A unifying implementation of stratum (aka strong) orthogonal arrays[⋆]

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Abstract

Constructions of so-called "strong orthogonal arrays" (SOAs) have been previously proposed. The approaches and notations taken in the different proposals vary widely. The SOAs and their constructions are reviewed using a unifying notation with a simple set of equations. In addition to providing a unifying overview, some constructions are improved, e.g., by enforcing column orthogonality via a bipartite pair matching algorithm where the original constructions pay no attention to column orthogonality. All constructions presented in the paper are implemented in the R package SOAs. As an aside, it is argued that "stratum" is a better choice than "strong" for the "S" in the acronym SOAs.

Keywords: experimental design, quantitative factors, strong orthogonal arrays, stratum orthogonal arrays, computer experiments

1. Introduction

He and Tang (2013, 2014) introduced so-called "Strong Orthogonal Arrays" (SOAs) and proposed their use for the construction of Latin Hypercube Designs (LHDs) for computer experiments. Subsequent authors built on their work and introduced multiple variants, among them Liu and Liu (2015), He, Cheng and Tang (2018), Zhou and Tang (2019), Shi and Tang (2020), and most recently Li, Liu and Yang (2021a). This author is attracted by the concept, but considers the adjective "strong" in its label as misleading: by a stretch of concept, SOAs can be seen as orthogonal arrays, but as very *weak* ones (low OA strength) only. For the sake of clarity, this paper explicitly distinguishes between OA strength and SOA strength, because these are related, but distinct, concepts. In order to avoid confusing use of the adjective "strong", this paper uses the acronym SOAs, but connects it with the alternate long form "Stratum Orthogonal Arrays". The rationale behind that expression: when columns are collapsed to strata, SOAs become strong(er) orthogonal arrays.

Table 1 shows a small SOA that is used for an informal explanation of terminology for this introduction. The four columns have $2^3 = 8$ levels each. Next to the SOA itself, the table shows column-wise stratum labels for $2^2 = 4$ or $2^1 = 2$ column-specific coarser strata. These stratum labels can also be considered as collapsed levels of coarser-grained columns, i.e., e.g., the stratum labels for two strata are obtained by collapsing original levels 0,1,2,3 into the new level 0 and original levels 4,5,6,7 into the new level 1. Collapsing levels is an unambiguous operation with a unique result, as displayed in the table. On the other hand, one can also expand a set of coarser levels (e.g., 0,1) to finer levels (e.g., 0,1,2,3 (from 0), and 4,5,6,7 (from 1)), which is not a unique operation but can be done in many different ways (see Section 2.6). All the constructions for SOAs can be viewed as particular methods for expanding the levels of a suitable s-level OA to s^ℓ levels, for some small ℓ (mostly 2 or 3), e.g. for expanding the levels of the 2-level OA in the last four columns of Table 1 to the $2^3 = 8$ levels of the SOA. For assessing the quality of an SOA, considerations are often restricted to small subsets of columns, e.g. columns X_1 and X_2; such margins of

[⋆] An online supplement provides additional proofs and examples.

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Table 1: An SOA with four 8-level columns in 16 runs, with column-wise stratum labels for four and two strata

Run no.	The SOA				Stratum labels for							
					four strata				two strata			
	X_1	X_2	X_3	X_4	$X_{1;4}$	$X_{2;4}$	$X_{3;4}$	$X_{4;4}$	$X_{1;2}$	$X_{2;2}$	$X_{3;2}$	$X_{4;2}$
1	4	5	0	3	2	2	0	1	1	1	0	0
2	6	7	2	1	3	3	1	0	1	1	0	0
3	4	4	5	7	2	2	2	3	1	1	1	1
4	6	6	7	5	3	3	3	2	1	1	1	1
5	5	1	1	7	2	0	0	3	1	0	0	1
6	7	3	3	5	3	1	1	2	1	0	0	1
7	5	0	4	3	2	0	2	1	1	0	1	0
8	7	2	6	1	3	1	3	0	1	0	1	0
9	0	5	1	6	0	2	0	3	0	1	0	1
10	2	7	3	4	1	3	1	2	0	1	0	1
11	0	4	4	2	0	2	2	1	0	1	1	0
12	2	6	6	0	1	3	3	0	0	1	1	0
13	1	1	0	2	0	0	0	1	0	0	0	0
14	3	3	2	0	1	1	1	0	0	0	0	0
15	1	0	5	6	0	0	2	3	0	0	1	1
16	3	2	7	4	1	1	3	2	0	0	1	1

the entire SOA are also called *projections* (of the SOA onto the respective margin), and one can consider one-dimensional (1D), two-dimensional (2D) or higher-dimensional (3D, 4D, ...) projections; projections simply ignore the presence of further columns of the SOA.

Arrays with many levels per column, such as SOAs, are primarily used for computer experiments with quantitative variables. The most well-known examples are LHDs, which were first proposed by McKay, Beckman and Conover (1979): for these, each column has as many levels as there are experimental runs. The most important property of LHDs is their “space-filling” behavior, which can be measured in a variety of ways (see Section 2.4). Many constructions are based on orthogonal arrays, e.g. Tang's (1993) proposal to expand the levels of an OA, Ye's (1998) proposal to obtain an LHD with orthogonal columns from a construction based on regular fractional factorial 2-level columns, or Xiao and Xu's (2018) maximin distance level expansion (MDLE) arrays. As was mentioned before, SOAs provide another and very structured way of expanding the levels of OAs. They have two key benefits: their low-dimensional stratification behavior (see below) is more refined and controlled than that of other OA expansions, and their space-filling properties can be improved with limited effort during construction, using a level permutation approach proposed by Weng (2014). It should be noted that there are SOA constructions for LHDs (e.g. 6 columns with 125 levels in 125 runs) or for non-LHD arrays with many levels for each column (e.g., the small SOA of Table 1 or an SOA in 81 runs with 12 27-level columns), but also for arrays with many columns at as few as 4 levels each (e.g. 40 columns at 4 levels each in 88 runs).

Every SOA has at least OA strength 1, i.e., it has equireplicated individual columns. Typically, OA strength 2, which would require equireplicated pairs of columns, is not attempted for an SOA; for example, OA strength 2 would require a multiple of 64 runs for the 8-level columns of Table 1. SOA strength is based on *stratum* balance in low-dimensional projections, i.e., equireplication is not required for individual level combinations, but for combinations of column-wise strata only. The SOA of Table 1 has SOA strength 3, which implies that $2^3 = 8$ equally-sized strata are obtained in 1D projections (obvious from the table), as well as 2D and 3D projections. Figure 1 shows example stratifications for 2D and 3D. The 3D charts show the $2 \cdot 2 \cdot 2$ equally-sized strata obtained by using two strata each for X_1, X_2 and X_3; this

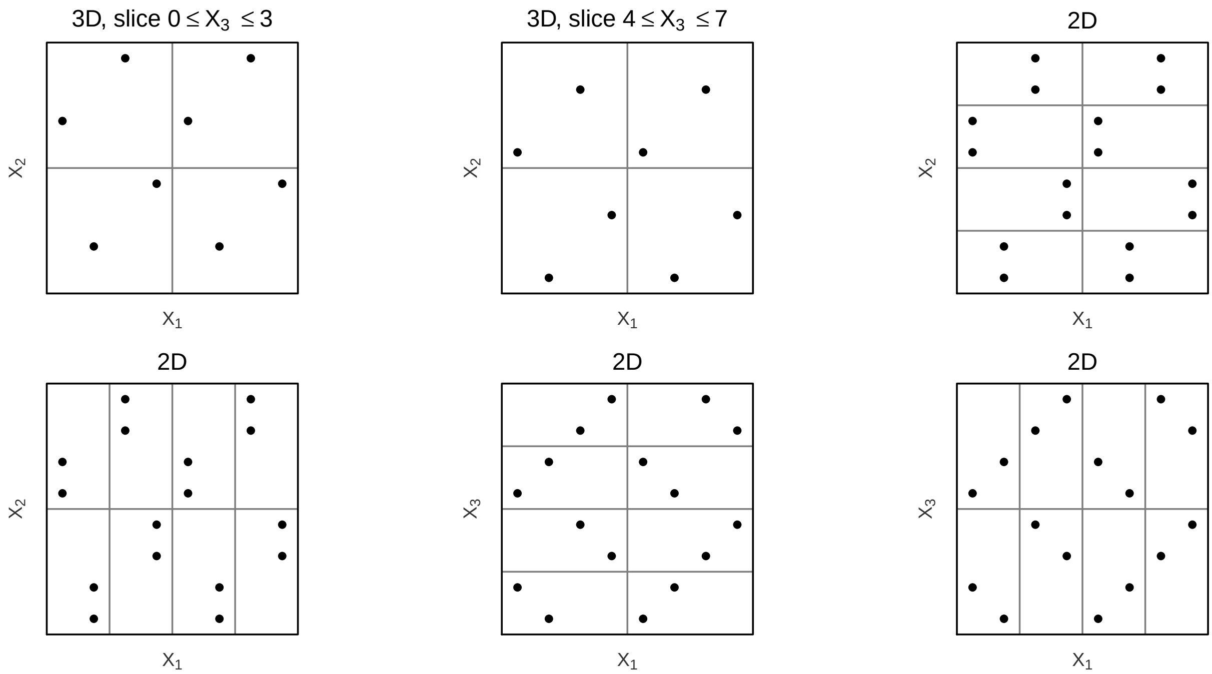

Figure 1: Illustration of stratification properties for the SOA of Table 1. The top row shows the 3D stratification of $X_1 \times X_2 \times X_3$ into $2 \cdot 2 \cdot 2 = 8$ strata (left and middle). The 2D plots show the stratifications of $X_1 \times X_2$ and $X_1 \times X_3$ into $2 \cdot 4 = 8$ strata and $4 \cdot 2 = 8$ strata. 1D stratification of each column into 8 equally-sized 1D strata is obvious from the table.

corresponds to the fact that the three columns $X_{1;2}, X_{2;2}, X_{3;2}$ of Table 1 form a full factorial. Likewise, the figure illustrates the various types of 2D stratifications which yield 8 equally-sized strata involving X_1: each of the column pairs $X_{1;2}$ with $X_{2;4}$, $X_{1;4}$ with $X_{2;2}$, $X_{1;2}$ with $X_{3;4}$ or $X_{1;4}$ with $X_{3;2}$ forms 8 strata with two elements each. It can be easily checked in Table 1 that analogous balance properties hold for all other triples or pairs of columns with comparable patterns of numbers of levels. Detail on OA strength and SOA strength is covered in Sections 2.3 and 3, respectively; Section 3.3 introduces more refined variants of SOA strength, including an extension (strength 3+) proposed in this paper.

This paper provides a unifying overview of diverse SOA constructions that have been proposed in recent years. It has been written with a clear focus on practically feasible constructions, which have been implemented in the R package SOAs (Grömping 2022b). All constructions are presented based on simple matrix equations. The unifying view on a diverse set of recent articles revealed a few opportunities for improvements:

- The construction for Shi and Tang's (2020) Family 3 is improved to achieve orthogonal columns, and Family 2 SOAs can be made to have a single pair of non-orthogonal columns only (see Section 4.2.2).
- For the constructions by He et al. (2018), a broadened choice of columns for one of the matrices together with a bipartite pair matching algorithm for matching columns between two matrices guarantees orthogonal columns where orthogonality is compatible with the situation at hand (see Sections 5.2 and 5.3).
- A small modification of the construction by Zhou and Tang (2019) (swapping two matrices) enables a larger strength than possible with the original construction in some cases (see Section 5.1).
- Both the construction by Zhou and Tang (2019) with the modification of the previous bullet and the construction by Li et al. (2021a) sometimes yield larger strength than advertised by their authors; implementation of the Weng (2014) optimization of space filling together with a slight modification of matrix construction increases the chance that this occurs (see Section 4.1.2).

