ENUMERATION OF STRENGTH 3 MIXED ORTHOGONAL ARRAYS

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ABSTRACT. We introduce methods for enumerating mixed orthogonal arrays of strength 3. We determine almost all mixed orthogonal arrays of strength 3 with run size up to 100.

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1. Introduction

S:introductionpaper

This paper is devoted to constructing all strength 3 orthogonal array (OAs) with a given parameter set and run size. The remainder of Section S:introductionpaper 1 is a review of notation. In Section SS:enuimeratentro 2, we define isomorphisms orthogonal array, so that only a single representative of each isomorphism class needs to be found. By encoding orthogonal arrays as colored graphs, we can define canonical orthogonal arrays in Section SS:usingcanonicalgraphs 3. This allows us to compute representatives of isomorphism classes efficiently using the nauty program McKayWebpage [10]. We can enumerate all canonical orthogonal arrays using backtrack search in the GAP computer algebra system ??. In Section SS:solveILP 5, we use integer linear programming methods combined with canonical orthogonal arrays to list isomorphism classes of extensions of a strength 3 OA. Another method for enumerating strength 3 OAs that have two distinct levels by backtrack search is discussed in Section SS:lexleastfrac ??. In the last section, we determine almost all (mixed???) orthogonal arrays of strength 3 and run size up to 100.

1.1. **Fractional factorial designs.** Fix d finite sets $Q_1, Q_2, \dots, Q_d$, called *factors*. The *(full) factorial design* with respect to these d factors is the cartesian product $D = Q_1 \times \dots \times Q_d$. A *fraction* F of D is a subset consisting of elements of D (possibly with multiplicity). We take $r_i := |Q_i|$ to be the number of *levels* of the ith factor. For our purposes, the factor sets have no internal structure, so we can always take $Q_i = \mathbb{Z}_{r_i} = \{0, 1, \dots, r_i - 1\}$. We say that F is *symmetric* if $r_1 = r_2 = \cdots = r_d$; otherwise, we say F is *mixed*.

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

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

the *design type* of F. We divide $\{1, \dots, d\}$ into *sections* $J_1, \dots, J_m$ corresponding to the distinct level sizes. So the kth section

$$J_k = \{a_1 + \cdots + a_{k-1} + 1, \dots, a_1 + \cdots + a_k\}$$

consists of all j such that R_j has s_k levels. To avoid confusion, we always use the index k to indicate the section and the index j to indicate the column.

For example

$$\begin{aligned} F = \{ & (0,0,0,0), (0,1,0,1), (0,0,1,1), (0,1,1,0), (1,0,0,0), (1,1,0,1), \\ & (1,0,1,1), (1,1,1,0), (2,1,1,1), (2,0,1,0), (2,1,0,0), (2,0,0,1), \\ & (3,1,0,0), (3,1,0,1), (3,1,1,0), (3,1,1,1) \} \end{aligned}$$

is a $4 \cdot 2^3$ mixed fractional design. We usually consider a fractional design as a matrix whose rows correspond to the elements of the multiset, in any order, and whose columns correspond to the factors. So the example above becomes

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

where T denotes transpose. We also refer to the rows of F as *runs*, so the number of rows is the *run size*.

A *subfraction* of F is obtained by choosing a subset of the factors (columns), and removing all other factors. A fraction is called *trivial* if it is a multiple of a full design, ie, it contains every possible row with the same multiplicity. Let t be a natural number. A fraction F is called *t-balanced* if, for each choice of t factors, the corresponding subfraction is trivial. In other words, every possible combination of coordinate values from a set of t factors occurs equally often.

Note that a fraction with strength t also has strength s for $1 \leq s \leq t$. The example above has strength 3 but not strength 4. A t-balanced fraction F is also called an *orthogonal array of strength t*.

We denote the set of all fractions with N runs and design type T by $\mathrm{OA}(N;T)$. The subset of orthogonal arrays of strength t is denoted $\mathrm{OA}(N;T;t)$. In keeping with the usual convetions, we write

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

to indicate that F is an *element* of $\mathrm{OA}(N; s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}; t)$.

We say that a triple of column vectors X, Y, Z are *orthogonal* if each possible value (x, y, z) appears in $[X|Y|Z]$ with the same frequency. So an array has strength three if, and only if, every triple of columns in the array is orthogonal.

1.2. **Permutations.** 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 write Sym_N instead of $\mathrm{Sym}(\{1, 2, \ldots, N\})$, for a natural number N. We usually write elements of Sym_N in *cycle notation*, so the permutation $p = (1, 2, 3)(4, 5)$ is defined by $1^p = 2,\ 2^p = 3,\ 3^p = 1,\ 4^p = 5,\ 5^p = 4$.

We 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

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

SS:enuimeratentro

2. Isomorphisms of orthogonal arrays

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.

Let N be a positive integer and let T be a design type. We define the *underlying set* of $\mathrm{OA}(N;T)$ to be

$$U := \{(i, j, x) \mid i = 1, \ldots, N, \quad j = 1, \ldots, d, \quad x \in Q_j\}.$$

In other words, U consists of all possible triples of a row i, a column j, and an entry F_{ij} for a matrix $F \in \mathrm{OA}(N;T)$. We can now encode F by its *lookup table*

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

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

E:PNd

$$\#\{x \mid (i, j, x) \in S\} = 1 \qquad \text{for all } i = 1, \ldots, N \text{ and } j = 1, \ldots, d. \tag{2.1}$$

We now define three group actions on the underlying 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.

The full group G of fraction transformations of U is defined as

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

E:PNd Using () we can prove that, for every $F \in \mathrm{OA}(N;T)$ and $g \in G$, there exists a unique $F' \in \mathrm{OA}(N;T)$ with $t(F') = t(F)^g$. So G acts faithfully on $\mathrm{OA}(N;T)$ via

$$F^g = F^{\pi(g)} := t^{-1}\left(t(F)^g\right).$$

Let F and F' be in $\mathrm{OA}(N;T)$. An *isomorphism* from F to F' is $g \in G$ such that $F^g = F'$. The *automorphism group* of an orthogonal array $F \in \mathrm{OA}(N;T)$ is the normalizer of F in the group G, ie,

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

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

The following result describes the structure of the full group G.

P:commutative laws **Proposition 1.**

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

So we can now identify G with $R \times (C \ltimes L)$ where $C \ltimes L = \prod_{k=1}^{m} \mathrm{Sym}_{s_k} \wr C_k$.

C:structureG **Corollary 2.** $|G| = N!\, a_1! \cdots a_m!\, (s_1!)^{a_1} \cdots (s_m!)^{a_m}$.

2.1. **A GAP computation.** We now give an example of the computation of an automorphism group in GAP, in order to clarify the concepts involved. Note that such computations can usually be carried out more efficiently with the techniques of Section 3 SS:usingcanonicalgraphs. 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

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

with $N = 4$ runs and design type $T = 2^4$. The underlying set is

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

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 GAP, we can find the homomorphic images in Sym_{32}:

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

[THIS IS WRONG!!!!]

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 setwise stabiliser. It has order 24 and generators

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

We can convert these back to a product of level column and row permutations. For example, 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 orthogonal arrays isomorphic to F is

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

by the Orbit Theorem [? AlperinBellBook].

3. Orthogonal arrays and colored graphs

SS:usingcanonicalgraphs

It is well known that all combinatiorial 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* [10 MckayWebpage] 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 cononical representative of an isomphism class of arrays.

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

- V is a finite set;

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

We call the elements of V *vertices*, the elements of E *edges*, and the elements of C *colors*. An isomorphism $G \to G' = (V', E', \gamma')$ is a one-to-one and onto map $s : V \to V'$ 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, $\gamma'(s(v)) = \gamma'(s(w))$.

We write $V(x)$ for the neighbors of a vertex $x \in V$.

Let F be an orthogonal array with runsize N and design type T. A colored graph $G_F = (V, E, \gamma)$ 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.
- The edge set contains edges $\{\rho_i, \sigma_{jv}\}$ and $\{\gamma_j, \sigma_{jv}\}$ 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.

Note that G is a tripartite graph with respect to the partition of V into row, column and level vertices. We have

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

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

A:labeling

$$f := \Big[[1, \ldots, N], [N+1, \ldots, N+n_S], [N+n_S+1, \ldots, N+n_S+a_1], \ldots, [N+n_S+1+\sum_{i=1}^{m-1} a_i, \ldots, |V|] \Big] \tag{3.1}$$

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

Example 1. Let D be the OA$(4; 2^3; 2)$

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

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

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

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

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

Example 2. Let D be the OA$(6; 3^1 \cdot 2^2; 1)$

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

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

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

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

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

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

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

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

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

L:basicfact1 **Lemma 3.** Φ *is an injection.*

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

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

L:propertiescoloredgraph **Lemma 4.** *Let D be an orthogonal array with factors Q_i and with run size N. Then*

(1) *G_D is tripartite with the vertex partition (R, S, C) given by* E:ver (??) *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.*

D:coloredaxiom **Definition 5.**

(i) *Given parameters U, N, the colored graphs which satisfy properties* $(1) - (5)$ *of Lemma* L:propertiescoloredgraph *4 are called the* colored graphs *of type U, N. They form a subset of $\mathcal{G}$, written $\mathcal{G}_{U,N}$.*

(ii) *By Lemma 4(1), vertices of R, S, C in a graph in $\mathcal{G}_{U,N}$ are called the* row-vertices*, the* symbol-vertices *and the* column-vertices *respectively.*

What we want to do now is, firstly, to find the column-vertex set C of g. It may happen that some vertices have the same valency even if they belong to distinct colors (row and column colors, for instance). This can usually be solved by computing the intersection of their neighbor sets. More precisely,

L:columnver **Lemma 6.** *Suppose that $\frac{N}{s_k} \in \mathbb{N}$ for all $k \in \{1, \ldots, m\}$, in which case $\frac{N}{s_k} > 1$ for at least one number k. Then, a subset C of the vertex set V of a graph g in $\mathcal{G}_{U,N}$ is the column-vertex set if and only if the valencies of vertices in C are $\{s_1, s_2, \ldots, s_m\}$ and their neighbor sets are mutually disjoint subsets of V.*

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

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

E:exspec0 **Example 3.** The example below is a strength 1 array $F := \mathrm{OA}(4; 4^4; 1)$

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

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

P:bijection **Proposition 7** (Constructing an array from a colored graph)**.** *Given parameters $U = s_1^{a_1} \cdot s_2^{a_2} \cdots s_m^{a_m}$ and run size N, such that $\frac{N}{s_k} \in \mathbb{N}$ for all $k \in \{1, \ldots, m\}$, and such that there is at least one k for which $\frac{N}{s_k} > 1$, we have*

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

Proof. We pick a colored graph $g \in \mathcal{G}_{U,N}$. Then g fulfills properties (1) – (5) of Lemma 4. We construct an array $F_g \in \mathcal{F}_{U,N}$ such that $\Phi(F_g) = g$. The process of constructing F_g starts from column-vertices, then locates symbol-vertices, and finally determines row-vertices.

