiplicity notation for automorphism group orders. The (IS) construction means a combination of integer linear formulation and employing symmetries of automorphism groups of OAs, all were introduced in part 2.1, and fully developed in Section 3 and 4 above.

N	Type; Strength t	#	Size of the automorphism group Aut(F)	Methods
80	$5 \cdot 4 \cdot 2^5$; $t = 3$	≥ 1		(IS), colored graph
80	$5 \cdot 4 \cdot 2^6$; $t = 3$	≥ 5	$2^2, 4^3$	(IS), colored graph
96	$6 \cdot 4^2 \cdot 2^5$; $t = 3$	≥ 1199	1^{411}, 2^{370}, 4^{250}, 8^{137}, 12, 16^{29}, 48	,,
96	$6 \cdot 4^2 \cdot 2^6$; $t = 3$	≥ 8	2^2, 4^2, 8^4	,,

Table 3: Hard-to-construct strength 3 and 4 OAs of sizes $N \leq 100$.

In [14], only one OA($80; 5 \cdot 4 \cdot 2^6; 3$) and one OA($96; 6 \cdot 4^2 \cdot 2^5; 3$) were found, however. For the most interesting one with size at most 100, OA($96; 6 \cdot 4^2 \cdot 2^6; 3$), we currently obtain at least 8 non-isomorphic OAs, and theirs distinct automorphism group sizes are 2,4 and 8.

Conclusion and potential future work

We have discussed mathematical and computational aspects of factor enlarging problem of mixed OAs with strength at least 2, provided a fix number of experiments. Our approach combining permutation groups and integer linear formulation provides a generic framework for enumerating mixed OAs of any strength with all feasible factor levels and with run sizes satisfying the Rao bound. The dual of the problem, namely fixing the factors and the strength, and try to find better lower bounds of the run sizes also is very interesting and challenging. Some techniques from Bose-Mesner or Terwilliger algebras, see Schrijver (2004) [20], and other approaches as semidefinite programming [see Laurent (2004) [11] and Vandenberghe-Boyd (1999) [25]] could be promising leads to go.

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Appendix A: Permutation group

Given a set X, a permutation of 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 of X. We denote Sym_N instead of $\mathrm{Sym}(\{1, 2, \ldots, N\})$, for a natural number N. We 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 say a group K acts on a set X if we have a group homomorphism $\phi : K \to \mathrm{Sym}(X)$. We abbreviate $x^{\phi(g)}$ by x^g. Let $p \in \mathrm{Sym}_N$. The action of p on a subset $B \subseteq \{1, 2, \ldots, N\}$ is given by $B^p := \{x^p : x \in B\}$. The action of p on a list of length N is given by

$$[y_1, y_2, \ldots, y_N]^p := [y_{1^{p^{-1}}}, y_{2^{p^{-1}}}, \ldots, y_{N^{p^{-1}}}].$$

In other words, we compute the ith position of Y^p by $Y^p[i] = y_{i^{p^{-1}}} = Y[i^{p^{-1}}]$.

Appendix B: Investigate the full group of a specific OA

To clarify the concepts involved, we compute of the automorphism group in G. A. P. Note that such computations can usually be carried out more efficiently with the techniques of Section 2.2. When applying permutations to a particular fraction F, we find it convenient to apply the level permutations first, then permute the columns in each sections independently, and finally permute the rows. Consider the design F with $N = 4$ runs and design type $T = 2^4$, giving the underlying set U:

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

$$\begin{aligned} U = \{\ & (1,1,1),(1,1,2),(1,2,1),(1,2,2),(1,3,1),(1,3,2),(1,4,1),(1,4,2), \\ & (2,1,1),(2,1,2),(2,2,1),(2,2,2),(2,3,1),(2,3,2),(2,4,1),(2,4,2), \\ & (3,1,1),(3,1,2),(3,2,1),(3,2,2),(3,3,1),(3,3,2),(3,4,1),(3,4,2), \\ & (4,1,1),(4,1,2),(4,2,1),(4,2,2),(4,3,1),(4,3,2),(4,4,1),(4,4,2)\ \}. \end{aligned}$$

Note that the 32 elements of this set have been placed in lexicographic order. We use this order to identify the triples with the integers 1 to 32.

We have $R = \mathrm{Sym}_4$, $C = \mathrm{Sym}_4$, $L = (\mathrm{Sym}_2)^4$. Using the `Action` command in G.A.P [8], we can find the homomorphic images in Sym_{32}:

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

Here $|T| = 32$ and G is a permutation group of order 9216 with a generating set consisting of the union of the generators of $\phi_R(R), \phi_C(C), \phi_L(L)$. Now

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

which we identify with $\{1,3,5,7,9,12,13,16,17,19,22,24,25,28,30,31\}$. So $\mathrm{Aut}(F)$ can now be computed as a stabilizer. It has order 24 and generators

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

Possibly convert these back to a product of level, column and row permutations, e.g., the last generator decomposes into the level permutations $(1,1,(1,2),(1,2))$, the column permutation $(2,3,4)$ and the row permutation $(1,2,3)$. The number of OAs isomorphic to F is $|G|/|\mathrm{Aut}(F)| = 9216/24 = 384$, by the Orbit Theorem.

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