The different constructions for SOAs combine many established concepts of experimental design theory, so that a self-contained presentation requires a substantial amount of basic facts (Section 2). Section 3 introduces SOAs, provides the equations used for the constructions in this paper, presents and illustrates the earliest constructions, details the practically relevant classes of SOAs and states necessary and sufficient requirements for obtaining the different classes, as far as they can be stated in general terms. Sections 4 and 5 provide further specific constructions in the unifying notation of this paper. Section 6 gives an overview of the constructions and their properties in terms of run sizes, numbers of columns and quality criteria. The discussion gives an overall assessment and an outlook at future developments, and three appendices provide details that would disrupt the flow but are nevertheless of interest; in particular, Appendix C (Tables 10 ff.) lists many example designs that are constructed throughout the paper, together with an overview of their properties and the ingredients of their construction. Furthermore, supplemental online material is available for this paper.

2. Notation and basic facts

$\lfloor\cdot\rfloor$ and $\lceil\cdot\rceil$ denote the floor and ceiling functions, respectively. Their application to matrices or vectors is element wise.

2.1. Matrix notation

Matrices and vectors are denoted with bold face capital or lower case letters, respectively. $\mathbf{1}_n$ and $\mathbf{0}_n$ denote a column vector of n identical elements (1 or 0), the superscript $\top$ denotes the transpose of a matrix or vector. Column vectors with single digit integer elements are parsimoniously written as a string of integers, e.g. $2 \cdot \mathbf{1}_5 = 22222$. $\otimes$ denotes the Kronecker product. Element wise application of a scalar function f to a matrix $\mathbf{M}$ is denoted by $f(\mathbf{M})$; analogously, element wise addition or subtraction between a scalar s and a matrix $\mathbf{M}$ is denoted by, e.g., $s + \mathbf{M}$. The $n \times m$ matrix $\mathbf{X}$ is written as

$$\mathbf{X} = (x_{i,j})_{i=1:n,j=1:m} = \begin{pmatrix} x_{11} & \dots & x_{1m} \\ \vdots & & \vdots \\ x_{n1} & \dots & x_{nm} \end{pmatrix} = (\mathbf{x}_1, \dots, \mathbf{x}_m) = \begin{pmatrix} \mathbf{x}^{(1)} \\ \vdots \\ \mathbf{x}^{(n)} \end{pmatrix}.$$

For a matrix $\mathbf{M}$ with c columns, $\mathbf{M}_{c_1:c_2}$ denotes the sub matrix of columns c_1 to c_2. The function *cyc* denotes a cyclic permutation of the columns, i.e., $cyc(\mathbf{M}) = (\mathbf{m}_2, \dots, \mathbf{m}_c, \mathbf{m}_1)$. The function $\mathcal{S}$ of Definition 1 simplifies the presentation of constructions for SOAs with orthogonal columns.

Definition 1. Let $\mathbf{M}$ be an $n \times m$ matrix with elements from $\{0, \dots, s-1\}$, m even. The function $\mathcal{S}$ returns an $n \times m$ matrix with the ℓth column given as

$$\mathcal{S}(\mathbf{M})_\ell = \begin{cases} \mathbf{m}_{\ell+1} & \ell \text{ odd} \\ s - 1 - \mathbf{m}_{\ell-1} & \ell \text{ even} \end{cases}, \quad \ell = 1, \dots, m.$$

2.2. Galois fields

A Galois field $GF(s)$ (see e.g. Appendix A of Hedayat et al. 1999) is a finite field over the elements $\{\alpha_0, \alpha_1, \dots, \alpha_{s-1}\}$; Galois fields exist whenever s is a prime or an integer power of a prime. Galois fields come with addition (neutral element α_0) and multiplication (neutral element α_1); for prime s, one can choose $\{\alpha_0, \alpha_1, \dots, \alpha_{s-1}\} = \{0, 1, \dots, s-1\}$ with $\mod s$ arithmetic. For non-prime prime powers, this paper also denotes the elements of the Galois field with the numbers $\{0, 1, \dots, s-1\}$, but uses suitable addition and multiplication tables that fulfill the requirements for a field, in line with the implementation of Galois fields in R package lhs (Carnell 2022). Tables 8 and 9 in Appendix A show the respective tables for prime powers 4, 8 and 9. Addition modulo a prime or non-prime s, as well as addition w.r.t. a Galois field $GF(s)$, will be denoted as $+_s$, multiplication as $\cdot_s$.

2.3. Orthogonal arrays

An OA is a rectangular table of symbols that typically stand for the levels of an experimental factor. In this paper, the columns of an OA stand for the factors, the rows for the level combinations used in experimental runs. An $\text{OA}(n, m, s_1^{m_1} \dots s_k^{m_k}, t)$ has n rows and m columns. m_1 columns have s_1 levels, $\dots$,m_k columns have s_k levels, $m_1 + \cdots + m_k = m$, and $s(i)$ denotes the number of levels of the ith column. The OA's strength is t, which means that any combination of t columns indexed by $i_1 \dots i_t$ has all $s(i_1) \cdot \dots \cdot s(i_t)$ level combinations the same number of times. SOAs are typically based on *symmetric* OAs, i.e., OAs with $s_1 = \cdots = s_k = s$; such OAs are denoted by $\text{OA}(n, m, s, t)$. Non-symmetric OAs are also called *asymmetric* or *mixed level*. An OA with n rows and m columns is called *saturated*, if $(s_1 - 1) \cdot m_1 + \cdots + (s_k - 1) \cdot m_k = n - 1$, in other words, if a factorial linear model that contains just the main effects for all m array columns leaves no degrees of freedom for error. For an $\text{OA}(n, m, s, t)$, the strength implies that $n = \lambda s^t$ for an integer λ that is called the index of the OA. As was mentioned before, the expression "strength" will have to be used in two different meanings in this paper about SOAs: "OA strength" will always be explicitly referred to as such, whereas the mere use of the word "strength" outside of this section always refers to "SOA strength", which is a different concept (see Definition 2).

OAs typically have small numbers of levels; many of the usual symmetric OAs have $s = 2$, $s = 3$ or at most $s = 4$, and mixed level OAs often have the majority of their factors at 2 or 3 levels, possibly with a few exceptions. There are various construction algorithms for symmetric OAs; these are, for example, explained in Hedayat, Sloane and Stufken (1999). They can typically construct OAs whose number of levels s is a power of a prime (e.g. 2, 3, 4, 5, 7, 8, 9, 11, 13, 16, ...). Construction algorithms for *regular* fractional factorial OAs take a specific role (see subsections below): An OA is called "regular", if its columns can be obtained as linear combinations of some linearly independent basic columns, based on modulo or Galois field arithmetic. Typical instances of basic columns would be the k columns in s levels each of an $s^k \times k$ full factorial array with s-level columns.

2.3.1. Regular saturated strength 2 fractions

Several constructions of SOAs make use of the regular saturated strength 2 $\text{OA}(s^k, (s^k - 1)/(s - 1), s, 2)$ that can be obtained for s-level columns with s a prime or prime power, using the so-called Rao-Hamming construction (see e.g. Section 3.4 of Hedayat et al.): It consists of a set of k linearly independent basic vectors on $GF(s)^{s^k}$ and all their linear combinations, where uniqueness is achieved by using only those coefficient vectors from $GF(s)^k$ for which the first non-zero element is 1. For example, an $\text{OA}(3^3, (3^3 - 1)/(3 - 1), 3, 2) = \text{OA}(27, 13, 3, 2)$ is obtained from the three basic vectors 012012012012012012012012012, 000111222000111222000111222 and 000000000111111111222222222 and their ten linear combinations with coefficient vectors 110, 120, 101, 102, 011, 012, 111, 112, 121, 122 (calculations modulo 3).

2.3.2. Yates matrix for regular 2-level fractions

Regular fractional factorial 2-level OAs are particularly well-understood (see e.g. Mee 2009). Note that they are often discussed in $-1/+1$ coding with multiplication instead of 0/1 coding with $+_2$ (remember that $+_2$ denotes addition modulo 2). The two approaches are equivalent, and this paper uses the latter because of consistency with the cases for $s \neq 2$.

Large catalogs of non-isomorphic regular 2-level fractions are available. These can be parsimoniously specified using the so-called Yates matrix column numbers, whose fascinating systematic is now explained. A Yates matrix of degree k is the $2^k \times (2^k - 1)$ matrix for all effects in a full factorial design with k basic columns, called basic factors in this section in order to avoid confusion with the Yates matrix column numbers. Starting from two basic factors, the principle of recursive construction is shown below:

$$Y(2) = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad Y(3) = \begin{pmatrix} Y(2) & \mathbf{0}_4 & Y(2) \\ Y(2) & \mathbf{1}_4 & Y(2) +_2 1 \end{pmatrix}, \quad Y(4) = \begin{pmatrix} Y(3) & \mathbf{0}_8 & Y(3) \\ Y(3) & \mathbf{1}_8 & Y(3) +_2 1 \end{pmatrix}, \quad \dots \tag{1}$$

If $\mathbf{e}_1, \mathbf{e}_2, \dots$ denote the basic factors, the Yates matrix column numbers have a systematic structure, and their binary representations indicate which effects are captured by them: $\mathbf{e}_j$ is in column 2^{j-1}, e.g. for $k = 4$, the four basic factors are in columns 1, 2, 4, and 8 (binary representations: 1=0001,2=0010,4=0100,8=1000). Further column numbers also indicate which interaction effect is represented by the column in a full factorial model, for example column 11 (binary representation 11=1011, with further leading zeroes for $k > 4$) captures the three-factor interaction of $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_4$. The structure of the Yates matrix implies that the first $2^u - 1$ columns capture the effects of basic factors $\mathbf{e}_1, \dots, \mathbf{e}_u$ and all their interactions. Likewise, the $2^{k-u} - 1$ Yates matrix columns numbered with multiples of 2^u capture the effects of the last $k - u$ basic factors and all their interactions. For example, for $k = 5$ and $u = 3$, columns 1 to 7 capture all effects related to the first three basic factors, whereas the three columns numbered with multiples of 8 (8, 16, 24) capture the design with the last $5 - 3 = 2$ basic columns. Computationally, instead of the recursive construction of Equation (1), if a function for creating a full factorial in k columns is available that allows one to specify the order of columns (first or last factor changing fastest, e.g. 01010101, 00110011 and 00001111 or 00001111, 00110011, and 01010101), the Yates matrix for k factors can be obtained by multiplying the full factorial in the k basic factors (fastest changing first) with the transpose of that same full factorial (but slowest changing first) (calculations modulo 2), and omitting the column of zeroes in the first position. In support of example constructions, the Yates matrix for 16 runs is shown in Table 13 of Appendix C.