Suppose that $g = (V, E)$. We collect vertices in V that have valencies s_1, s_2, $\ldots$, s_m such that their neighbors are mutually disjoint subsets of V. From Lemma 6, these vertices are uniquely determined and they form column vertices of g. Let C be the set of these column-vertices. For each $c \in C$, we track its neighbors by property 3 of Lemma 4. That is, if $c \in C_k$ for some $k = 1, \ldots, m$, then c is adjacent with vertices $V(c) := \{v_1, \ldots, v_{s_k}\}$; where $v_i \in V \setminus (C \cup R)$ since g is tripartite and satisfies properties (3) and (5) of Lemma 4. So v_i are symbol-vertices.

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

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

On the other hand, by Definition D:coloredaxiom 5(i), it is clear that $\Phi(\mathcal{F}_{U,N}) \subseteq \mathcal{G}_{U,N}$. Hence, $\Phi(\mathcal{F}_{U,N}) = \mathcal{G}_{U,N}$. □

C:bijection **Corollary 8.** *Provided that $\frac{N}{s_k} \in \mathbb{Z}^{\times}$ for all $k \in \{1, \dots, m\}$, and that there is at least a number $\frac{N}{s_k} > 1$, with Lemma L:basicfact1 3, we have the mapping Φ is a bijection between the set $\mathcal{F}_{U,N}$ of orthogonal arrays of type U, N and the set $\mathcal{G}_{U,N}$ of colored graphs of type U, N.*

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

L:bijection1 **Lemma 9.** *Let G_F, G_D be the two colored graphs which are formed by two orthogonal arrays $F, D \in \mathcal{F} = \mathcal{F}_{U,N}$. Then F and D are isomorphic arrays if and only if G_F and G_D are isomorphic graphs.*

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

The 'only if' part can be seen as follows. If G_F and G_D are isomorphic graphs, we can find a permutation q on vertices (of G_F) such that $G_D = G_F^q$. Now since $G_F, G_D \in \mathcal{G}_{U,N}$, the graphs G_F, G_D satisfy all the conditions in Lemma L:propertiescoloredgraph 4. So they are tripartite and q is a color-preserving permutation. This permutation therefore can be factored as a product of three permutations q_R, q_S, q_C which act on row, symbol and column vertices of G_F independently. Since the numbering of vertices in G_F and G_D are the same, the triple q_R, q_S, q_C induce row, symbol and column permutations q_r, q_s, q_c acting on F. The composed map $q_r\, q_s\, q_c$ takes F to D. □

E:ex3 **Example 4.** We construct an $\mathrm{OA}(6; 3 \cdot 2^2; 1)$ from the colored graph described by Figure F:cg6 1. Here $m = 2, d = 3, s_1 = 3, s_2 = 2$, the column vertex set $C = \{14, 15, 16\}$ since their neighbor sets $\{7, 8, 9\}, \{10, 12\}$, and $\{11, 13\}$ are mutually disjoint. Vertices $1, 2, \dots 6$, for instance, also have valency 3, but they cannot represent the first column-vertex (3-level column) since their neighbors are not disjoint. Now the first column-vertex is 14, its neighbor $V(14) = \{7, 8, 9\}$ (represent levels 0,1,2 in column 1) lead us to row-vertices 1,2; 3,5 and 4,6 respectively. The symbol vertices are $[[7, 8, 9], [10, 12], [11, 13]]$; those correspond to levels 0,1,2 in column 1, levels 0,1 in column 2 and levels 0,1 in column 3 of F. The array

Table 1. A counterexample in constructing OA from colored graph

cnt-ex

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

obtained is

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

E:exspec **Example 5** (counterexample, cf. Example E:exspec0 3). We wish to construct an OA$(4; 4^4; 1)$ from the colored graph with adjacencies as in Table cnt-ex 1. Notice that $\frac{N}{s_1} = 4/4 = 1$, so we cannot distinguish between column-vertices and row-vertices. In other words, there are two candidate sets for column-vertices, $\{21, 22, 23, 24\}$ and $\{1, 2, 3, 4\}$. If we choose the first candidate to be column vertex set, then the latter will be row vertex set, and vice versa. Hence, the partition (R, S, C) is not determined uniquely by the colored graph. If we take $\{21, 22, 23, 24\}$ as the column-vertices, and take the partition

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

then the result obtained is the array in Example E:exspec0 3.

3.1. **Finding the canonical graph.** . For any colored graph G, denote by canon(G) the *canonical labeling graph* computed using *nauty*. It consists of a vertex

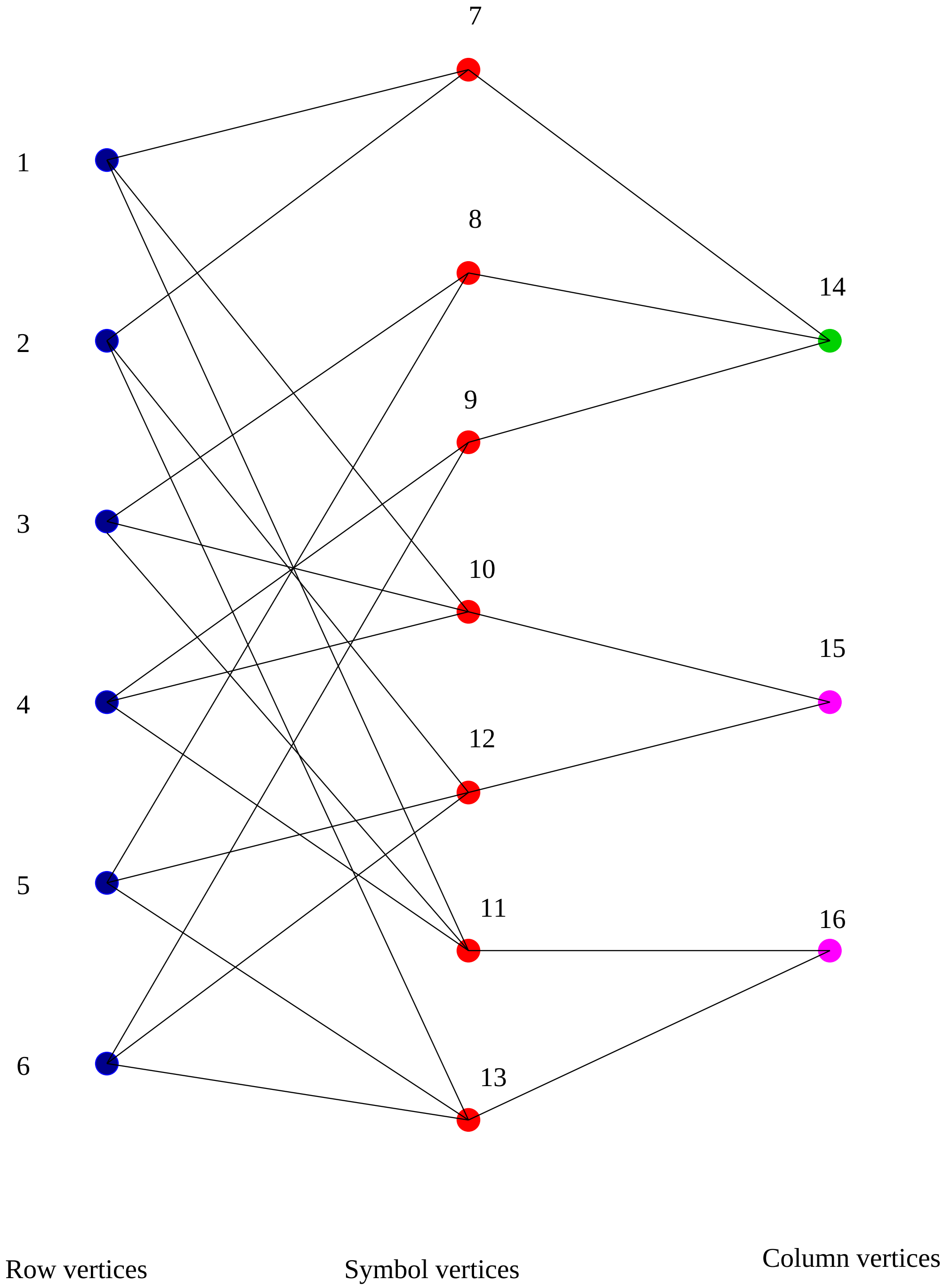

FIGURE 1. The colored graph of a 6 runs OA F:cg6

relabeling permutation, p, say and new adjacencies. Hence, canon(G) is determined fully by these adjacencies.

The vertex-relabeling p is of the form

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

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

Let $G_F := \Phi(F)$ and $G_D := \Phi(D)$ be the colored graphs of arrays F and D respectively. As a result of Lemma L:bijection1 9, we have

C:testingisoarray **Corollary 10.** *F and D are isomorphic arrays* $\iff$ canon(G_F) = canon(G_D).

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

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

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

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

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

Example 6. Let D be an OA$(16; 4^1 \cdot 2^2; 2)$.

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

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

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

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

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

The relabeling permutation is

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

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

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

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

Table 2. Adjacency relations of a colored graph

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

4. Backtrack search for arrays with two level sizes

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

Definition 11 (Column lexicographically-least orthogonal arrays)**.**

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

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

artial-full-colored-leaf

Definition 12.

(1) *For $1 \le i \le N$, $1 \le j \le d$, denote by F_{ij} the subset of entries of a putative fraction F consisting of $j-1$ columns completely made, and column j built only to row i. We call it a partial fraction up to the jth column and up to the ith row. For convenience, let $F_{0,0}$ be the empty fraction.*

(2) *A full-partial fraction, denoted F_j, of a putative fraction F, is a partial fraction $F_{N,j}$. So the first j columns have been built, for $j = 1, 2, \ldots, d$.*

(3) *In a partial fraction F_{ij}, a hth row $F_{ij}[h, -] = (p_1, p_2, \ldots, p_j)$, for $h = 1, \ldots, i$, is called a partial row, where $1 \le p_l \le r_l$ for $l = 1, \ldots, j$.*

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

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

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

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

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

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

R:first-t-layers **Remark 1.** *Up to the first t columns, T has only one leaf for each layer.*

E:constructalllex **Example 7.** Find $F = \mathrm{OA}(16; 4^1 \cdot 2^3; 3)$. In the first four layers, including the root, of the tree T, there is only one leaf. Let us build F step by step.
Layer 0: $F_{0,0} = []$.
Layers 1,2,3: Columns 1,2,3 are made trivially.
Layer 4: A (4,2,2)-triple occurs once, and a (2,2,2)-triple occurs twice, so there is only one possibility for building the leaf $F_{16,4}$ in this layer. This gives a unique solution for this design, given by (E:F16a 4.1).

E:F16a

$$F = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \end{bmatrix}^T \tag{4.1}$$

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

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

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

D:howto-compute-nij **Definition 13.** *Let $n_{i,j} \geq 1$ be the number of symbols that can be plugged into position $F[i, j]$, and let $X_{i,j} = \{x_1, x_2, \ldots, x_{n_{i,j}}\}$ be the set of these symbols, for $1 \leq i \leq N$, $1 \leq j \leq d$. At the first jth layer of the tree T such that there exist a row-index i and $n_{i,j} \geq 2$, we create a stack*

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

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

Branches(T) is declared globally to store branching leaves during depth-first search. The general strategy is: if we find a branching point, then we add branching leaves to the stack, and follow one of these ramifying leaves. Then either new branching points are found and their branching leaves are updated into Branches(T); or rows can be formed without extending Branches(T) until the whole column has been built. More clearly, during branching at layer j on each leaf $J := [(i, x_l); j]$, if we detect another row-index i_2 such that $n_{i_2,j} \geq 2$, then we replace J in Branches(T) by $n_{i_2,j}$ new branching leaves of the form $[(i, x_l), (i_2, y_k); j]$ where

$y_k \in X_{i_2,j} \ldots$ Whenever a leaf F_j in layer j is fully colored, we call that leaf *inspected*. Then we delete the corresponding branching leaf in Branches(T) (not in tree T), and start forming column $j+1$ from F_j. Hence Branches(T) can consist of branching leaves on distinct layers.