2.3.3. Balance

A full factorial $\mathrm{OA}(n, m, s_1^{m_1} \dots s_k^{m_k}, m)$ with $n = \lambda \cdot s_1^{m_1} \cdot \dots \cdot s_k^{m_k}$ contains $\lambda \geq 1$ copies of each possible level combination of the m array columns, and thus has strength m. If one considers the numbers of levels $s_1, \dots, s_k$ as given, better balance is not achievable. OAs of strength t exhibit such perfect balance at least in any tD projection, $1 \leq t \leq m$. This paper uses the term *balance* in a non-technical sense. It refers to the degree of perfection an array achieves in comparison to the balance properties of a full factorial or to the lower-dimensional balance properties of a strength t OA. The term *balance* is also used to refer to the balance properties of SOAs that are of a different nature than those of OAs.

2.3.4. GWLP and GMA

The imbalance of an OA for qualitative factors is often measured by the so-called generalized word length pattern (GWLP). Xu and Wu (2001) proposed to obtain the GWLP using a model matrix based on a normalized orthogonal coding (which is, e.g., implemented in function `contr.XuWu` from the R package DoE.base, Grömping 2022a): The GWLP for an OA with m columns is the row vector $(A_0, A_1, A_2, \dots, A_m)$, where $A_0 = 1$ and A_j, $j = 1, \dots, m$, measures the confounding of the j factor interactions with the intercept (=overall mean because of the normalized orthogonal coding). The GWLP can, e.g., be calculated using function `GWLP` of R package DoE.base. It is a generalization of the more well-known word length pattern for regular 2-level fractional factorials, for which the normalized orthogonal coding is the $-1/+1$ coding, and a j-factor interaction contributes "+1" to A_j if its model matrix column is constantly either $+1$ or -1 (i.e., the interaction effect cannot be separated from the overall mean), or contributes 0 to A_j if its model matrix column consists of the same number of -1 values and $+1$ values ($n/2$ values each). The GWLP entries A_j of a strength t OA are zero for all $1 \leq j \leq t$, which indicates the balance implied by the strength. The smallest positive j for which $A_j > 0$ is called the resolution of the OA (i.e., the resolution is $t+1$, if t denotes the maximum strength). Xu and Wu (2001) introduced the GWLP-based ranking criterion "generalized minimum aberration" (GMA), which works as follows: a design with higher OA strength (or higher resolution) is better; for two designs with resolution R, the design with the smaller A_R is better; if A_R is the same, the design with the smaller A_{R+1} is better, and so forth. A GMA design is an overall best design according to this criterion (it is not necessarily unique).

SOAs are based on OAs with at least strength 2 and have themselves maximum OA strength 1 in most situations, i.e., resolution II (resolution is denoted as a Roman numeral). Their A_2 value can thus be used to measure their imbalance in terms of the GWLP; however, since SOAs are typically created for quantitative variables, the GWLP is not necessarily a suitable metric for assessing their quality. Nevertheless, using a GMA OA in the construction for an SOA can be beneficial (see e.g. Section 2.6.1).

2.3.5. Obtaining OAs

The literature provides many constructions for symmetric OAs whose numbers of levels are powers of a prime, for example by Bose (1938), Bush (1952), Bose and Bush (1952), or Addelman and Kempthorne (1961). Such OAs can, e.g., be created using several `create...` functions from R package lhs (Carnell 2022, based on C code by Owen 1994). Besides construction algorithms, literature and web pages provide catalogs of OAs: Hedayat et al. (1999) list many OAs, and the website by Sloane (without date) has many further OAs. Other websites with catalogs of OAs are provided by Kuhfeld (2010) and Eendebak and Schoen (2010). The R package DoE.base (Grömping 2022a) holds a catalog with all OAs available from the website by Kuhfeld (which are mostly saturated strength 2 OAs) and some larger strength 2 OAs, as well as another catalog of strength 3 OAs; the available OAs can be inspected using a function `show.oas`.

2.4. Latin hypercube designs and space filling criteria

Projections of a symmetric s-level OA of OA strength t onto a 1D, 2D, ..., tD marginal space have exactly $s, s^2, \ldots, s^t$ distinct level combinations. For the typically small s, there are thus very few distinct level combinations in lower-dimensional projections. The benefit of OAs lies in their implicit replication that allows the estimation of low order interaction effects and random error. As soon as random error becomes irrelevant, like in computer experiments, the small number of level combinations in low order projections becomes a disadvantage. Therefore, LHDs have been proposed especially for computer experiments with quantitative factors in order to provide a good exploration of the entire experimental space.

An LHD for m quantitative variables in n runs is an OA$(n, m, n, 1)$, i.e., each column has as many levels as there are rows (=runs). Note that some authors write about latin hypercube *designs*, others about latin hypercube *samples*; both are two slightly different versions of the same concept. LHDs are usually specified in terms of integer levels. In latin hypercube *sampling*, one often works with real numbers in $[0, 1]^m$, where the integer numbers from the LHD approach correspond to intervals within $[0, 1]$. This paper works with LHDs, but the difference is unsubstantial since it is straightforward to go back and forth between LHD and latin hypercube sample.

There is a large amount of literature on quality criteria for LHDs. It is commonly agreed that LHDs should be "space-filling", i.e., fill the m-dimensional space as well as possible. Popular metrics to assess their space-filling properties are the minimum interpoint distance (which should be as large as possible, maximin distance, advocated by Johnson, Moore and Ylvisaker 1990) or the maximum interpoint distance (which should be as small as possible, minimax distance), or various criteria that measure discrepancy from uniformity in some way (and should be small). This paper uses the maximin distance criterion, as well as the so-called ϕ_p criterion which is commonly used in the SOA literature and was first proposed by

Morris and Mitchell (1995) with the intention to mimic the maximin distance criterion:

$$\phi_p(\mathbf{X}) = \left(\sum_{\{i,j\} \subset \{1,\ldots,n\}, i \neq j} d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})^{-p} \right)^{1/p},$$

where $d()$ is a suitable distance function, chosen independently of p, e.g. Minkowski with $q = 2$ (euclidean) or $q = 1$ (manhattan), and $x^{(i)}$ is the observation vector for the ith unit, i.e., the ith row of the matrix $\mathbf{X}$ that represents the runs. For large p, minimizing ϕ_p is known to be a good substitute for the maximin distance criterion. $d(c \cdot \mathbf{x}^{(i)}, c \cdot \mathbf{x}^{(j)}) = c \cdot d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$, and $\phi_p(c\mathbf{X}) = \phi_p(\mathbf{X})/c$, so that normalized versions d_{ij}^* and ϕ_p^* for range $[0,1]$ can be easily obtained, which is helpful when comparing arrays with different numbers of levels.

Recently, Tian and Xu (2022) proposed a space-filling pattern in a spirit similar to the GWLP (see Section 2.3.4). Their criterion has not been considered in this paper, but might become an important tool for assessing space-filling of SOAs in the future.

2.5. Orthogonal columns

For an OA, "orthogonal" refers to combinatorial balance which is invariant to level coding. In this paper, when talking about "orthogonal columns", "orthogonal" refers to geometric orthogonality in n-dimensional space, which can be measured by correlation between columns: two columns are geometrically orthogonal if their correlation is zero. Combinatorial orthogonality implies geometric orthogonality, but the reverse is not true. Geometric orthogonality is of interest for quantitative experimental variables only, and it is heavily dependent on level coding. LHDs with orthogonal columns have been discussed in the literature (e.g. Ye 1998). The benefit of geometric orthogonality is that estimated coefficients in simple main effect linear regression do not change, regardless whether one does or does not include other columns in the model. The expression "3-orthogonality", which was introduced by Bingham, Sitter and Tang (2009), describes a stronger orthogonality property: 3-orthogonal arrays guarantee that columns are not only orthogonal to each other and to the constant column, but also to products of pairs of other columns and to squares of other columns. This effectively means that main effect estimates are uncorrelated with the estimates of second order effects. 3-orthogonality thus prevents misleading conclusions on main effects from neglecting relevant second order effects, and makes estimation of second order models more efficient. To the author's knowledge, Ye (1998) was the first author to propose 3-orthogonal LHDs; his construction produces 2^k or $2^k + 1$ runs with $2k - 2$ columns (but does not yield SOAs).

Note that orthogonality or 3-orthogonality does not imply space filling; thus, it is advisable to consider additional space-filling criteria, because the default constructions can exhibit strong patterns that leave large holes unfilled. For example, an unoptimized orthogonal SOA in 125 runs seems to arrange the design points in parallel diagonal stripes that are less space-filling than would be desirable, while even one round of optimization towards lowering ϕ_p substantially improves this behavior as can be seen from the 2D projections in Figure 2, and by comparing the ϕ_p values (0.0395 reduced to 0.013 by the optimization). Note, however, that the right-hand side figure also shows systematic holes in several of the projections.

2.6. Expanding levels

An early proposal for obtaining LHDs by expanding the levels of OAs was by Tang (1993). Two simple techniques to expand an OA(n, m, s, t) to a symmetric OA with OA strength $t' \geq 1$ and with columns in $s \cdot \ell$ levels are presented in Sections 2.6.1 and 2.6.2. Level expansion of OAs is easy to implement. The quality of the resulting array strongly depends on the level orderings within the initial OA, and also within replacements. Depending on the size of ℓ, the space to optimize over can be huge.

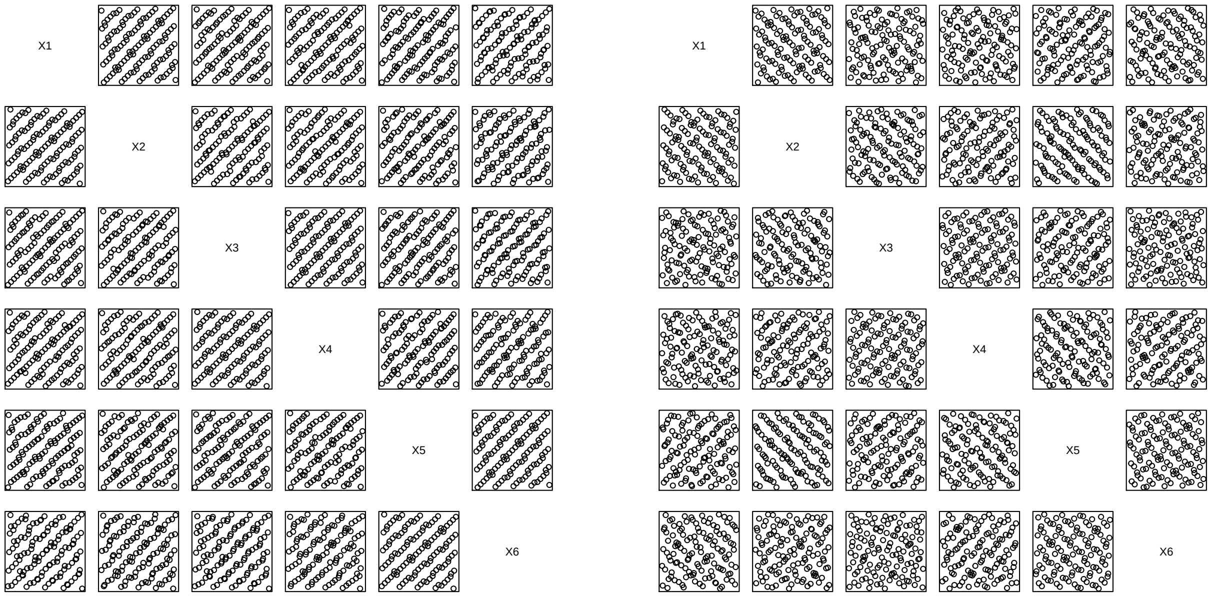

Figure 2: 2D projections of unoptimized (left) and optimized (right) SOA in 125 runs with six orthogonal columns at 125 levels each

2.6.1. Expanding levels within the OA

This type of expansion returns an array with the same number of rows as the in-going OA. It can be applied, if ℓ divides n/s. An $\text{OA}(n, m, s \cdot \ell, t')$ can be obtained by expanding the levels of each column in the following way: allocate

- new levels $0, \dots, \ell - 1$ to the n/s runs with old level 0,
- new levels $\ell, \dots, 2\ell - 1$ to the n/s runs with old level 1,
- $\dots$,
- and new levels $(s-1)\ell, \dots, s\ell - 1$ to runs with old level $s - 1$,

conducting all allocations in an equireplicated way.