At the first t layers (see Remark R:first-t-layers 1) where branching happens at row i, we initialize

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

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

P:sol_for_findingLLF

Proposition 14. *For $j = t+1, \ldots, d$, a* fully colored leaf *$F_{N,j}$ in the layer j is lex-least in its isomorphic class, if we follow the two following operations during constructing $F[-,j]$:*

(1) For any pair of adjacent partial rows, u and v, say, of $F_{N,j}$, where the jth column $F[-,j]$ has not been formed yet from row v, we choose $v[j] \in \{v[j-1], \ldots, r_j\}$ if $u[k] = v[k]$ for all $1 \leq k \leq j-1$, otherwise we choose $v[j] \in \{1, \ldots, r_j\}$.

(2) When column $F[-,j]$ is formed completely, ie, $F_{N,j}$ is made, we permute this column with each of the previous columns (with the same number of levels) and sort rows of the resulting fraction. If the sorted fraction is lexicographically less than $F_{N,j}$ then we discard $F_{N,j}$, (subtree from that leaf has no descendant on layer d); otherwise we accept $F_{N,j}$, go to Step 3.

(3) Applying each level permutations to nonbinary columns of $F_{N,j}$ and compare with the full-partial orthogonal arrays found so far. If the result equals one of them, we disrecard $F_{N,j}$; otherwise accept it as an orthogonal array being lexicographically least up to column j.

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

If employ these operations, we have

Corollary 15.

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

Proof. Using Proposition P:sol_for_findingLLF 14 with $j = d$ tells us that Assertion 1. is correct. Now suppose that there are two distinct fully-colored leaves at layer d in T, say F, K, which are isomorphic, and $F < K$. It implies that there is a non-trivial permutation p such that $K^p = F$. By Assertion 1., $K < K^p$, so $F < K^p$, contradiction. Assertion 2. follows. □

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

Backtrack algorithm extends a column

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

Output: A fully-colored leaf F_j in layer j.

[2] Extend-columnF_{j-1}, Branches(T)) Compute $n_{i,j}$, # symbols which can be plugged into $F[i,j]$, Definition D:howto-compute-nij 13 $\exists\imath : n_{i,j} \geq 2$ detect feasible branching points split the leaf F_{j-1} into $n_{i,j}$ branches where the newly-formed leaves are different only at entry $F[i,j]$ add to Branches(T) leaves $J = [(i,x_l);j]$ in which $x_l \in X_{i,j}$ form a unique leaf $F[i,j]$ at layer j depth-first form column j build up (rows of) each of leaves in layer j from the row $i+1$ update Branches(T) during the process $i = N$, a fully-colored leaf F_j in the layer j has been made Return F_j see Definition D:define-partial-full-colored-leaf 12(2) Using this procedure we extend the tree T from a fully-colored leaf, until the number of columns j meets d. We record that solution, go back to the nearest branching point of that solution (ie, its parent), and try its next sibling. These tasks are described in the following algorithm LEX-LEAST-FRACTIONs. Backtrack algorithm computes all non-isomorphic orthogonal arrays

Input: Design type U, run size N, and strength t.

Output: All non-isomorphic orthogonal arrays $\mathrm{NF}(F) \in \mathcal{F}$.

[2] Lex-Least-Fractions$U$, N, t Initialize a rooted tree T having $t+1$ layers, each layer has only one leaf Let F_t denote the leaf at layer $(t+1)$ it has t columns Let $j := t+1$; Branches$(T) := []$ (global variable); $K := F_t$; Branches$(T) \neq [\,]$ or $j < d$ Compute $K :=$ EXTEND-COLUMN(K, Branches(T)) K is at distance d to root of T record K as a solution on T; Return all leaves at layer d of the tree T. Note that this algorithm could be generalized to more than two section orthogonal arrays. However, our C code Brouwer03 [5] presently deals with two section orthogonal arrays only.

SS:solveILP

5. Use of integer linear programming and symmetry

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

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

O:transformrules

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

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

Example 8. Let $F = \mathrm{OA}(16; 4 \cdot 2^2; 3) = [S_1|S_2|S_3]$:

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

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

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

Remark 2. Although the constancy of frequencies is a necessary and sufficient condition (by definition) for the existence of X, we observe that the linear constraints P found using rules of Observation 1 forms a set of necessary conditions.

For instance, appending a blocking factor X (see Definition 57, page 96 in [2]) with 4 levels to an array $\mathrm{OA}(16; 4 \cdot 2^3; 3)$ means constructing an $\mathrm{OA}(16; 4 \cdot 2^3 \cdot 4; 2)$. We have $s = 4$, X is orthogonal to S_1 if and only if each pair $(a, x) \in [S_1, X]$ occurs once ($\frac{16}{4 \cdot 4} = 1$). This implies that $x_1 + x_2 + x_3 + x_4 = 1 \cdot (0 + 1 + 2 + 3) = 6$, $x_i \in \{0, 1, 2, 3\}$. Of the two possibilities $[0, 1, 2, 3]$ and $[0, 3, 0, 3]$ only the first is valid, the second is discarded since the frequencies of 0 and 3 are 2 in $\mathrm{OA}(16; 4 \cdot 4; 2)$, which is prohibited.

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

$$AX = b,$$

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

E:originalX (5.1) $$X = (x_1, \ldots, x_N) \in \{0, 1, \ldots, s-1\}^N \subseteq \mathbb{N}^N$$

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

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

E:reducedmatform
$$M\,X = c, \tag{5.2}$$

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

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

(1) build the system (5.2) [E:reducedmatform] using Observation 1 [O:transformrules];
(2) find all solution vectors $X = (x_1, \ldots, x_N)$ in $\{0, 1, 2, \ldots, s-1\}^N$;
(3) collect non-isomorphic, canonical orthogonal arrays of the set of all arrays $[F|X]$ into a set L; if L is empty, conclude F has no extension; otherwise go back to Step 1 for each array in L until the number of factors meets the number of columns required.

The first step is already done. The method to solve the last step was given in Subsection 3 [SS:usingcanonicalgraphs]. What we need to find in Step 2, in fact, are the non-isomorphic vectors X (under row-index permutations) in the whole solution set. We show how to find them in the next sections. We then discuss how to combine the automorphism group $\mathrm{Aut}(F)$ of F in finding non-isomorphic vectors X. Notice that, when extending OAs, the group size tends to grow proportionally with the number of solutions.

5.3. **Another backtrack approach.** . The system P described by (5.2) [E:reducedmatform] can be solved over $\mathbb{N}_{\geq 0}$ by depth-first branching at the variables x_i $(i = 2, \ldots, N)$. If P has no solution, then F is not extendable; we try another array having the same parameters as F but not isomorphic to F. We identify P with its polynomials, ie, $P = \{f_1, f_2, \ldots, f_m\}$, in which the f_i are linear polynomials in the indeterminates $x_2, \ldots, x_N$. In particular, when the x_is are binary, we can use the following fact.

L:modulo2
Lemma 16 (Finding binary solutions of an integral polynomial)**.** *Let f be an arbitrary polynomial in P, and put the polynomial $p = f \bmod 2$. Denote by V_f, V_p the sets of indeterminates occurring in f and p, respectively. Put $C = V_f \setminus V_p$, $n_f = |V_f|$, $n_p = |V_p|$, $n_C = |C|$. We denote the set of solutions of the equation $f = 0$ by S_f, and the set of solutions of the equation $p = 0$ mod 2 by S_p. Let S_p^i be the solution set of the equation $p = i$ for $i = 0, \ldots, n_p$. Then $S_f \subseteq S_p$, and S_p is a disjoint union of $\frac{n_p}{2}$ sets S_p^i, for odd (even) integers $i = 0, \ldots, n_p$ if the constant coefficient of f is odd (even). Moreover, the maximum number of solutions of $f = 0$ is $2^{n_f - 1}$.*

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

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

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

Lemma 17. *For $g \in \mathrm{Aut}(F)$, g induces $g_1 \in G_D$ and generates the image D^{g_1} which is isomorphic to D.*

Proof. We have

ideauserowperm
$$D^{g_1} = [F|X]^{g_1} = [F^g|X^{g_R}] = [F|X^{g_R}] \tag{5.3}$$

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

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

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

The first step is to localize the formation of a vector X of the form (E:originalX 5.1) by taking the derived designs of strength $t - 1$. We get the r_1 derived designs $F_1, \ldots, F_{r_1}$, each of which is an $\mathrm{OA}(r_1^{-1}N; r_2 \cdots r_d; t-1)$. Clearly, if a solution vector X exists, then it is formed by r_1 sub-vectors u_i of length $\frac{N}{r_1}$:

E:list-form-vector-X
$$X = [u_1; u_2; \ldots; u_{r_1}], \text{ where } u_i = \left(x_{\frac{(i-1)N}{r_1}+1}, \ldots, x_{\frac{iN}{r_1}}\right). \tag{5.4}$$

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

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

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

Define the stabilizer in G of F_i by

izers-of-derived-designs
$$\begin{aligned} N_G(F_i) &:= \mathrm{Normalizer}\big(G, \mathrm{RowInd}(F_i)\big) \\ &= \big\{h \in G : \mathrm{RowInd}(F_i)^h = \mathrm{RowInd}(F_i)\big\}. \end{aligned} \tag{5.5}$$

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

$$L(F_i) := \text{Centralizer}\big(N_G(F_i), J(F_i)\big), \tag{5.6}$$

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

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

$$F_{i_1,\dots,i_m} = \text{OA}\left(\frac{N}{r_1 r_2 \cdots r_m}; r_{m+1} \cdots r_d; t-m\right) \tag{5.7}$$

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

$$\text{RowInd}(F_{i_1,\dots,i_m}) := \bigcap_{j=1}^{m} \big\{l \in \{1, 2, \dots, N\} : F[l, j] = i_j\big\}. \tag{5.8}$$

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

$$N_G(F_{i_1,\dots,i_m}) := \text{Normalizer}\big(G, \text{RowInd}(F_{i_1,\dots,i_m})\big),$$
$$L(F_{i_1,\dots,i_m}) := \text{Centralizer}\big(N_G(F_{i_1,\dots,i_m}), J(F_i)\big), \text{ for } 1 \leq i_j \leq r_j.$$

Definition 18. *$L(F_{i_1,\dots,i_m})$ is called the subgroup associated with the derived design $F_{i_1,\dots,i_m}$, for $1 \leq i_j \leq r_j$, $j = 1, 2, \dots m$. 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.