Xiao and Xu (2018) proposed an algorithm for optimizing this type of expansion, which they called MDLE for “maximin distance level expansion”. In particular, they showed that it is beneficial to start from a GMA OA, which has itself been optimized for maximin distance by level permutations, before applying level expansion (the maximization of the minimum distance can be omitted for 2-level starting OAs). Xiao and Xu proposed to use a threshold acceptance (TA) algorithm. Their approach is computationally more demanding than the optimization proposed by Weng (2014, see Section 2.8), but also yields better results. Since Xiao and Xu did not impose any structural constraints on the level expansion, the optimization space for MDLE is larger than that for SOAs. MDLE designs will not be covered in this paper.

2.6.2. Expanding levels by expanding each row

This type of expanding an $\text{OA}(n, m, s, t)$ returns an $\text{OA}(n \cdot \ell, m, s \cdot \ell, t')$ with $t' \geq 1$. There are no requirements for $\ell \geq 2$, except that it is an integer. In the $\text{OA}(n, m, s, t)$, insert a vector

- $0, \dots, \ell - 1$ instead of positions with level 0,
- $\ell, \dots, 2\ell - 1$ instead of positions with level 1,
- $\dots$,
- $(s-1)\ell, \dots, s\ell - 1$ instead of positions with level $s - 1$.

Of course, level permutation can also greatly affect the properties of arrays obtained by this type of expansion.

2.7. Collapsing levels

Collapsing the levels $0, \ldots, s^v - 1$ of a column in s^v levels into only s^u levels $0, \ldots, s^u - 1$, $u < v$, can be simply done with the formula $x_{s^u} = \lfloor x_{s^v}/(s^{v-u}) \rfloor$, where $\lfloor \cdot \rfloor$ denotes the floor function.

If an array was obtained by level expansion, collapsing its levels (again) to s levels either recovers the original array (in case of Section 2.6.1) or a replicate of the original array (in case of Section 2.6.2). In either case, the collapsed array inherits its balance properties from the original array.

For SOAs with columns in s^v levels, stratifications into collapsed columns are often considered, e.g. 2D stratifications of s^3-level columns into $s^2 \times s$ or $s \times s^2$, 3D stratifications of s^4-level columns into $s^2 \times s \times s$ or $s \times s^2 \times s$ or $s \times s \times s^2$. In order to avoid both repetitive writing and complex notation, this paper uses the single representative with exponents sorted from largest to smallest to include all stratifications with the same multi-set of numbers of levels, e.g. "all $s^2 \times s \times s$ stratifications" includes all the 3D stratifications that were listed above for s^4 level factors.

2.8. Optimization by level permutations

As was mentioned before, while combinatorial properties are invariant to the level coding of array columns, column orthogonality or space filling properties heavily depend on level coding. Column orthogonality is typically guaranteed by a construction mechanism (see Sections 3.2.2, 4.1 and 5.1); space filling properties can be optimized by adequate level permutations that do not destroy structural requirements.

A brute force method for level permutations would conduct all combinations of conceivable non-distinct level permutations and select the best outcome. For many situations, such an approach is prohibitive. Weng (2014) suggested to proceed in a reduced version that is adopted in this paper and is now explained. This section assumes the quality criterion ϕ_p for space filling.

Let ν denote the number of permutation applications; ν could e.g. be $3m$, if each of the m columns of three m-column matrices with s levels each is subjected to separate level permutation, like in Equation (4) of the next section. The total number of permutations for a brute force search would be $(s!)^\nu$. In Weng's approach, the number of actual permutations that have to be conducted is far smaller:

a) Start with a random tuple Π_0 of ν permutations of the levels $\{0, 1, \ldots, s-1\}$.
b) Obtain ν one-neighbors of Π_0, by replacing each single permutation in the tuple by another random permutation, keeping all other positions in the tuple unchanged versus Π_0.
c) Assess ϕ_p for Π_0 and all its one-neighbors from step b.
d) If Π_0 is already best in step c, proceed to step e. Else restart step b with the best tuple of level permutations as the new Π_0.
e) Inspect the current tuple of level permutations and all its two-neighbors, in the sense that two permutations are modified ($\binom{\nu}{2}$ such two-neighbors).
f) If Π_0 is best in step e, declare it the winner. Else restart step b with the best tuple of level permutations from step e as the new Π_0.

Weng applied her approach to the He and Tang (2013) constructions and gave examples for which this reduced method came close to the optima found in previous brute-force searches, and she also emphasized that omission of the step with two-neighbors does not lead to satisfactory results. When applying her approach to other constructions, care must be taken that the structural requirements of a construction are not destroyed by level permutations.

3. SOAs

This section provides a formal look at SOAs and their properties, starting with the definition of an (O)SOA of strength t:

Definition 2 (SOA and OSOA)**.** Let $\mathbf{D}$ denote an $\text{OA}(n, m, s^t, 1)$.

(i) $\mathbf{D}$ is an SOA of strength t, denoted as $\text{SOA}(n, m, s^t, t)$ $(m \geq t)$, if and only if all j-dimensional $s^{u_1} \times \cdots \times s^{u_j}$ projections for columns $i_1 < \cdots < i_j$, $1 \leq j \leq t$ produce s^t equally-sized strata, where the i_ℓth column is collapsed to s^{u_ℓ} levels, $u_\ell \geq 1$, and $\sum_1^j u_\ell = t$.

(ii) An $\text{SOA}(n, m, s^t, t)$ whose correlation matrix is the m-dimensional identity matrix is called an $\text{OSOA}(n, m, s^t, t)$.

Example 1. Figure 1 visualized selected projections from the $\text{SOA}(16, 4, 2^3, 3)$ of Table 1, and the table also shows the coarsened columns $X_{j;4}$ and $X_{j;2}$, $j = 1, \ldots, 4$. For checking that the entire SOA has SOA strength 3, one has to verify that 1) each 1D projection, i.e., each individual column X_j, $j = 1, \ldots, 4$, yields $2^3 = 8$ equally-sized strata, 2) each 2D combination of a column $X_{j;4}$ with a column $X_{j';2}$, $j \neq j'$, yields 8 equally-sized strata ($2^2 \times 2^1$ type stratification), and 3) each 3D combination of columns $X_{j;2}$, $X_{j';2}$, $X_{j'';2}$, j, j', j'' distinct, also yields 8 equally-sized strata ($2^1 \times 2^1 \times 2^1$ type stratification). The SOA of Table 1 is not an OSOA, because X_1 is correlated with X_3 and X_2 is correlated with X_4.

3.1. Equations and general results

An SOA is an $\text{OA}(n, m, s^k, 1)$; any $\text{OA}(n, m, s^k, 1)$ can be represented in terms of an equation of k $\text{OA}(n, m, s, 1)$, which underpins the usefulness of equations for the construction of SOAs:

Lemma 1. *Let* $\mathbf{D}$ *denote an* $OA(n, m, s^k, 1)$*.*

(i) $\mathbf{D}$ *can be written as*

$$\mathbf{D} = \sum_{j=1}^{k} s^{k-j} \mathbf{A}_j, \tag{2}$$

where the $\mathbf{A}_j$ *are* $OA(n, m, s, 1)$*.*

(ii) *In Equation (2),* $\lfloor \mathbf{D}/s^{k-1} \rfloor = \mathbf{A}_1$*.*

Proof. The proof for (i) is constructive by collapsing levels, successively obtaining $\mathbf{A}_1$ to $\mathbf{A}_k$:

- $\mathbf{A}_1 = \lfloor \mathbf{D}/s^{k-1} \rfloor$ (which also proves (ii)),
- for $1 < \ell \leq k$, $\mathbf{A}_\ell = \left\lfloor \left(\mathbf{D} - \sum_{j=1}^{\ell-1} s^{k-j}\mathbf{A}_j\right) \Big/ s^{k-\ell} \right\rfloor$.

All the thus-obtained $\mathbf{A}_\ell$ are obviously $\text{OA}(n, m, s, 1)$: It suffices that each level occurs equally often in each individual column, which directly follows from the fact that each of the levels $0, 1, \ldots, s^k - 1$ occurs equally often in $\mathbf{D}$. □

Example 2. The matrix $\mathbf{A}_1 = \lfloor \mathbf{D}/s^{k-1} \rfloor$ for constructing the SOA $\mathbf{D}$ of Table 1 $(s = 2, k = 3)$ is shown in the last four columns of the table. The matrix $\mathbf{A}_2$ is obtained as $\mathbf{A}_2 = \lfloor (\mathbf{D} - 4 \cdot \mathbf{A}_1)/2 \rfloor$ and consists of the columns 0101010101010101, 0101010101010101, 0101010101010101 and 1010101010101010, and the matrix $\mathbf{A}_3$ is obtained as $\mathbf{A}_3 = \mathbf{D} - 4 \cdot \mathbf{A}_1 - 2 \cdot \mathbf{A}_2$ and consists of the columns 0000111100001111, 1100110011001100, 0011110011000011 and 1111111100000000.

All SOA constructions in this paper are presented in terms of constructions for the matrices in Equation (2). Equation (2) can be seen as an especially structured way of conducting level expansion according to Section 2.6.1 for the matrix $\mathbf{A}_1$; the properties of $\mathbf{A}_1$ are therefore of particular importance. Note that the matrix $\mathbf{A}_1$ from Equation (2) trivially has OA strength t for an SOA of SOA strength t, because it yields s^t equally-sized strata for each t-column projection.

The most frequently used special cases $k = 2$ and $k = 3$ are handled in simplified notation: switching from $\mathbf{A}_1$, $\mathbf{A}_2$, $\mathbf{A}_3$ to $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ will improve readability of constructions by avoiding several subscript levels.

This paper mainly considers constructing SOAs in s^2 levels from

$$\mathbf{D} = s\mathbf{A} + \mathbf{B} \tag{3}$$

and SOAs in s^3 levels from

$$\mathbf{D} = s^2\mathbf{A} + s\mathbf{B} + \mathbf{C}. \tag{4}$$

The following two lemmas state existence criteria for such SOAs.