5.7. **Using the subgroups $L_{i_1,\dots,i_m}$.** . Recall that $\text{Z}(P)$ is the set of all solutions X. From (5.3), the vector X^g can be pruned from $\text{Z}(P)$, for any solution X and any permutation $g \in \text{Aut}(F)$. This follows from the fact that D^g is an isomorphic array of $D = [F|X]$. For a fixed m-tuple of symbols $i_1, \dots, i_m$, let $V_{i_1,\dots,i_m}$ be the set of solutions of $F_{i_1,\dots,i_m}$ (being an $\text{OA}((r_1 r_2 \cdots r_m)^{-1} N; r_{m+1} \cdots r_d; t-m)$) for $1 \leq m \leq t-1$. For any sub-vector $u \in V_{i_1,\dots,i_m}$, from (5.8) and (5.4), let

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

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

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

Proposition 19. *For any pair of sub-vectors $u, v \in V_{i_1,\dots,i_m}$, if $v \ = \ u^{g_R}$ for some $g_R \in L_{i_1,\dots,i_m}$, we have $\text{Z}(u) = \text{Z}(v)$.*

We prove this proposition in the next two lemmas. In Lemma 20, without loss of generality, it suffices to give the proof for the first strength 2 derived array. The induction step will be presented in Lemma 22.

L:strength2deriveddesign **Lemma 20** (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*

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

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 $\boldsymbol{u}^* := [u_2; \dots; u_{r_1}] \in \mathrm{Z}_X(u_1)$, then $X = [u_1; u_2; \dots; u_{r_1}]$ is in $\mathrm{Z}(P)$. We view $h \in \mathrm{Aut}(F)$, so

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

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

Corollary 21. *We can wipe out all solutions $Y = [v_1; v_2; \dots; v_{r_1}] \in \mathrm{Z}(P)$ if $v_1 \in u_1^{L_1}$, the L_1- orbit of u_1 in V_1. In other words, if $V_1 \neq \emptyset$, then it suffices to find the first sub-vector of vector X by selecting $|V_1|/|L_1|$ representatives u_1 from the L_1-orbits in V_1.*

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

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

Next, if $t \geq 3$ we extend the proof of Proposition 19 for $2 \leq m \leq t - 1$.

L:derm1 **Lemma 22** (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 20, 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

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

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

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

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

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

E:row-index-set-derived-design D:subgroups-associated-derived-des

From (5.8) and Definition 18, we know $L(f_j) := \text{Centralizer}\big(N_G(f_j), J(f_j)\big)$ consists of row permutations acting locally on

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

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

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

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

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

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 $\text{Z}_X(u_{1,1}) = \text{Z}_Y(v_{1,1})$. In fact, we only need to have $\text{Z}_X(u_{1,1}) \subseteq \text{Z}_Y(v_{1,1})$. Let any sub-vector

$$\boldsymbol{u}^* := \big[\; [u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \big] \in \text{Z}_X(u_{1,1}),$$

and $h \in L(f_1)$. Then we have $X = [u_1; u_2; \ldots; u_{r_1}] \in \text{Z}(P)$, and

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

Hence, $Y = \big[\, [v_{1,1}; u_{1,2}; \ldots; u_{1,r_2}]; u_2; \ldots; u_{r_1} \,\big]$ is a solution vector and $\boldsymbol{u}^* \in \text{Z}_Y(v_{1,1})$. 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, $j = 1, \ldots, r_2$. □

E:strength-t-minus-m-derived-design

5.8. **Operations on derived designs.** . Recall from (5.7) that the symbols $i_1, \ldots, i_m$ (where $1 \le i_j \le r_j$) indicate the derived design having symbol i_j in column j, for $j = 1, \ldots, m$. Let

E:definesigmagroup

$$\sigma := G \times \tau \tag{5.9}$$

be the *direct product* of G and τ, where $\tau := \text{Sym}(s)$ is the group acting on the symbols of column X.

We consider each derived design as an agent that receives data from its lower strength derived designs, make some appropriate operations, then pass the result to its parent design. Notice that strength 1 and strength t designs require special operations. Recall from Definition 18 that $L_{i_1,\ldots,i_m}$ are the subgroups associated with the derived designs $F_{i_1,\ldots,i_m}$ having strength $t-m$. When $m = t-1$, we write $L_{i_1,\ldots,i_{t-1}}$ for the subgroup associated with the strength 1 derived design $F_{i_1,\ldots,i_{t-1}}$.

D:subgroups-associated-derived-des

ted with derived designs

The agents of derived designs can be described as follows.

(1) At 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 $F_{i_1,\dots,i_{t-1}}$.

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

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

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

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

(3) At the (global) design F:

Input: the sub-vectors from strength $t-1$ derived designs;

Operation: find the representatives of σ-orbits in the Cartesian product $V = V_1 \times V_2 \times \ldots \times V_{r_1}$, where V_i had been already pruned by the subgroup L_i ($i = 1, 2, \dots, m$);

Output: solution vectors X which are non-isomorphic up to $\sigma = G \times \tau$, defined in (E:definesigmagroup 5.9).

We propose the following three-step procedure: [0] 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

◇ 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 $V_{i_1,\dots,i_{m-1}}$.
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 $u_i \in V_i$.

◇ Step 2: *Pruning at strength t design F*. 2a) Select the representative vectors X from the σ-orbits of V, V consists of vectors of length N, being formed by sub-vectors found from Step 1

2b) append vectors X to F to get strength t orthogonal arrays $[F|X]$, 2c) compute and store their canonical arrays into a list Lf, return Lf.

◇ Step 3: *Repeating step.* # current columns $<$ d Call PRUNING-USES-SYMMETRY(f, d) for each $f \in Lf$ Return Lf

E:multstep1 **Example 9.** Let $U := \big[[3,1],[2,3]\big]$, $F = \mathrm{OA}(24; 3.2^3; 3)$,

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

$\mathrm{Aut}(F)$ has order 12288. Compute $G = \mathrm{Row}(\mathrm{Aut}(F))$, and update it by $G = \mathrm{Stabilizer}(G, [1])$, which is a permutation group of size 768. The three strength 2 derived designs give 8, 8, and 16 candidates respectively, so we have to check $8.8.16 = |V| = 1024$ possibilities.

The row permutation subgroups of the three strength 2 derived designs are

$L_0 = [(), (7,8), (5,6), (5,6)(7,8), (3,4), (3,4)(7,8), (3,4)(5,6), (3,4)(5,6)(7,8)]$,

$L_1 = [()]$, and

$L_2 = [(), (23,24), (21,22), (21,22)(23,24), (19,20), (19,20)(23,24),$
$(19,20)(21,22), (19,20)(21,22)(23,24), (17,18), (17,18)(23,24), (17,18)(21,22),$
$(17,18)(21,22)(23,24), (17,18)(19,20), (17,18)(19,20)(23,24),$
$(17,18)(19,20)(21,22), (17,18)(19,20)(21,22)(23,24)]$

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.

Observe that $\mathrm{Aut}(F)$ decomposes the rows of F into row-orbits $O_1, \ldots, O_l$. If $\mathrm{Aut}(F)$ acts intransitively on the rows of F, then $l > 1$. For each of the orbits O_j, let $\mathrm{RowInd}(O_j) \subseteq \{1, \ldots, N\}$ be the row indices of O_j in F. We can define the normalizers and the centralizers of O_j as in (5.5) and in (5.6). But the subgroups found in this way help reducing isomorphic vectors only when the group G has very large size. This is not the case when arrays have many columns.

5.9. **A mixed approach using linear algebra and symmetries.** Recall that the extension of an orthogonal array F with run size N to a new array $[F|X]$ is reduced to solving a linear system P having matrix form (5.2):

$$M.X = c.$$

Recall that $G = \mathrm{Row}(\mathrm{Aut}(F))$ is the group of all row permutations induced by the automorphism group $\mathrm{Aut}(F)$, and that $\mathrm{Z}(P)$ is the set of solutions of (5.2) over the set $\{0, 1, \ldots, s-1\}$ as a subset of $\mathbb{N}$. Denote by $\mathbb{Q}^N$ the vector space of dimension N over the rationals. For any solution X, we view $X \in S$, where S is the solution set of (5.2) over $\mathbb{Q}$. The set S in fact is an affine space in $\mathbb{Q}^N$; and $\mathrm{Z}(P) = S \cap \{0, 1, \ldots, s-1\}^N$. Moreover, $\mathrm{Z}(P)$ is a subset of $\bigcap_{g \in G} S^g$. Indeed, since $\mathrm{Z}(P)^g = \mathrm{Z}(P)$ for all $g \in G$, we have $\mathrm{Z}(P) \subseteq S^g$, for all $g \in G$. We call the intersection $\bigcap_{g \in G} S^g$ the *G-invariant core* of $\mathrm{Z}(P)$, (by definition it is the maximal G-invariant subset of S). The G-invariant core $\bigcap_{g \in G} S^g$ of $\mathrm{Z}(P)$ is still an affine space since the image S^g of S is an affine space, and intersecting two affine spaces results in again an affine space. The idea is that even though S has large dimension, it is likely that the G-invariant core of $\mathrm{Z}(P)$ could have smaller dimension.

Example 10. Consider extending array $\mathrm{OA}(72; 6 \cdot 3 \cdot 2^2; 3)$ to $\mathrm{OA}(72; 6 \cdot 3 \cdot 2^3; 3)$. The solution space has dimension 36, using G we can reduce it to dimension 20.

5.10. **Computing the G-invariant core of the solution set $\mathrm{Z}(P)$.** . First we compute the intersection of two affine spaces. We identify S with the pair $[v, B]$, where v is a specific vector in S and B is a basis of S (over $\mathbb{Q}$). Let $n := N - \mathrm{rank}(M)$ be the dimension of S, then $|B| = n$, and

E:formrationalsolutionsS (5.10)
$$S = v + \langle B \rangle = v + \sum_{i=1..n} b_i B_i, \text{ where indeterminates } b_i \in \mathbb{Q}.$$

Observation 2. Let $p \in G$, the affine image S^p can be determined by the vector v^p and the basis $B^p := \{u^p : u \in B\}$. In other words,

:formrationalsolutionsSp (5.11)
$$S^p = v^p + \langle B^p \rangle = v^p + \sum_{i=1..n} c_i B_i^p, \text{ where } c_i \in \mathbb{Q}.$$

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

$$v^p - v = \sum_{i=1..n} b_i B_i - \sum_{i=1..n} c_i B_i^p = \big[B_1|B_2|\dots|B_n| - B_1^p| - B_2^p|\dots| - B_n^p\big][b_1, \dots, b_n, c_1, \dots, c_n]^t$$

has solution $b_1, \dots, b_n, c_1, \dots, c_n$.

Hence, if $S \cap S^p \neq \emptyset$, its basis and specific vector can be found by substituting $b_1, \dots, b_n$ back into (5.10), (or $c_1, \dots, c_n$ into (5.11)). We prune the integral solution set Z(P) by computing its G-invariant core. Let H be a set of generators of G. We compute $\bigcap_{g\in G} S^g$ using the following procedure. Computing G-invariant core

A:find-invariantcore

Input: the affine solution space S of (5.2), and the generators H;
Output: the affine space $\bigcap_{g\in G} S^g$.

[2] Find-G-invariant-core S, H Set $Y := S$; $W := Y$; update $Y := \bigcap_{g\in H} Y^g \cap Y$; $Y = W$; return Y.

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

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

:formrationalsolutionsSZ

$$X^T = (0, x_2, x_3, \dots, x_N)^T = u + \sum_{i=1..n} y_i C[i], \tag{5.12}$$

where pivotal variables $y_i \in \mathbb{Z}$. Hence, solving P in terms of indeterminates $(x_j) \in \{0, 1, \dots, s-1\}^N$ $(j = 1, \dots, N)$ is reduced to finding all integral (pivotal) tuples $(y_i) \in \mathbb{Z}^n$ $(i = 1, \dots, n)$ such that each coordinate x_j is in $\{0, 1, \dots, s-1\}$.

Although very often $n < N$, this approach is useful if a few more inequalities would be found and used to delete out some (not all) isomorphic vectors in each isomorphic class retaining the non-isomorphic vectors. From that point, the search for non-isomorphic vectors becomes feasible.

5.11. **Imposing extra constraints on the system.** . For each generator p of G such that at least one of its cycles has even length, we extract those *even length cycles* into a set K. We do not use odd length cycles of p. Then, for each $h \in K$, we form an extra inequality whose left hand side is the sum of X's coordinates with odd indices, and the right hand side is the sum of X's coordinates with even indices of the cycles in h. In more details, we have

:LinearAlgebra-and-group

Lemma 23. *If $K \neq []$, for each $h \in K$ having the form*

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

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

E:extra-inequalities

$$x_{i_1} + x_{j_1} + x_{j_3} + \dots \leq x_{i_2} + x_{j_2} + x_{j_4} + \dots \tag{5.13}$$

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

Proof. Suppose $h = \prod_i (i_1, i_2) \quad \prod_j (j_1, j_2, j_3, j_4) \ldots \in K$, 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 (5.13). □

For example, let $h = (1,2)(7,8,9,10)(13,16)$ be a permutation in K, $(h^{-1} = (1,2)(7,10,9,8)(13,16))$, we can impose the following inequality

$$x_1 + x_7 + x_9 + x_{13} \leq x_2 + x_8 + x_{10} + x_{16}$$

on the original system P. Indeed, suppose that $Z = [z_1, z_2, z_3, \ldots, z_{16}]$ is a solution, and

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

The image

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

satisfies the constraint (5.13), since (*) means

$$x_2 + x_8 + x_{10} + x_{16} \geq x_1 + x_9 + x_7 + x_{13}.$$

5.12. **Finding pivotal variables y_i such that $X \in \{0, 1, \ldots, s-1\}^N$.** . Having obtained Formula (5.12) of X, and found extra inequalities (using Lemma 23), we now find integral (pivotal) tuples $(y_i) \in \mathbb{Z}^n$ by a recursive procedure. Let $ExtraS$ be the set of these extra inequalities, and let Y be the set of coordinates of X in terms of $(y_i)_{i=1,\ldots,n}$. We split Y into 3 subsets:

$$\begin{aligned} &Y_1 := \{\text{ monomials}\}, \\ (5.14) \quad &Y_2 := \{\text{ monomials with constant, and be grouped with respect to } y_i\}, \\ &Y_3 := \{\text{ polynomials with at least two indeterminates } y_i\}. \end{aligned}$$

For $t = 3$ we cut vector X into $r_1 r_2$ sub-vectors

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

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

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

We use $ExtraS$ and L_X as *certificates* to prune vector solutions during the search. That is, whenever we find a sub-vector (or partial vector) by using Y, we substitute it into $ExtraS$ to check whether $ExtraS \leq 0$ (ie, each polynomial p in $ExtraS$ must be less than or equal 0), and to L_X to see whether all of its components have strength 1. Note that components in L_X are still considered valid when they depend on variables y_i; the same reasoning is applied for non-positiveness of polynomials in $ExtraS$. If all conditions are all right, we enlarge the sub-vector (in all feasible possibilities) until the length of vectors equals to n. Then the column vector X is found back by (5.12). A combination of depth-first and breath-first schemes to find all solutions $(y_i) \in \mathbb{Z}^n$ is presented in the following algorithm.

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

Input: Y; $ExtraS$ and L_X
Output: All vectors $(y_i)_{i=1,\dots,n} \in \mathbb{Z}^n$

[2] Compute-pivotals Y, $ExtraS$, L_X split $Y = Y_1 \cup Y_2 \cup Y_3$ by (5.14), form all partial vectors by making the hypercube from variables of Y_1, prune them using $ExtraS \le 0$, and L_X; substitute each valid partial vector back to Y, $Y_1 = \emptyset$; only keep intermediate valid nodes in the search tree; $\diamond$ Since $Y = Y_2 \cup Y_3$, extend the valid partial vectors made above by all possible vectors of Y_2 collect the full vector solutions whose lengths equal n $\diamond$ always certificate newly extended nodes using $ExtraS$ and L_X return the representatives in the $\sigma := G \times \tau$-orbits (5.9) of $Z(P)$.

Example 11. Extending $F = \mathrm{OA}(16; 2^3; 3)$ to $[F\ X] = \mathrm{OA}(16; 2^3 \cdot 4; 3)$. Here $N = 16$, the group of row permutations G has size 768, generated by the following permutations:

$$\big[(15,16),(13,14),(11,12),(9,10),(7,8),(5,6),(3,4),(3,6)(4,5)$$
$$(9,10)(11,14)(12,13),(3,10,5,4,9,6)(7,11,14)(8,12,13)\big],$$

from which we find 169 extra inequalities . After reducing the affine solution space by these symmetries, we get an 8-dimensional G-core S, and the solution vector $X \in \{0,1,2,3\}^{16}$ in terms of $(y_i) \in \mathbb{Z}^8$ $(n = 8)$ is

$$\begin{aligned} X = (x_j) =&(0, y_1+6, y_2+6, -y_1-y_2-6, y_3, -y_1-y_3, y_4, y_1-y_4+6,\\ &y_5, -y_1-y_5, y_6+6, y_1-y_6, y_7+6, y_1-y_7, y_8, -y_1-y_8) \end{aligned}$$

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

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

into $Y_1 = \{y_3, y_4, y_5, y_8\}$; $\quad Y_2 = \big\{[y_1+6],[y_6+6, y_2+6],[y_7+6]\big\}$; and

$$Y_3 = \{-y_1-y_8, -y_1-y_5, -y_1-y_3, -y_1-y_2-6, y_1-y_7, y_1-y_6, y_1-y_4+6\}.$$

We form all partial solutions from Y_1, pruning at each those sub-vectors (having length 4) by using 169 inequalities of $ExtraS$, and by employing the fact that each of the four vectors $(0, y_1+6, y_2+6, -y_1-y_2-6)$, $(y_3, -y_1-y_3, y_4, y_1-y_4+6)$, $(y_5, -y_1-y_5, y_6+6, y_1-y_6)$, and $(y_7+6, y_1-y_7, y_8, -y_1-y_8)$ has strength 1. At each iteration, when ever $Y_1 = \emptyset$, we generate all valid partial solutions from Y_2, concatenate them with partial solutions of y_3, y_4, y_5, y_8, and prune again. This results in 35 vectors; of these only one vector forms an $\mathrm{OA}(16; 2^3 \cdot 4; 3)$.

6. A collection of strength 3 orthogonal arrays

6.1. **Introduction.** This section is organized as follows. Subsection 6.2 recalls known results and presents parameters of strength 3 orthogonal arrays (OAs) with $8 \le N \le 100$. Subsection 6.3 presents the construction of OAs with $72 \le N \le 100$. Finally, we use the methods of Section ?? to obtain a table of many isomorphism classes of OAs with run size at most 100 in Subsection 6.4. For convenience, we abbreviate methods used for constructing and enumerating orthogonal arrays. The abbreviations are listed in Table 3. It is also convenience to use abbreviations for specific lower bounds and for particular nonexistence proofs. These too are listed in Table 3.

Notation	Name	Reference
(A)	Arithmetic	ManNguyen-Memphis-paper [3]
(B)	Backtrack search for $s_1^a s_2^b$ OAs	SS:lexleastfrac ??
(C)	Colored graphs	SS:usingcanonicalgraphs 3
(Con)	Concatenation	ManNguyen-Memphis-paper [3]
(La)	Latin squares	ManNguyen-Memphis-paper [3]
(H)	Hadamard construction	ManNguyen-Memphis-paper [3]
(I)	Integer linear programming (ILP)	SS:solveILP 5
(IS)	ILP with symmetry	SS:solveILP 5
(J) and (L)	Juxtaposition and Linear code	ManNguyen-Memphis-paper [3]
(M) and (O)	Multiplication and Even sum	
(O'), (Br)		BrouwerWebpage [6]
(Q)	Quasi-multiplication	ManNguyen-Memphis-paper [3]
(S) and (T)	Split and Trivial design	
(X), (X_6)		Brouwer04 [4]
(X_3), (X_4), (X_5)	explicit constructions	,,
(X_1), (X_7), (***)	mixed additive codes	
(3^5)		Hedayat97 [8]
(Rao)	the *generalized Rao bound*	Rao [11]
(Del)	the *Delsarte bound*	Delsarte [7]
(Div)	the divisibility condition	
(5.1)	$\nexists$ OA$(24; 3 \cdot 2^5; 3)$, Sec. 5.1	Brouwer04 [4]
(5.9)	$\nexists$ OA$(64; 4^5 \cdot 2^3; 3)$, Sec. 5.9	,,
(5.10)	$\nexists$ OA$(64; 4^3 \cdot 2^9; 3)$, Sec. 5.10	,,

tab-5 TABLE 3. An overview of constructions, lower bounds on run sizes

SS:parametersOAs

6.2. **Parameter sets of OAs with run size $8 \le N \le 100$.** The *divisibility condition* for the run size of an orthogonal array F gives a necessary condition for the existence of F in terms of its parameters.

L:Divisibilitycondition

Lemma 24. *In an* OA$(N; r_1 \cdot r_2 \cdots r_d; t)$*, the run size N must be divisible by the least common multiple* (lcm) *of all numbers $\prod_{i \in I} r_i$ where $|I| = t$.*

Proof. This says that the t times derived design has an integral run size. □

For example, in an OA$(N; 3^5 \cdot 2; 3)$, N must be a multiple of 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 Brouwer04 [4], we constructed all orthogonal arrays of strength 3 with run sizes N at most 64. We extend that to the cases $72 \le N \le 100$ in this paper.

L:allparameters

Lemma 25. *The following are the only nontrivial parameter sets for mixed orthogonal arrays of strength 3 and run size at most 100 allowed by* (Div), (Rao), and (Del).