Lemma 2 (recast from He and Tang 2013)**.** *An SOA*$(n, m, s^2, 2)$ $\mathbf{D}$ *exists if and only if* $n \times m$ *matrices* $\mathbf{A}$ *and* $\mathbf{B}$ *can be found such that* $\mathbf{A}$ *is an* $OA(n, m, s, 2)$*, and all pairs* $(\mathbf{a}_\ell, \mathbf{b}_\ell)$ *are* $OA(n, 2, s, 2)$*. These arrays are related by Equation (3).*

Lemma 3 (Shi and Tang, quoting He and Tang 2013)**.** *An SOA*$(n, m, s^3, 3)$ $\mathbf{D}$ *exists if and only if* $n \times m$ *matrices* $\mathbf{A}$*,* $\mathbf{B}$ *and* $\mathbf{C}$ *can be found such that* $\mathbf{A}$ *is an* $OA(n, m, s, 3)$*, and all triples* $(\mathbf{a}_\ell, \mathbf{a}_j, \mathbf{b}_j)$*,* $(\mathbf{a}_\ell, \mathbf{b}_\ell, \mathbf{c}_\ell)$ *are* $OA(n, 3, s, 3)$*,* $\ell \neq j$*. These arrays are related by Equation (4).*

Similar statements can also be made for larger strengths.

The following trivial lemma shows that it is generally easy to assign a column $\mathbf{c}_\ell$ for given columns $\mathbf{a}_\ell$ and $\mathbf{b}_\ell$ such that strength 3 is achieved, as long as an SOA is based on 2-level OAs whose columns are taken from a saturated regular fractional factorial $\mathbf{S}$.

Lemma 4. *If all columns of the matrices* $\mathbf{A}$*,* $\mathbf{B}$ *and* $\mathbf{C}$ *have been chosen from a saturated fractional factorial 2-level design* $\mathbf{S}$*, the matrix* $\mathbf{C}$ *fulfills the assumptions of Lemma 3, iff* $\mathbf{c}_\ell$ *does not coincide with any of* $\mathbf{a}_\ell$*,* $\mathbf{b}_\ell$ *or* $\mathbf{a}_\ell +_2 \mathbf{b}_\ell$*.*

The next lemma will be used for improving a construction to yield orthogonal columns.

Lemma 5. *Let* $\mathbf{A}$*,* $\mathbf{B}$ *and* $\mathbf{C}$ *be* $OA(n, m, s, 2)$ *such that their combination into a single matrix* $(\mathbf{A} \vdots \mathbf{B} \vdots \mathbf{C})$ *is an* $OA(n, 3m, s, 2)$*. Then Equation* (4) *yields a matrix* $\mathbf{D}$ *with orthogonal columns.*

Proof. $\mathbf{D} = s^2\mathbf{A} + s\mathbf{B} + \mathbf{C}$. The correlation matrix of $\mathbf{D}$ can be obtained with the usual rules for calculating correlation matrices of sums and products with scalars. The strong assumptions of the lemma imply the requested orthogonality property. □

Example 3. The matrices $\mathbf{A} = \mathbf{A}_1$, $\mathbf{B} = \mathbf{A}_2$ and $\mathbf{C} = \mathbf{A}_3$ for the SOA of Table 1 were given in Example 2. All their columns are taken from a regular 2-level OA. SOA strength 3 was verified directly in Example 2. It can also be verified using Lemma 3: matrix $\mathbf{A}$ has OA strength 3, all triples $(\mathbf{a}_\ell, \mathbf{a}_j, \mathbf{b}_j)$ have OA strength 3 (straightforward to see), and all triples $(\mathbf{a}_\ell, \mathbf{b}_\ell, \mathbf{c}_\ell)$ have OA strength 3; the latter can be most easily ascertained using Lemma 4. Matrix $\mathbf{B}$ has OA strength 1 only, so that the orthogonal columns result of Lemma 5 cannot be applied (and we saw already that the columns are not orthogonal).

The following subsection presents the early constructions of strength 2 to strength 4 or 5 (O)SOAs. Later sections will provide constructions for refined strength classifications.

3.2. Early constructions for (O)SOAs

3.2.1. SOAs of strengths 2 to 5 by He and Tang (2013)

He and Tang (2013) introduced SOAs, based on so-called generalized orthogonal arrays (GOAs), for strengths $t = 2, \ldots, 5$. Recasting them to the form of Equation (2) is straightforward, because it only

Table 2: Constructions by He and Tang 2013 of an SOA(n, m', s^t, t) based on an $n \times m$ matrix $\mathbf{V}$, which is an OA(n, m, s, t). m' is given in (5), further notations were explained in Section 2.1.

t	$\mathbf{D} =$	Matrices
2	$s\mathbf{A} + \mathbf{B}$	$\mathbf{A} = \mathbf{V}, \mathbf{B} = cyc(\mathbf{A})$
3	$s^2\mathbf{A} + s\mathbf{B} + \mathbf{C}$	$\mathbf{A} = \mathbf{V}_{1:(m-1)}, \mathbf{B} = (\mathbf{v}_m, \dots, \mathbf{v}_m), \mathbf{C} = cyc(\mathbf{A})$
4	$s^3\mathbf{A}_1 + s^2\mathbf{A}_2 + s\mathbf{A}_3 + \mathbf{A}_4$	$\mathbf{A}_1 = \mathbf{V}_{1:m'}, \mathbf{A}_2 = \mathbf{V}_{(m'+1):(2m')}, \mathbf{A}_3 = cyc(\mathbf{A}_2), \mathbf{A}_4 = cyc(\mathbf{A}_1)$
5	$s^4\mathbf{A}_1 + s^3\mathbf{A}_2 + s^2\mathbf{A}_3 + s\mathbf{A}_4 + \mathbf{A}_5$	$\mathbf{A}_1 = \mathbf{V}_{1:m'}, \mathbf{A}_2 = \mathbf{V}_{(m'+1):(2m')}, \mathbf{A}_3 = \mathbf{1}_{m'}^\top \otimes \mathbf{v}_m,$ $\mathbf{A}_4 = cyc(\mathbf{A}_2), \mathbf{A}_5 = cyc(\mathbf{A}_1)$

requires a re-grouping of matrix columns: He and Tang's $n \times t$ GOA matrices $\mathbf{B}_1^{GOA}, \dots, \mathbf{B}_m^{GOA}$ for m SOA columns hold the first columns of the $n \times m$ matrices $\mathbf{A}_j$, $j = 1, \dots, t$, in $\mathbf{B}_1^{GOA}$, the second columns in $\mathbf{B}_2^{GOA}$, ..., the last columns in $\mathbf{B}_m^{GOA}$. The formulas in Table 2 state the resulting constructions for an SOA(n, m', s^t, t) from an OA(n, m, s, t), which is named $\mathbf{V}$. The number of columns m' obtainable from the m columns of $\mathbf{V}$ can be calculated as

$$m'(m, t) = \begin{cases} \lfloor 2m/t \rfloor & t \text{ even} \\ \lfloor 2(m-1)/(t-1) \rfloor & t \text{ odd} \end{cases}. \tag{5}$$

The relevant specific cases are $m'(m, 2) = m$, $m'(m, 3) = m - 1$, $m'(m, 4) = \lfloor m/2 \rfloor$ and $m'(m, 5) = \lfloor (m-1)/2 \rfloor$. The matrices in the construction equations have m' columns each. In Table 2, the rows for $t = 2$ and $t = 3$ correspond to Equations (3) and (4).

He and Tang (2013) themselves did not consider the use of level permutations in SOA construction. As Weng's (2014) algorithm greatly improves space filling of the resulting SOAs, it is recommended to apply it to this construction, permuting levels of the columns of all t in-going matrices (i.e., $m \cdot t$ candidate level permutations).

Example 4. The SOA$(16, 4, 8, 3)$ of Table 1, also listed in Table 11 (subtable HT) of Appendix C, has been constructed with He and Tang's method for $t = 3$, using the OA$(16, 8, 2, 3)$ shown in Table 13 in the role of $\mathbf{V}$. The construction matrices were given in Example 2. Apart from level permutations, $\mathbf{A}$ consists of $\mathbf{V}_{1:4}$, all four columns of $\mathbf{B}$ are $\mathbf{v}_5$, and $\mathbf{C} = cyc(\mathbf{A})$. Properties of the SOA are shown in Table 10 (row for HT, 8 levels). In particular, level permutations improved the ϕ_p value from about 0.171 to about 0.134.
Appendix C (Table 12, subtable HT) also lists an SOA$(16, 7, 4, 2)$ obtained from He and Tang's construction for $t = 2$, also using the OA$(16, 8, 2, 3)$ of Table 13 in the role of $\mathbf{V}$. As shown in Table 10, this SOA has a good initial ϕ_p, which was not improved by level permutations.

Example 5. The SOA$(27, 3, 27, 3)$ of Figure 3 was obtained using the OA$(27, 4, 3, 3)$ (available in R package DoE.base as `L27.3.4`) in the role of $\mathbf{V}$: apart from level permutations, the matrix $\mathbf{A}$ consists of its first three columns, matrix $\mathbf{B}$ of three copies of the fourth column, and $\mathbf{C} = cyc(\mathbf{A})$ (construction code: `set.seed(7626); SOA27_3 <- SOAs(L27.3.4, noptim.repeats = 3)`).

3.2.2. OSOAs of strengths 2 to 4 by Liu and Liu

Liu and Liu presented constructions for OSOAs. They chose signed levels centered at zero, which is quite common for the orthogonal column case. Nevertheless, for keeping the same notation for all constructions, we will continue to use $0, \dots, s-1$ for the OA levels and $0, \dots, s^t - 1$ for the levels of the OSOA. Strength $t = 4$ already requires a large number of rows per column, so that designs with larger strengths are not considered. The constructions correspond to Theorem 2 of Liu and Liu for even strength and to Theorem 4 of Liu and Liu for odd strength. They use the equations of Table 2, based on the matrices provided below. The connections of those matrices to Liu and Liu's exposition are detailed in Chapter 1 of the Supplemental Material.

Lemma 6 (Liu and Liu 2015 Theorems 2 and 4)**.** *The subsequent t-specific constructions ($t = 2, 3, 4$) based on an $OA(n, m, s, t)$ named* $\mathbf{V}$ *create an $OSOA(n, m', s^t, t)$, where m' is provided in the constructions. If $t > 2$ and $m' > 2$, the columns are 3-orthogonal.*

If $\mathbf{V}$ is an $\text{OA}(n, m, s, 2)$, the $m' = 2\lfloor m/2 \rfloor$ columns of the matrix $\mathbf{A}$ are obtained as

$$\mathbf{a}_\ell = \begin{cases} \mathbf{v}_{\ell+1} & \ell \text{ odd} \\ \mathbf{v}_{\ell-1} & \ell \text{ even} \end{cases}, \quad \ell = 1, \dots, m', \tag{6}$$

and $\mathbf{B} = \mathcal{S}(\mathbf{A})$ with $\mathcal{S}$ from Definition 1. Using $\mathbf{A} = \mathbf{V}_{1:m'}$ would yield a different but comparable construction.