$\mathrm{OA}(4m; 2^a; 3)$	$4 \le a \le 2m$, m even, $2 \le m \le 24$,
$\mathrm{OA}(4m; m \cdot 2^3; 3)$	m even, $2 \le m \le 24$,
$\mathrm{OA}(8m; m \cdot 2^a; 3)$	$3 \le a \le 7$, $3 \le m \le 12$,
$\mathrm{OA}(8m; m \cdot 4 \cdot 2^a; 3)$	$2 \le a \le 4$, m even, $4 \le m \le 12$,
$\mathrm{OA}(9m; m \cdot 3^b; 3)$	$3 \le b \le 4$, $m = 3, 6, 9$,
$\mathrm{OA}(36; 3^2 \cdot 2^a; 3)$	$1 \le a \le 2$,
$\mathrm{OA}(48; 3 \cdot 2^a; 3)$	$3 \le a \le 15$,
$\mathrm{OA}(48; 4 \cdot 3 \cdot 2^a; 3)$	$2 \le a \le 9$,
$\mathrm{OA}(48; 4 \cdot 2^a; 3)$	$3 \le a \le 11$,
$\mathrm{OA}(54; 3^b \cdot 2^a; 3)$	$a = 0, 1$, $b \ge 1$, $a + b \ge 4$, $a + 2b \le 19$,
$\mathrm{OA}(60; 5 \cdot 3 \cdot 2^a; 3)$	$a = 2$,
$\mathrm{OA}(64; 4^c \cdot 2^a; 3)$	$a \ge 0$, $c \ge 1$, $a + c \ge 4$, $a + 3c \le 18$,
$\mathrm{OA}(72; 6^2 \cdot 2^a; 3)$	$1 \le a \le 6$,
$\mathrm{OA}(72; 6 \cdot 3^b \cdot 2^a; 3)$	$0 \le b \le 1$, $1 \le a \le 11$,
$\mathrm{OA}(72; 4 \cdot 3^2 \cdot 2^a; 3)$	$a = 1$,
$\mathrm{OA}(72; 3^b \cdot 2^a; 3)$	$1 \le b \le 2$, $1 \le a \le 23$,
$\mathrm{OA}(80; 5 \cdot 4^b \cdot 2^a; 3)$	$0 \le b \le 1$, $1 \le a \le 15$,
$\mathrm{OA}(80; 4 \cdot 2^a; 3)$	$2 \le a \le 19$,
$\mathrm{OA}(81; 9 \cdot 3^b; 3)$	$b \le 4$,
$\mathrm{OA}(81; 3^b; 3)$	$3 \le b \le 14$,
$\mathrm{OA}(84; 7 \cdot 3 \cdot 2^a; 3)$	$a \le 2$,
$\mathrm{OA}(90; 5 \cdot 3^2 \cdot 2^a; 3)$	$a = 1$,
$\mathrm{OA}(96; 8 \cdot 6^b \cdot 2^a; 3)$	$0 \le b \le 1$ $a + b \ge 3$, $a \le 11$,
$\mathrm{OA}(96; 8 \cdot 3^b \cdot 2^a; 3)$	$0 \le b \le 1$ $a + b \ge 3$, $a \le 11$,
$\mathrm{OA}(96; 6 \cdot 4^b \cdot 2^a; 3)$	$1 \le b \le 2$, $a + b \ge 3$, $3b + a \le 15$,
$\mathrm{OA}(96; 4^c \cdot 3^b \cdot 2^a; 3)$	$0 \le b \le 1$, $0 \le c \le 2$, $a + b + c \ge 4$, $3(c-1) + 2b + a \le 23$,
$\mathrm{OA}(100; 5^2 \cdot 2^a; 3)$	$1 \le a \le 2$.

Proof. The cases with N at most 64 were given in [4] (Brouwer04). The first five cases depending on parameters m were also determined there. We consider now cases with $72 \le N \le 100$.

(i) Applying (Rao) to $\mathrm{OA}(12, 6 \cdot 2^a; 2)$ of $\mathrm{OA}(72; 6^2 \cdot 2^a; 3)$ gives $1 \le a \le 6$.
$\mathrm{OA}(72; 6 \cdot 3^b \cdot 2^a; 3)$ with $0 \le b \le 1$, $1 \le a \le 11$: When $b = 1$, we use the derived designs $\mathrm{OA}(12, 3 \cdot 2^a; 2)$, and find $a \le 9$. When $b = 0$, we use the derived designs $\mathrm{OA}(12, 2^a; 2)$, which leads to $a \le 11$.
Applying (Div) to $\mathrm{OA}(18, 3^2 \cdot 2^a; 2)$ of $\mathrm{OA}(72; 4 \cdot 3^2 \cdot 2^a; 3)$ we find $a = 1$.
$\mathrm{OA}(72; 3^b \cdot 2^a; 3)$ with $1 \le b \le 2$: Applying (Rao) to $\mathrm{OA}(24, 3^{b-1} \cdot 2^a; 2)$s, we have $24 \ge 1 + 2(b-1) + a$. In other words:

$$1 \le b \le 2, \quad a + b \ge 4 \text{ (to avoid trivial designs) and } a + 2b \le 25.$$

Hence $3 \le a \le 23$ for $b = 1$, and $2 \le a \le 21$ for $b = 2$. If $b = 2$ then $a \le 20$ by (Del) [9, Section 9.2] (Hedayat99).

(ii) $\mathrm{OA}(80; 5 \cdot 4^b \cdot 2^a; 3)$ with $a \ge 8$: Applying (Rao) to the derived designs $\mathrm{OA}(16; 4^b \cdot 2^a; 2)$ of $\mathrm{OA}(80; 5 \cdot 4^b \cdot 2^a; 3)$, the parameters must satisfy:

$$0 \le b \le 1, \quad a + b \ge 3 \text{ and } 3b + a \le 15.$$

If $b = 0$, $a \le 15$; and if $b = 1$ then $a \le 12$.

(iii) $\mathrm{OA}(81; 9\cdot 3^b; 3)$: $b \le 4$ by applying (Rao) to $\mathrm{OA}(9, 3^b; 2)$.
$\mathrm{OA}(81; 3^b; 3)$: the derived designs $\mathrm{OA}(27; 3^{b-1}; 2)$ must satisfy that $27 \ge 1+2(b-1)$, ie, $b \le 14$.

(iv) $\mathrm{OA}(84; 7\cdot 3\cdot 2^a; 3)$: we have $a \le 2$ by applying (Div).

(v) $\mathrm{OA}(90; 5\cdot 3^2\cdot 2^a; 3)$: we have $a \le 1$ by applying (Div).

(vi) $\mathrm{OA}(96; 8\cdot 6^b\cdot 2^a; 3)$ with $0 \le b \le 1$ $a+b \ge 3$, $a \le 11$: applying (Rao) to $\mathrm{OA}(12; 6^b\cdot 2^a; 2)$, we get $a+b \ge 2$, $12 \ge 1+5b+a$, or $a+5b \le 11$. If $b=0$, $a \le 11$, and if $b=1$, $a \le 6$.
$\mathrm{OA}(96; 8\cdot 3^b\cdot 2^a; 3)$ with $0 \le b \le 1$ $a+b \ge 3$, $a \le 11$. Indeed, the derived designs $\mathrm{OA}(12; 3^b\cdot 2^a; 2)$ shows that $a \le 11$ if $b=0$; and $a \le 4$ if $b=1$.
$\mathrm{OA}(96; 6\cdot 4^b\cdot 2^a; 3)$ and $b > 0$. Use (Rao) for $\mathrm{OA}(16; 4^b\cdot 2^a; 2)$ to see that the parameters must satisfy

$$1 \le b \le 2, \quad a+b \ge 3, \text{ and } 3b+a \le 15.$$

When $b=2$, $a \le 9$; and when $b=1$, $a \le 12$.
$\mathrm{OA}(96; 4^c\cdot 3^b\cdot 2^a; 3)$ with $b+c > 0$. When $c > 0$, use Rao for $\mathrm{OA}(16; 4^{c-1}\cdot 3^b\cdot 2^a; 2)$; when $c=0$, use Rao for $\mathrm{OA}(32; 3^{b-1}\cdot 2^a; 2)$. The parameters must satisfy

$$0 \le b \le 1, \quad 0 \le c \le 2, \quad a+b+c \ge 4, \text{ and } \quad 3(c-1)+2b+a \le 23.$$

That is, when $c=2$, if $b=1$, $a \le 18$; if $b=0$, $a \le 20$. When $c=1$, if $b=1$, $a \le 21$; if $b=0$, $a \le 20$.

(vii) By (Div), $a < 3$ in $\mathrm{OA}(100; 5^2\cdot 2^a; 3)$. □

SS:construction_N>64

6.3. **Constructing OAs with run size** $72 \le N \le 100$**.** Since there is no OA of strength 3 with run size larger 64 and less than 72, we list parameters for OAs with $72 \le N \le 100$ in Table 4. In the fourth column of Table 4 we show the constructions for OAs with $72 \le N \le 100$ whose parameters were indicated in Lemma 25. We skip all cases found by Construction (M). When the gap between the total number of known columns with the upper bound is positive, we mention the next open cases. The question marks ? written in the last column of Table 4 indicate that we have not proved yet the nonexistence of OAs with corresponding values.

Basic constructions. We consider case by case with respect to the run sizes.

(i) $N = 72$: $\mathrm{OA}(72; 9\cdot 2^a; 3)$ with $2 \le a \le 6$: this has the form $\mathrm{OA}(8m; m\cdot 2^a; 3)$ where $3 \le a \le 7$, $3 \le m \le 12$. Since $m = 9$ is an odd number, using Construction (X) we get $a = 6$.
$\mathrm{OA}(72; 6^2\cdot 2^a; 3)$ exists for $a \le 2$ by (IS) and (O).
$\mathrm{OA}(72; 6\cdot 3\cdot 2^a; 3)$ exists for $a \le 4$ by (IS) and (O').
$\mathrm{OA}(72; 4\cdot 3^2\cdot 2^a; 3)$ exists for $a \le 1$ by (T), but not for $a = 2$ by Div.
$\mathrm{OA}(72; 3^2\cdot 2^a; 3)$: See a construction of the case $a = 12$, $b = 2$ at [6]. When $b = 1$, $a \le 20$; an $\mathrm{OA}(72; 3\cdot 2^a; 3)$ exists obviously. The open cases are $13 \le a \le 20$.

(ii) $N = 80$: $\mathrm{OA}(80; 5\cdot 4^b\cdot 2^a; 3)$ with $a \ge 1$: For $b = 1$, $a \le 12$, we get $a = 5$ by juxtaposing two arrays $\mathrm{OA}(40; 2\cdot 5\cdot 2^5; 3)$; and $a = 6$ by the arithmetic method in [3].