If $\mathbf{V}$ is an $\text{OA}(n, m, s, 3)$, the first $\widetilde{m} = 2\lfloor m/4 \rfloor$ columns of the matrices $\mathbf{A}$ and $\mathbf{B}$ are obtained as

$$\mathbf{a}_\ell = \begin{cases} \mathbf{v}_{2\ell+1} & \ell \text{ odd} \\ \mathbf{v}_{2\ell-3} & \ell \text{ even} \end{cases}, \quad \mathbf{b}_\ell = \mathbf{v}_{2\ell}, \quad \ell = 1, \dots, \widetilde{m}, \tag{7}$$

and $\mathbf{C}_{1:\widetilde{m}} = \mathcal{S}(\mathbf{A}_{1:\widetilde{m}})$ with $\mathcal{S}$ from Definition 1. If $m - 2\widetilde{m} < 3$, $m' = \widetilde{m}$. Otherwise, $m' = \widetilde{m} + 1$, and the additional column can be obtained as follows:

$$\mathbf{a}_{m'} = \mathbf{v}_m, \quad \mathbf{b}_{m'} = \mathbf{v}_{m-1}, \quad \mathbf{c}_{m'} = \mathbf{v}_{m-2}. \tag{8}$$

If $\mathbf{V}$ is an $\text{OA}(n, m, s, 4)$, the $m' = 2\lfloor m/4 \rfloor$ columns of the matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ are obtained as

$$\mathbf{a}_{1;\ell} = \begin{cases} \mathbf{v}_{2\ell+2} & \ell \text{ odd} \\ \mathbf{v}_{2\ell-3} & \ell \text{ even} \end{cases}, \quad \mathbf{a}_{2;\ell} = \begin{cases} \mathbf{v}_{2\ell+1} & \ell \text{ odd} \\ \mathbf{v}_{2\ell-2} & \ell \text{ even} \end{cases}, \tag{9}$$

together with $\mathbf{A}_3 = \mathcal{S}(\mathbf{A}_2)$ and $\mathbf{A}_4 = \mathcal{S}(\mathbf{A}_1)$ with $\mathcal{S}$ from Definition 1.

Hence, among the t matrices for a strength t construction, the last $\lfloor t/2 \rfloor$ matrices are obtained from the first $\lfloor t/2 \rfloor$ matrices by applying function $\mathcal{S}$. The permutation approach by Weng (2014) can thus be applied independently to the columns of the first $\lceil t/2 \rceil$ matrices. This can be implemented by independently permuting the levels of the columns of $\mathbf{V}$. (Level permutations seem to be less powerful for this construction than for some others.)

Example 6. Appendix C lists both an $\text{OSOA}(16, 7, 4, 2)$ (Table 12, subtable LL) and an $\text{OSOA}(16, 4, 8, 3)$ (Table 11, subtable LL) of this construction; both were obtained using the $\text{OA}(16, 8, 2, 3)$ listed in Table 13 in the role of $\mathbf{V}$. Before level permutations, the strength 2 construction uses $\mathbf{A} = (\mathbf{v}_2, \mathbf{v}_1, \mathbf{v}_4, \mathbf{v}_3, \mathbf{v}_6, \mathbf{v}_5, \mathbf{v}_8)$ and $\mathbf{B} = \mathcal{S}(\mathbf{A}) = (\mathbf{v}_1, 1 - \mathbf{v}_2, \mathbf{v}_3, 1 - \mathbf{v}_4, \mathbf{v}_5, 1 - \mathbf{v}_6, \mathbf{v}_7)$ and the strength 3 construction uses $\mathbf{A} = (\mathbf{v}_3, \mathbf{v}_1, \mathbf{v}_7, \mathbf{v}_5)$, $\mathbf{B} = (\mathbf{v}_2, \mathbf{v}_4, \mathbf{v}_6, \mathbf{v}_8)$, and $\mathbf{C} = \mathcal{S}(\mathbf{A}) = (\mathbf{v}_1, 1 - \mathbf{v}_3, \mathbf{v}_5, 1 - \mathbf{v}_7)$. Table 10 shows the resulting properties. The $\text{OSOA}(16, 7, 4, 2)$, whose matrix $\mathbf{A}$ has OA strength 3, must have 3D projections that fulfill the criteria of SOA strength 3; it has SOA strength 2 only, because the 2D properties for SOA strength 3 are violated. Note, however, that it has 3-orthogonal columns, despite having SOA strength 2 only. Furthermore, note that level swaps according to Weng (2014) improved ϕ_p for the 8-level design, but not for the 4-level one.

The following conjecture has not been proven, but was found to hold true for various example OAs

(OA(81, 3, 10, 3), OA(243, 3, 20, 3), OA(125, 5, 6, 3), OA(729, 9, 10, 3), OA(256, 2, 19, 3) (a non-regular OA from Mee 2009, Section 8.2.2).

Conjecture 1 (3-orthogonality for strength 2 constructions by Liu and Liu)**.** *Using the Liu and Liu construction for strength 2 on an OA of strength 3 always yields 3-orthogonal columns.*

For strength 2, a wide variety of OSOAs can be constructed with this technique. The constructions for larger strengths require relatively many runs per column. For example, one can obtain an OSOA(64, 16, 8, 3) from an OA(64, 32, 2, 3), an OSOA(81, 4, 27, 3) from an OA(81, 10, 3, 3), an OSOA(64, 4, 16, 4) from an OA(64, 8, 2, 4) or an OSOA(256, 8, 16, 4) from an OA(256, 17, 2, 4). The considerable benefit of the constructions for $t > 2$ is that they are guaranteed to produce 3-orthogonal columns, which implies that main effects are uncorrelated to second order effects in linear regression models (see Section 2.5). If Conjecture 1 holds true, basing the strength 2 construction on a strength 3 $\mathbf{V}$ can yield 3-orthogonal columns for about twice as many columns as is possible with the strength 3 construction (but at fewer levels for each column).

3.3. Classes of SOAs

In the previous sections, we saw general results for strength 2 and 3 SOAs and early constructions by He and Tang (2013) for SOAs with strengths 2 to 5 and by Liu and Liu (2015) for OSOAs with strengths 2 to 4. In the following, this paper considers constructions for strength 3 and four more refined classes of SOAs, all of which provide less balance than strength 4 but more balance than strength 2. This is because strength 4 or higher is usually prohibitive in terms of run size, while strength 2 without further balance criteria is often not satisfactory.

Table 3: Number of equally-sized strata for low-dimensional projections of refined classes of (O)SOAs

	strength	1D	2D	3D	4D
s^2 levels	2	s^2	s^2	−−	−−
	2+	s^2	s^3	−−	−−
	3−	s^2	s^3	s^3	−−
s^3 levels	2*	s^3	s^3	−−	−−
	3	s^3	s^3	s^3	−−
	3+	s^3	s^4	s^4	−−
s^4 levels	4	s^4	s^4	s^4	s^4

Table 3 summarizes the stratification properties for the classes of (O)SOAs considered in the following, namely (O)SOAs of strengths 2+, 3−, 2*, 3, or 3+; the border cases of strengths 2 and 4 are included for reference. 1D projections consider a single column, 2D projections two columns collapsed to s^a and s^b levels, with $a + b$ equal to the exponent in the table entry, 3D projections three columns collapsed to s^a, s^b and s^c levels with $a + b + c$ equal to the exponent in the table entry, and so forth. Note that the expression "strength 3+" is coined here (see Definition 4 below), in obvious analogy to the expression "strength 2+" used by He, Cheng and Tang (2018).

Figure 3 illustrates strength 3 stratification properties, using an SOA$(27, 3, 3^3, 3)$ from the He and Tang (2013) construction. In comparison, Figure 4 shows an unoptimized OSOA$(n, m, s^3, 2^*)$ from the Li et al. (2021a) construction (to be presented in Section 4.1). Obviously, strength 2* instead of 3 sacrifices stratification properties in 3D while the stratification properties for 2D and 1D projections are unchanged. SOA$(n, m, s^2, 3-)$ stratify like Figure 3, except for having fewer levels so that the bottom right plot would have three points in each of nine rows and columns, respectively, and the points would also be less dispersed in the other plots. An SOA$(n, m, s^2, 2+)$ is not only coarser than the SOA shown in Figure 3

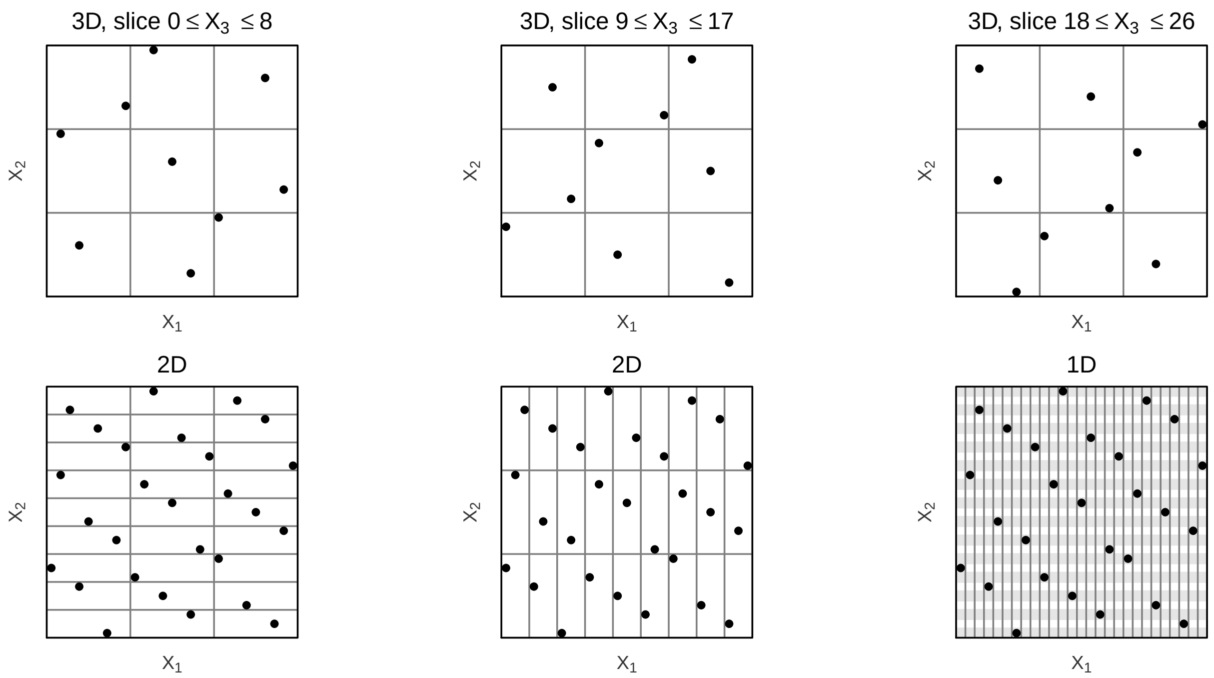

Figure 3: Illustration of stratification properties for an SOA(27,3,27,3) from the He and Tang construction. Each stratum contains exactly one element. The top row shows the 3D stratification of $X_1 \times X_2 \times X_3$ into $3 \cdot 3 \cdot 3 = 27$ strata. The bottom row shows the stratification of $X_1 \times X_2$ into $3 \cdot 9 = 27$ strata (left) or $9 \cdot 3 = 27$ strata (middle), and the stratification of X_1 and X_2 into 27 1D strata each (right).