N	Levels	Existence	Construction	Upper bound	Nonexistence
72	$18 \cdot 2^a$	$a \leq 3$	(M)	3	
72	$9 \cdot 2^a$	$a \leq 6$	(IS)	7	$a = 7$, (X)
72	$6^2 \cdot 2^a$	$a \leq 2$	(IS)	3	$a = 3$, (O)
72	$6 \cdot 3 \cdot 2^a$	$a \leq 4$	(IS)	5	$a = 5$, (O')
72	$6 \cdot 2^a$	$a \leq 11$	(M)	11	
72	$4 \cdot 3^2 \cdot 2^a$	$a \leq 1$	(T)	13	$a = 2$, (Div)
72	$3^2 \cdot 2^a$	$a \leq 12$	(B) and (IS)	20	$a = 13$?
72	$3 \cdot 2^a$	$a \leq 12$	(B) and (IS)	23	$a = 13$?
80	$20 \cdot 2^a$	$a \leq 3$	(M)	3	
80	$10 \cdot 4 \cdot 2^a$	$a \leq 2$	(O)	4	$a = 3$, (O)
80	$10 \cdot 2^a$	$a \leq 7$	(M)	7	
80	$5 \cdot 4 \cdot 2^a$	$a \leq 6$	(A), (La), (IS)	8	$a = 7$?
80	$5 \cdot 2^a$	$a \leq 9$	(B)	15	$a = 10$?
80	$4 \cdot 2^a$	$a \leq 19$	(M)	19	
81	$9 \cdot 3^b$	$b \leq 4$	(***)	4	
81	3^b	$b \leq 10$	(L)	14	$b = 11$,
84	$7 \cdot 3 \cdot 2^a$	$a \leq 2$	(M)	4	$a = 3$, (Div)
88	$22 \cdot 2^a$	$a \leq 3$	(M)	3	
88	$11 \cdot 2^a$	$a \leq 6$	(IS)	7	$a = 7$, (X)
90	$5 \cdot 3^2 \cdot 2^a$	$a = 1$	(T)	6	$a = 2$, (Div)
96	$24 \cdot 2^a$	$a \leq 3$	(M)	3	
96	$12 \cdot 4 \cdot 2^a$	$a \leq 4$	(IS) and (L)	4	
96	$12 \cdot 2^a$	$a \leq 7$	(M)	7	
96	$8 \cdot 6 \cdot 2^a$	$a \leq 2$	(IS) or (O)	3	$a = 3$, (O)
96	$8 \cdot 3 \cdot 2^a$	$a \leq 4$	(IS) or (J)	5	$a = 5$, (O')
96	$8 \cdot 2^a$	$a \leq 11$	(M)	11	
96	$6 \cdot 4^2 \cdot 2^a$	$a \leq 6$	(La), (IS)	9	$a = 7$?
96	$6 \cdot 4 \cdot 2^a$	$a \leq 8$	(S)	12	$a = 9$?
96	$6 \cdot 2^a$	$a \leq 15$	(M)	15	
96	$4^2 \cdot 3 \cdot 2^a$	$a \leq 7$	(S)	18	$a = 8$?
96	$4^2 \cdot 2^a$	$a \leq 20$	(Q)	20	
96	$4 \cdot 3 \cdot 2^a$	$a \leq 9$	(S)	21	$a = 10$?
96	$3 \cdot 2^a$	$a \leq 16$	(J)	31	$a = 17$?
100	$5^2 \cdot 2^a$	$a \leq 2$	(T)	15	$a = 3$, (Div)

tab-7 TABLE 4. Parameters of $\mathrm{OA}(N; s_1^c \cdot s_2^b \cdot s_3^a; 3)$s with $72 \leq N \leq 100$

If we take the derived designs at the 4-factor, then $a \leq 8$ WuZhangWang [?]. For $b = 0$, $a \leq 15$, we obtain $a = 9$ by juxtaposing an array $\mathrm{OA}(32; 2^{16}; 3)$ and $\mathrm{OA}(48; 3 \cdot 2^9; 3)$. Hence, the open cases are $7 \leq a \leq 8$ for $b = 1$; and are $10 \leq a \leq 15$ for $b = 0$.

(iii) $N = 81$: $\mathrm{OA}(81; 9 \cdot 3^b; 3)$, $b \leq 4$: by (B) and (***).
$\mathrm{OA}(81; 3^b; 3)$: $3 \leq b \leq 10$: by (L); see Hedayat99 [9, Section 5.9] for nonexistence of $b = 11$.

(iv) $N = 88$: $\mathrm{OA}(88; 11 \cdot 2^a; 3)$ with $2 \leq a \leq 6$: $a = 6$ is obtained similarly as in the case $\mathrm{OA}(72; 9 \cdot 2^6; 3)$).

(v) $N = 96$: $\mathrm{OA}(96; 6 \cdot 4^b \cdot 2^a; 3)$: For $b = 2$, $a \leq 9$. We get $a = 3$ by juxtaposing an $\mathrm{OA}(32; 2 \cdot 4^2 \cdot 2^3; 3)$ and an $\mathrm{OA}(64; 4 \cdot 4^2 \cdot 2^8)$. Furthermore, an $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^4; 3)$ was constructed by Construction (Q) in ManNguyen-Memphis-paper [3].

We make an $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^5; 3)$ by (La). An $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^6; 3)$ is found by (IS). For $b = 1$, $a \leq 12$. We get $a = 8$ from splitting a 4-level factor in $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^6; 3)$. Hence, for $b = 2$, the open cases are $7 \leq a \leq 9$; and for $b = 1$, $a \leq 12$, the open case is $\mathrm{OA}(96; 6 \cdot 4 \cdot 2^9; 3)$.

$\mathrm{OA}(96; 4^c \cdot 3^b \cdot 2^a; 3)$:

The case $b = 0$. We use Construction (Q).

The case $b = 1$. For $c = 2$, we consider $\mathrm{OA}(96; 4^2 \cdot 3 \cdot 2^a; 3)$, a is bounded above by 13 WangWu [12]. We employ Construction (A) below for the case $a = 5$, and we split the 6-level factor in $\mathrm{OA}(96; 6 \cdot 4^2 \cdot 2^6; 3)$ to get $a = 7$. For $c = 1$, then $a \leq 20$ (by Del) in $\mathrm{OA}(96; 4 \cdot 3 \cdot 2^a; 3)$. Splitting the 6-level factor in $\mathrm{OA}(96; 6 \cdot 4 \cdot 2^8; 3)$ gives $\mathrm{OA}(96; 4 \cdot 3 \cdot 2^9; 3)$. For $c = 0$, then $a \leq 31$ in $\mathrm{OA}(96; 3 \cdot 2^a; 3)$. Juxtaposing three $\mathrm{OA}(32; 2^{16}; 3)$ gives $\mathrm{OA}(96; 3 \cdot 2^{16}; 3)$.

So the open cases are $\mathrm{OA}(96; 4^2 \cdot 3 \cdot 2^8; 3)$, $\mathrm{OA}(96; 4 \cdot 3 \cdot 2^{10}; 3)$, and $\mathrm{OA}(96; 3 \cdot 2^{17}; 3)$.

Enumerate-all-isoclasses

6.4. **Enumerating isomorphism classes.** Notice that the methods of ILP and automorphism groups in Section S:EnumerationMethods ?? now are implemented for extension of binary columns only. We have

Theorem 26. *The numbers of isomorphism classes of strength 3 orthogonal arrays with run size $8 \leq N \leq 100$ are as indicated in Table* tab-8 *5.*

In the table, we use multiplicity notation for automorphism group orders. We abbreviate n^1 to n, where n is a group size. In the third column of the table, number 0 indicates that there is no array. This conclusion is based on the Rao bound, the Delsarte bound, the divisibility condition (on the run size) or by explicit nonexistence proofs. In these cases, a particular name of lower bound or an explicit nonexistence proof is indicated. Open cases are indicated by '≥ 0', ie, we do not know whether an array exists or not with the parameters given in the first and second column. That means exhaustive computing (Constructions (B) and (IS)) fails to construct those arrays, or no proof of nonexistence has been found yet for the time being. For series having more than 5000 non-isomorphic arrays, we only list the number of arrays, not giving the automorphism group size. The actual OAs will be put at OA3webpage [1].

Table 5: Non-isomorphic OAs of strength 3 with $8 \leq N \leq 100$ tab-8

N	Type	#	Size of the automorphism group	Methods
8	2^4	1	192	(I)
16	$4 \cdot 2^3$	1	192	(I)
16	$4 \cdot 2^4$	0		(Rao)
24	$6 \cdot 2^3$	1	1728	(IS)
24	$6 \cdot 2^4$	0		(Rao)
24	$3 \cdot 2^3$	2	288^1, 12288^2	(IS)
24	$3 \cdot 2^4$	3	48, 384, 1152	(IS)
24	$3 \cdot 2^5$	0		(5.1)
27	3^4	1	1296	(IS)
27	3^5	0		(Rao)
32	$8 \cdot 2^3$	1	27648	(IS)
32	$4^2 \cdot 2^2$	2	128, 512	(IS)

continued on next page

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Table 5 (continued)

N	Type	#	Size of the automorphism groups	Methods
32	$4^2 \cdot 2^3$	2	128, 384	(IS)
32	$4^2 \cdot 2^4$	2	512, 1536	(IS)
32	$4^2 \cdot 2^5$	0		(Rao)
32	$4 \cdot 2^3$	3	1152, 24576, 12582912	(IS)
32	$4 \cdot 2^4$	7	$64, 96^2, 384, 1152, 1536, 4608$	(IS)
32	$4 \cdot 2^5$	7	$16, 32, 64, 128^2, 256, 512$	(IS)
32	$4 \cdot 2^6$	11	$24^2, 64^4, 128, 256^2, 768, 1536$	(IS)
32	$4 \cdot 2^7$	8	$84, 96^2, 128, 384, 768^2, 10752$	(IS)
32	$4 \cdot 2^8$	0		(Rao)
36	$3^2 \cdot 2^2$	3	576, 8192, 196608	(IS)
36	$3^2 \cdot 2^3$	0		(Div)
40	$10 \cdot 2^3$	1	691200	(IS)
40	$10 \cdot 2^4$	0		(Rao)
40	$5 \cdot 2^3$	9	$5760, 73728^4, 12582912^4$	(B)
40	$5 \cdot 2^4$	28	$32^4, 96^8, 192^4, 288^4, 2304^4, 4608^3, 23040$	(B)
40	$5 \cdot 2^5$	2	1^2	(IS)
40	$5 \cdot 2^6$	1	60	(IS)
40	$5 \cdot 2^7$	0		(X)
48	$12 \cdot 2^3$	1	24883200	(IS)
48	$12 \cdot 2^4$	0		(Rao)
48	$6 \cdot 4 \cdot 2^2$	3	128, 192, 2304	(IS)
48	$6 \cdot 4 \cdot 2^3$	0		(O)
48	$6 \cdot 2^3$	24	$34560^1, 294912^7, 25165824^{12}, 28991029248^3$	(B)
48	$6 \cdot 2^4$	122	$64^{24}, 96^4, 128^{12}, 288^{19}, 384^{36}, 1152^7, 3456^4, 9216^7, 13824^4, 23040^4, 138240$	(B)
48	$6 \cdot 2^5$	578	$8^{264}, 16^{66}, 24^{20}, 32^{117}, 48^{10}, 64^{45}, 128^{12}, 256^{24}, 384^4, 512^{12}, 4608^4$	(B)
48	$6 \cdot 2^6$	1879	$2^{120}, 4^{606}, 8^{192}, 12^{56}, 16^{177}, 24^{28}, 32^{354}, 48^{37}, 64^{126}, 72^{14}, 96^{20}, 128^{105}, 384^4, 512^{24}, 1536^{12}, 13824^4$	(B)
48	$6 \cdot 2^7$	1525	$2^{120}, 4^{120}, 6^{192}, 8^{150}, 12^{170}, 16^{174}, 24^{30}, 32^{240}, 64^{63}, 96^{10}, 128^{30}, 168^{21}, 192^{42}, 256^{21}, 288^{14}, 384^{82}, 768^{21}, 1536^{21}, 96768^4$	(B)
48	$6 \cdot 2^8$	0		(Rao)
48	$4 \cdot 3 \cdot 2^2$	5	1152, 8192, 98304, 1048576, 4194304	(IS)
48	$4 \cdot 3 \cdot 2^3$	35	$4^3, 8^7, 16^9, 24, 32^2, 48^4, 64, 96^3, 144, 192, 288, 384, 1152$	(IS)
48	$4 \cdot 3 \cdot 2^4$	19	$4^8, 8^{10}, 16$	(IS)
48	$4 \cdot 3 \cdot 2^5$	0		(O')
48	$4 \cdot 2^3$	6	$12582912, 764411904, 20639121408^2, 541653102231552$	(B)
48	$4 \cdot 2^4$	4	256, 384, 512, 3072	(B)
48	$4 \cdot 2^5$	29	$4^6, 8^4, 16^9, 32^4, 160^3, 768, 1536, 15360$	(B)
48	$4 \cdot 2^6$	130	$2^{40}, 4^{40}, 8^{18}, 16^{17}, 20^2, 24, 32^4, 40^2, 48, 80^2, 96, 160, 960$	(B)
48	$4 \cdot 2^7$	619	$2^{434}, 4^{119}, 6^2, 8^{33}, 12^9, 16^6, 24^5, 32^6, 96^4, 192$	(B)
48	$4 \cdot 2^8$	2356	$2^{1872}, 4^{390}, 8^{62}, 12^6, 16^3, 24^{14}, 32, 48^4, 64^3, 384$	(B)
72	$18 \cdot 2^3$	1	6320730931200	(IS)
72	$18 \cdot 2^4$	0		(Rao)
72	$9 \cdot 2^3$	534	$17418240, 61931520^{22}, 1509949440^{141}, 173946175488^{255}, 118747255799808^{115}$	(B)
72	$9 \cdot 2^4$	12857		,,
72	$9 \cdot 2^7$	0		(X)

continued on next page

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Table 5 (continued)