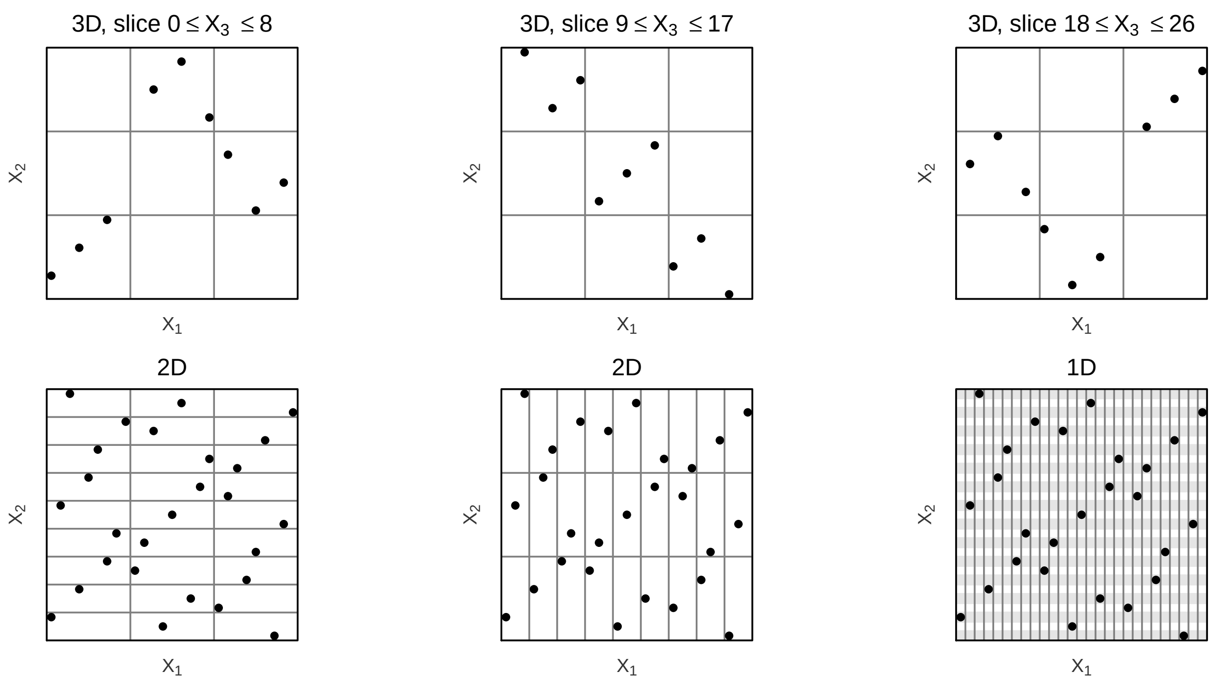

Figure 4: Illustration of stratification properties for three columns of an OSOA(27,4,27,2*) from the Li et al. construction.

but may also have 3D stratification behavior similar to Figure 4. Strength 3+ will be discussed after defining it.

Definition 3 (Properties α, β, γ, Shi and Tang 2020)**.**

$$\begin{array}{llll} \bullet & \text{property } \alpha: & \text{all } s^2 \times s^2 \text{ stratifications in 2D} & \text{yield } s^4 \text{ equally-sized strata.} \\ \bullet & \text{property } \beta: & \text{all } s^2 \times s \times s \text{ stratifications in 3D} & \text{yield } s^4 \text{ equally-sized strata.} \\ \bullet & \text{property } \gamma: & \text{all } s^3 \times s \text{ stratifications in 2D} & \text{yield } s^4 \text{ equally-sized strata.} \end{array} \tag{10}$$

Definition 4 (Strength 3+)**.** A strength 3 SOA has strength 3+ iff it fulfills all three properties of Definition 3.

Figure 5 illustrates the stratification properties of an OSOA$(16, 3, 2^3, 3+)$: The OSOA projects onto $16 = 2^4$ equally-sized strata in 3D (property β) and 2D (properties α in the top row γ in the bottom row), i.e., it has the properties of strength 4 SOAs for 2D and 3D projections. So far, to the author's knowledge, strength 3+ constructions for $s > 2$ are not known.

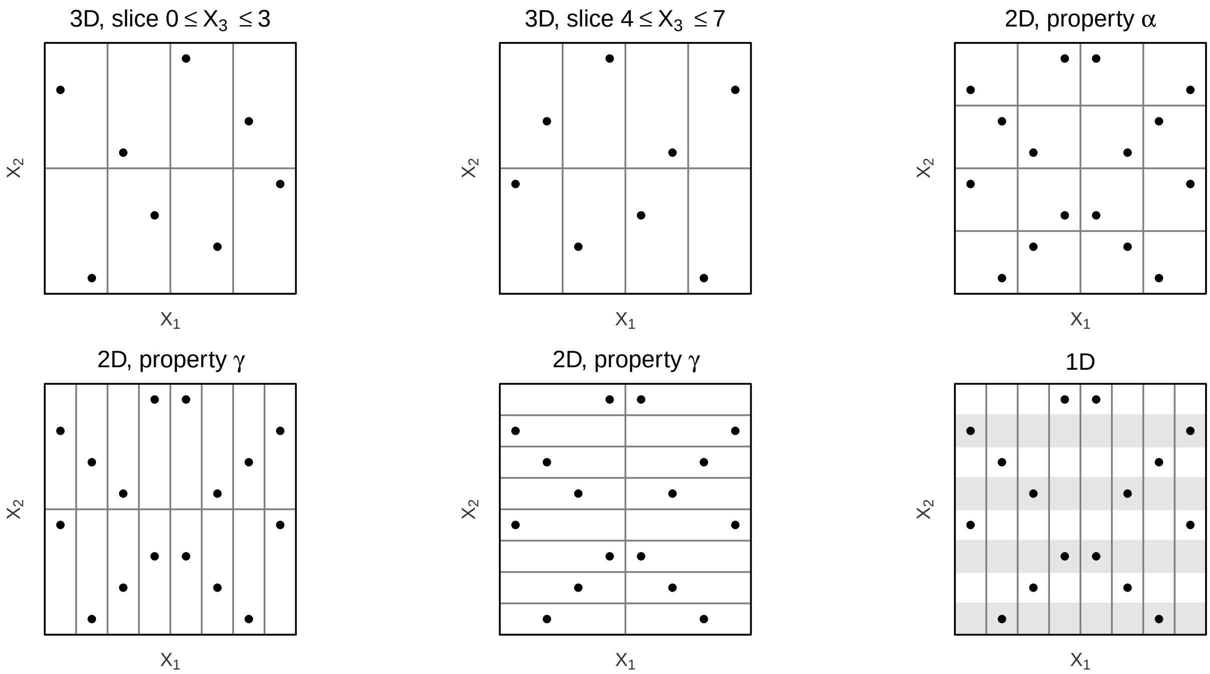

Figure 5: Illustration of stratification properties for SOA strength 3+, based on the rightmost design of Table 11 in Appendix C. The top row shows the 3D stratification of $X_1 \times X_2 \times X_3$ into $4 \cdot 2 \cdot 2 = 16$ strata (left and middle). The 2D plots show the stratification of $X_1 \times X_2$ into $4 \cdot 4 = 16$ strata (top right), $8 \cdot 2 = 16$ strata (bottom left) or $2 \cdot 8 = 16$ strata (bottom middle), and the 1D plot depicts the obvious stratification of X_1 and X_2 into 8 1D strata each (right).

Remark. SOAs whose strength t has no modifier ($-$, * or $+$) always have columns with s^t levels. Modifiers were introduced for more flexibility in this respect, and for denoting partial fulfillment of strength requirements.

(i) One might argue that the introduction of strengths $3-$ and 2^* is somewhat redundant, because it would suffice to communicate the numbers of levels with the strengths 3+, 3 or 2+: strengths 3+, 3 and 2^* indicate s^3 levels, strengths $3-$ and 2+ indicate s^2 levels for each column, i.e., the pairs $(3+, s^3)$, $(3, s^3)$, $(2+, s^3)$, $(3, s^2)$ and $(2+, s^2)$ would be sufficient. Nevertheless, we use the established notation from the literature, and its natural extension by 3+.

(ii) Tian and Xu (2022) proposed to separate the number of levels s^ℓ entirely from the SOA strength t, calling the resulting designs generalized SOAs (GSOAs). A GSOA with s^ℓ-level columns, $\ell > t$, can be easily obtained by level expansion from an SOA(n, m, s^t, t), as long as n is a multiple of s^ℓ. A GSOA with reduced number of levels could be obtained by collapsing column levels, but specific construction algorithms are likely to yield more columns.

OSOAs have orthogonal columns. SOAs without the "O" tend to have correlated columns, but whenever space filling behavior is optimized in some way, correlations are typically not too severe, so that it may be acceptable to use non-orthogonal SOAs, as long as they achieve better space filling properties. For example, the optimized 27 run SOA from Figure 3 even has uncorrelated columns (while the unoptimized version had correlation almost +0.2 for all pairs).

3.4. Further results on achieving balance properties

Lemmas 2 and 3 stated existence and construction hints for strength 2 and strength 3 (O)SOAs. He, Cheng and Tang (2018) ascertained the following construction for strength 2+ (their proposition 1):

Lemma 7 (He, Cheng and Tang 2018)**.** *An SOA*$(n, m, s^2, 2+)$ *exists if and only if* $n \times m$ *matrices* $\mathbf{A}$ *and* $\mathbf{B}$ *can be found such that* $\mathbf{A}$ *is an OA*$(n, m, s, 2)$*,* $\mathbf{B}$ *is an OA*$(n, m, s, 1)$*, and all triples* $(\mathbf{a}_\ell, \mathbf{a}_j, \mathbf{b}_j)$ *are OA*$(n, 3, s, 3)$ *for* $\ell \neq j$*. These arrays are linked through Equation (3).*

Zhou and Tang (2019) gave conditions for obtaining an OSOA of strength 2+ (their Theorem 1 and Remark 1):

Lemma 8 (Zhou Tang 2019)**.** *If the matrix* $\mathbf{B}$ *in Lemma 7 is an OA*$(n, m, s, 2)$ *or a column-orthogonal OA*$(n, m, s, 1)$*, Equation (3) yields an OSOA*$(n, m, s^2, 2+)$*.*

In the light of this lemma, it is advisable to bring $\mathbf{B}$ as close to strength 2 as possible for strength 2+ SOAs, in order to achieve column orthogonality, where possible. Zhou and Tang furthermore gave conditions for making the SOA obtained from Equation (3) achieve strength 3− (their Lemma 1):

Lemma 9 (Zhou Tang 2019)**.** *If the matrix* $\mathbf{A}$ *in Lemma 7 is an OA*$(n, m, s, 3)$*, Equation (3) yields an SOA*$(n, m, s^2, 3-)$*.*

Li, Liu and Yang (2021a) stated their rules for strength 2^* w.r.t. their specific construction only. In general terms, strength 2^* is attained, whenever the conditions of Lemma 3 are fulfilled, except for weakening the requirement for $\mathbf{A}$ to strength 2 instead of strength 3.