N	Type	#	Size of the automorphism groups	Methods
72	$6^2 \cdot 2^2$	2394	64^{930}, 96^{720}, 192^{320}, 384^{183}, 512^{231}, 41472^{10}	(B)
72	$6^2 \cdot 2^3$	0		(O)
72	$6 \cdot 3 \cdot 2^2$	9	98304, 589824, 2097152, 8388608, 16777216, 536870912, 805306368, 3221225472, 9663676416	
72	$6 \cdot 3 \cdot 2^3$	231	1^5, 2^{28}, 4^{47}, 6, 8^{68}, 12^2, 16^{47}, 24^2, 32^{14}, 48^9, 64^6, 96, 576	(IS)
72	$6 \cdot 3 \cdot 2^4$	289	1^{215}, 2^{33}, 3^3, 4^{22}, 8^9, 12^1, 16^4, 48^2	(IS)
72	$6 \cdot 3 \cdot 2^5$	0		(O')
72	$6 \cdot 2^3$	82	28991029248^4, 782757789696^{13}, 21134460321792^{21} 2567836929097728^{19}, 138663194171277312^{21}, $81879229526197539962884^4$	(B)
72	$6 \cdot 2^4$	156	256^{36}, 512^{72}, 3072^{32}, 4096^{12}, 110592^4	,,
72	$6 \cdot 2^5$	64296		,,
72	$6 \cdot 2^{12}$	0		(Rao)
72	$4 \cdot 3^2 \cdot 2$	17	8192, 49152, 65536, 196608, 524288^4, 4194304^4, 8388608, 9437184, 268435456, 402653184, 1610612736	(IS)
72	$4 \cdot 3^2 \cdot 2^2$	0		(Div)
72	$3^2 \cdot 2^2$	9	3693514644397228032, 657366253849018368, 21540577406124633882624, 36520347436056576, 19967499960663932928, 5135673858195456, 56358560858112, 427972821516288, 39582418599936	(B)
72	$3^2 \cdot 2^3$	465	3456, 4096, 8192^2, 16384^7, 24576^2, 32768^5, 49152, 65536^{11}, 98304,131072^2, 196608^{11}, 262144^{27}, 393216^3, 524288^{23},786432^5, 1048576^{23},1179648, 1572864^9, 2097152^{16} 2359296^3, 3145728^{23}, 4194304^{50},4718592^5, 6291456^8, 8388608^{20} 9437184^{10}, 12582912^2, 14155776, 16777216^5, 18874368^{13}, 25165824^3 28311552, 33554432^2, 37748736^8, 42467328, 50331648, 67108864^{24} 75497472^4, 84934656^2, 113246208, 134217728^{26}, 50994944^4, 169869312 226492416, 268435456^9, 301989888^3, 339738624^4, 402653184^9, 536870912 679477248^3, 805306368^8, 1073741824^{10}, 1358954496, 1610612736, 2038431744, 2147483648, 2293235712, 3057647616, 4076863488, 4586471424^2, 4831838208^2, 5435817984^2, 9663676416, 10871635968, 12230590464, 17179869184, 24461180928, 34359738368, 43486543872, 48922361856^3, 68719476736^2, 97844723712, 103079215104^2, 110075314176, 137438953472,146767085568, 206158430208^4, 293534171136^2, 990677827584, 1761205026816, 3710851743744, 7421703487488, 160489808068608, 213986410758144, 29249267520503808	(B)
72	$3^2 \cdot 2^{13}$	≥ 0		
72	$3 \cdot 2^3$	6	24, 48^4, 288	(B)

continued on next page

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Table 5 (continued)

N	Type	#	Size of the automorphism groups	Methods
72	$3 \cdot 2^4$	89	805306368, 1207959552, 2717908992, 6442450944, 10871635968, 16307453952, 19327352832, 21743271936^2, 24461180928, 32614907904^2, 48922361856^5, 65229815808, 73383542784, 86973087744, 110075314176, 220150628352^2, 440301256704^3, 521838526464, 880602513408^3, 1043677052928^2, 1981355655168, 2348273369088, 2641807540224^4, 3962711310336^3, 5283615080448^5, 7044820107264^2, 7421703487488^2, 7925422620672^3, 21134460321792, 35664401793024^2, 42268920643584^2, 71328803586048^2, 75144747810816, 106993205379072, 142657607172096^2, 213986410758144^4, 320979616137216, 427972821516288^2, 5777633090469888, 17332899271409664^4, 34665798542819328^5, 48693796581408768^2, 138663194171277312, 277326388342554624^2, 227442304239437611008, 1819538433915500888064, 5458615301746502664192	,,
72	$3 \cdot 2^{13}$	≥ 0		
80	$20 \cdot 2^3$	1	632073093120000	(IS)
80	$20 \cdot 2^4$	0		(Rao)
80	$10 \cdot 4 \cdot 2^2$	≥ 1	921600	
80	$10 \cdot 4 \cdot 2^3$	0		(O)
80	$10 \cdot 2^3$	6	174182400, 495452160, 9059696640, 695784701952, 237494511599616, 759982437118771200	(B)
80	$10 \cdot 2^5$	635	1^4, 2^{28}, 4^{97}, 8^{155}, 16^{122}, 24^6, 32^{88}, 48^{10}, 64^{31}, 96^{10}, 128^{17}, 144^4, 192^2, 256^7, 288^{16}, 384^2, 512^4, 576^7, 768^2, 1024^3, 1152^3, 2304^6, 4608^3, 9216^3, 18432^1, 36864^2, 73728^1, 1843200^1	(B)
80	$10 \cdot 2^6$	33071		,,
80	$10 \cdot 2^8$	0		(Rao)
80	$5 \cdot 4 \cdot 2^2$	25	49152, 196608, 1048576, 2097152^2, 4194304, 8388608^3, 16777216, 25165824, 134217728^2, 268435456^3, 536870912^2, 2147483648^2, 68719476736^2, 137438953472, 274877906944, 1099511627776	(IS)
80	$5 \cdot 4 \cdot 2^7$	≥ 0		
80	$5 \cdot 2^3$	50		(B)

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Table 5 (continued)

N	Type	#	Size of the automorphism groups	Methods
80	$5 \cdot 2^4$	2174	46080, 49152^{4}, 65536^{16}, 73728^{8}, 98304^{4}, 131072^{20}, 524288^{58}, 1048576^{85}, 1179648^{3} 2097152^{140}, 3145728^{26}, 4194304^{180}, 6291456^{53}, 8388608^{126}, 12582912^{8}, 16777216^{76}, 33554432^{50}, 37748736^{4}, 67108864^{77}, 134217728^{250}, 150994944^{8}, 268435456^{103}, 402653184^{20}, 536870912^{57}, 805306368^{144}, 1073741824^{160}, 1610612736^{32}, 2147483648^{56}, 2415919104^{14}, 3221225472^{20}, 4294967296^{16}, 12884901888^{8}, 34359738368^{39}, 38654705664^{4}, 68719476736^{66}, 103079215104^{20}, 137438953472^{16}, 206158430208^{69}, 274877906944^{4}, 412316860416^{68}, 618475290624^{7}, 1236950581248^{8}, 1649267441664^{4}, 4947802324992^{7}, 6597069766656^{4}, 19791209299968^{3}, 35184372088832^{4}, 105553116266496^{8}, 211106232532992^{4}, 316659348799488^{4}, 2533274790395904^{4}, 5066549580791808^{3}, 25332747903959040^{1}	,,
80	$5 \cdot 2^{10}$	≥ 0		
80	$4 \cdot 2^3$	17		(B)
80	$4 \cdot 2^4$	303	16777216, 25165824^{5}, 33554432, 50331648^{3}, 75497472^{6}, 100663296^{3}, 150994944^{3}, 201326592, 301989888^{19}, 603979776^{21}, 905969664^{4}, 1207959552^{6}, 1811939328^{35}, 2415919104^{2}, 3623878656^{61}, 7247757312^{8}, 10871635968^{20}, 14495514624^{5}, 21743271936^{15}, 43486543872^{31}, 86973087744^{25}, 130459631616, 173946175488^{10}, 260919263232^{9}, 347892350976, 521838526464^{4}, 695784701952, 1043677052928, 4174708211712	(B)
80	$4 \cdot 2^{20}$	0		(Rao)
81	$9 \cdot 3^3$	3	324, 864, 69984	(B), (L)
81	$9 \cdot 3^4$	2	324, 3888	(B)
81	$9 \cdot 3^5$	0		(Rao)
81	3^4	32	31104, 49152, 196608^{2}, 786432, 1048576^{2}, 1572864, 3145728, 4718592, 6291456^{2}, 8388608, 25165824^{2}, 28311552, 37748736^{2}, 100663296, 301989888^{2}, 603979776, 1207959552, 1358954496, 1811939328, 5435817984, 8153726976, 86973087744, 3522410053632, 285315214344192, 380420285792256, 1326443518324400147398656	(B)
84	$7 \cdot 3 \cdot 2^2$	≥ 1	241920	
84	$7 \cdot 3 \cdot 2^3$	0		(Div)
88	$22 \cdot 2^3$	1	76480844267520000	(IS)
88	$22 \cdot 2^4$	0		(Rao)
88	$11 \cdot 2^3$	4428	1916006400, 4459069440^{37}, 63417876480^{442}, 3478923509760^{1554}, 712483534798848^{1855}, 759982437118771200^{539}	(B)
88	$11 \cdot 2^7$	0		(X)
90	$5 \cdot 3^2 \cdot 2^2$	0		(Div)

continued on next page

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Table 5 *(continued)*

N	Type	#	Size of the automorphism groups	Methods
96	$24 \cdot 2^4$	0		(Rao)
96	$12 \cdot 4 \cdot 2^5$	0		(Rao)
96	$12 \cdot 2^3$	12812		(B)
96	$12 \cdot 2^8$	0		(Rao)
96	$8 \cdot 3 \cdot 2^5$	0		(O')
96	$8 \cdot 2^{12}$	0		(Rao)
100	$5^2 \cdot 2^2$	8198		(B)
100	$5^2 \cdot 2^3$	0		(Div)

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