The following results of this section hold for $s = 2$ only. Shi and Tang (2020) provided necessary and sufficient conditions under which properties α, β and γ of Definition 3 are fulfilled (their Proposition 1):

Lemma 10 (Shi and Tang 2020)**.** *Let* $\mathbf{D} = s^2\mathbf{A} + s\mathbf{B} + \mathbf{C}$ *an SOA*$(n, m, 8, 3)$*,* $n = 2^k$*, and let the columns of* $\mathbf{A}$*,* $\mathbf{B}$ *and* $\mathbf{C}$ *be chosen from the saturated regular OA*$(n, 2^k - 1, 2, 2)$*. The properties (10) are obtained under the following conditions:*

(i) $\mathbf{D}$ *projects into* s^4 *equally-sized* $s^2 \times s^2$ *strata (property* α*)*
iff $(\mathbf{a}_\ell, \mathbf{b}_\ell, \mathbf{a}_j, \mathbf{b}_j)$ *has strength 4 for all* $\ell \neq j$*.*
(ii) $\mathbf{D}$ *projects into* s^4 *equally-sized* $s^2 \times s \times s$ *strata (property* β*),*
iff $(\mathbf{a}_\ell, \mathbf{a}_j, \mathbf{a}_u, \mathbf{b}_u)$ *has strength 4 for all triples* (ℓ, j, u) *with distinct elements.*
(iii) $\mathbf{D}$ *projects into* s^4 *equally-sized* $s^3 \times s$ *strata,*
iff $(\mathbf{a}_\ell, \mathbf{a}_j, \mathbf{b}_j, \mathbf{c}_j)$ *has strength 4 for all* $\ell \neq j$ *(property* γ*).*

Let us briefly consider the performance of the strength 3 construction of He and Tang (2013; see Table 2) with a regular fractional factorial 2-level matrix $\mathbf{V}$ w.r.t. the criteria: Part (i) of the lemma implies that this construction cannot produce SOAs with property α, because all columns of $\mathbf{B}$ are identical (disregarding level permutation). Part (ii) implies that the construction produces an SOA with property β iff all quadruples of columns of $\mathbf{V}$ that contain column $\mathbf{v}_m$ have strength 4. Part (iii) implies that the construction cannot produce an SOA with property γ for all quadruples $(\mathbf{a}_\ell, \mathbf{a}_j, \mathbf{b}_j, \mathbf{c}_j)$, because $\mathbf{a}_\ell = \mathbf{c}_j$ for some pairs (ℓ, j).

3.5. OAs as OSOAs

We now take a brief look at using OAs as SOAs. First, note that any OA$(n, m, \ell, 2)$ has orthogonal columns. We consider OAs with s^k levels relative to the underlying s, when considering their strengths as SOAs. Note that a given OA can be considered together with different s, if its number of levels permits (e.g. $81 = 3^4 = 9^2$).

(i) Any OA$(n, m, s^2, 2)$ is, by construction, also an OSOA$(n, m, s^2, 2+)$, and it additionally fulfills property α.
(ii) An OA$(n, m, s^2, 2)$ may be an OSOA$(n, m, s^2, 3-)$ or even an OSOA$(n, m, s^2, 3+)$ (see example below).
(iii) Any OA$(n, m, s^2, 3)$ is an OSOA$(n, m, s^2, 3-)$ and additionally fulfills property α (and further balance properties for which no labels have been defined in the SOA literature).
(iv) Any OA$(n, m, s^3, 2)$ is, by construction, also an OSOA$(n, m, s^3, 2^*)$ that fulfills properties α and γ.
(v) Any OA$(n, m, s^3, 3)$ is, by construction, also an OSOA$(n, m, s^3, 3+)$.

For example, an OA$(81, 10, 9, 2)$ with $s = 3$ is an OSOA$(81, 10, 9, 2+)$ and fulfills property α. Similarly, an OA$(729, 28, 27, 2)$ with $s = 3$ is an OSOA$(729, 28, 27, 2^*)$, which competes, for example, with an OSOA$(729, 28, 27, 3)$ from the Liu and Liu method that can be created from the OA$(729, 56, 3, 3)$ provided in Section 5.12 of Hedayat et al. (1999); the OA does not have 3-orthogonal columns, whereas the Liu Liu-based OSOA has 3-orthogonal columns, but is not an OA. The 16 8-level columns from the OA$(128, 8^{16}16^1, 2)$ from the Kuhfeld (2010) collection with $s = 2$ are an OSOA$(128, 16, 8, 3+)$ $(s = 2)$ and are thus an example for (ii); the Shi and Tang method permits one to obtain strength 3+ in 128 runs with up to 31 8-level columns; if one only needs 16, it might be a better idea to use the OA, as its space-filling properties are not much worse. An OA$(729, 10, 9, 3)$ with $s = 3$ is an OSOA$(729, 10, 9, 3-)$ with property α (and further balance properties for which no labels have been defined in the SOA literature). For quantitative variables in computer experiments, the OSOA$(729, 28, 27, 3)$ discussed above is presumably more attractive; or if one only wants 9 levels, an OSOA of strength 2+ can be obained for a large number of columns (up to 121 from the ZT construction and even up to 301 from the HCT construction). Nevertheless, if only 10 columns are needed, the OA may be the best choice.

4. Constructions for further (O)SOAs in s^3 levels

This section covers constructions in terms of Equation (4). The strength 3 constructions by He and Tang (2013) and Liu and Liu (2015) were already covered in Section 3.2. The following two sub sections provide the construction of OSOAs of strength 2^* or 3 by Li, Liu and Yang (2021a) and the construction of strength 3 or 3+ 8-level SOAs by Shi and Tang (2020).

4.1. Li, Liu and Yang's construction of OSOAs of strength 2^* *or* 3

Li et al. (2021a) proposed a procedural algorithm, based on two OA$(n, m, s, 2)$ called $\mathbf{A}$ and $\mathbf{B}$. The constructions are related to the construction by Liu and Liu (2015; see Section 3.2.2). A key difference is that Li et al. considered separate matrices $\mathbf{A}$ and $\mathbf{B}$ and made more lenient assumptions on $\mathbf{B}$, rather than taking the columns of both these matrices from a single OA $\mathbf{V}$ that is subjected to strong assumptions.

For odd m, the last column of both matrices $\mathbf{A}$ and $\mathbf{B}$ is omitted, so that one can require m to be even. The algorithm constructs OSOA$(n, m, s^3, \text{strength})$ of strengths 2^* or 3. It yields

- strength 3 for $m = n/2 - 2$ columns with 8 levels, where n is a multiple of 8, based on doubled Hadamard matrices,
- strength 2^* for $m' = 2\lfloor m/2 \rfloor$ columns with s^3 levels, based on an arbitrary OA$(n/s, m, s, 2)$, $\mathbf{V}$. This has the special case, where $n = s^k$ and $\mathbf{V}$ is the regular saturated OA$(n/s, (s^{k-1} - 1)/(s - 1), s, 2)$.
- strength 3, if the $\mathbf{V}$ from the previous bullet has strength 3.

Proposition 1. *Li et al.'s (2021) algorithm based on the $n \times m$ matrices $\mathbf{A}$ and $\mathbf{B}$ can be restated as follows with $m' = 2 \cdot \lfloor m/2 \rfloor$:*

$$\mathbf{D} = s^2 \mathbf{A}_{1:m'} + s\mathbf{B}_{1:m'} + \mathbf{C}$$

with

$$\mathbf{C} = \mathcal{S}(\mathbf{A}_{1:m'}) \tag{11}$$

with $\mathcal{S}$ from Definition 1.

This representation will be used here, because it fits in nicely with Equation (4) and related results; note the close similarity to the Liu and Liu (2015) construction for strength 3. Chapter 2 of the Supplemental Material contains the proof for the proposition.

Depending on the properties of $\mathbf{A}$ and $\mathbf{B}$, the construction generates OSOA$(n, m', s^3, 2^*)$ or OSOA$(n, m', s^3, 3)$, where $m' = 2\lfloor m/2 \rfloor$. Note that one does not need to assume that $\mathbf{A}$ and $\mathbf{B}$ are subsets of columns from a saturated regular OA. Li et al. provided the following general results:

Lemma 11 (Li et al. 2021)**.** *Let $\mathbf{D} = s^2\mathbf{A} + s\mathbf{B} + \mathbf{C}$ with $\mathbf{C}$ chosen according to Equation (11), and let $\mathbf{A}$ and $\mathbf{B}$ be OA$(n, m, s, 2)$.*

(i) *If all three-column sets $(\mathbf{a}_i, \mathbf{a}_j, \mathbf{b}_j), i \neq j$, are OA$(n, 3, s, 3)$, $\mathbf{D}$ is an OSOA$(n, m, s^3, 2^*)$ (Theorem 2 in Li et al.).*
(ii) *If in addition to (i) $\mathbf{A}$ is an OA$(n, m, s, 3)$, $\mathbf{D}$ is an OSOA$(n, m, s^3, 3)$ (Theorem 3 in Li et al.).*

4.1.1. Obtain an OSOA from a general OA

Let $\mathbf{V}$ be an OA$(n/s, m, s, 2)$, and $m' = 2\lfloor m/2 \rfloor$. Li et al.'s construction of $n \times m'$ matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ for obtaining an OSOA$(n, m', s, 2^*)$ via Equation (4) can be stated as follows:

$$\mathbf{A} = (\mathbf{V}^\top, \mathbf{V}^\top +_s 1, \ldots, \mathbf{V}^\top +_s (s-1))^\top, \quad \mathbf{B} = (\mathbf{V}^\top, \mathbf{V}^\top, \ldots, \mathbf{V}^\top)^\top, \tag{12}$$

with $\mathbf{C}$ again obtained from Equation (11). According to Lemma 11, $\mathbf{D}$ generally has strength 2^*. If $\mathbf{V}$ has OA strength 3, the OSOA $\mathbf{D}$ also has strength 3. Section 4.1.2 will provide a modification for $\mathbf{A}$ that preserves the benefits of Equation (12) and improves the chances for good space-filling and for obtaining strength 3 even if $\mathbf{V}$ only has OA strength 2.

Level permutations according to Weng (2014) can be applied to the columns of $\mathbf{V}$ or separately to the columns of $\mathbf{A}$ and $\mathbf{B}$ (see also next section); the construction of matrix $\mathbf{C}$ from $\mathbf{A}$ must always follow Equation (11). Li et al. emphasized that the construction (12) does not require s to be a prime power. Thus, it can, e.g., be used for constructing an OSOA$(432, 6, 216, 2^*)$ from the symmetric 6-level portion of the OA$(72, 16, 2^5 3^3 4^1 6^7, 2)$ from Warren Kuhfeld's collection.

Example 7. Table 11 (subtable LLY) in Appendix C lists an OSOA$(16, 4, 8, 3)$ of this construction, which uses the first four columns of the OA$(8, 7, 2, 2)$ of Table 13 in the role of $\mathbf{V}$: apart from level permutations, $\mathbf{A}$ stacks $\mathbf{V}$ with $\mathbf{V} +_2 1 = 1 - \mathbf{V}$, $\mathbf{B}$ stacks two identical copies of $\mathbf{V}$, and $\mathbf{C} = \mathcal{S}(\mathbf{A})$. The resulting design is the same as the design by the Liu and Liu construction, except for row permutations; thus, the matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are also the same, except for a common permutation of rows, again with level swaps according to the algorithm by Weng (2014) for improved space filling.

Example 8. The OSOA$(27, 4, 27, 2^*)$ that was depicted in Figure 4 was obtained using this construction with the OA$(9, 3, 4, 2)$ of the Kuhfeld collection (available as `L9.3.4` in R package DoE.base) in the role of $\mathbf{V}$. For the unoptimized OSOA, $\mathbf{A}$ stacks $\mathbf{V}$, $\mathbf{V} +_3 1$, $\mathbf{V} +_3 2$, whereas $\mathbf{B}$ stacks three identical copies of $\mathbf{V}$, and $\mathbf{C} = \mathcal{S}(\mathbf{A}) = (\mathbf{a}_2, 2 - \mathbf{a}_1, \mathbf{a}_4, 2 - \mathbf{a}_3)$ (created with code `OSOAs(L9.3.4, optimize=FALSE)`). The Liu and Liu construction cannot construct a strength 3 OSOA in 27 runs with 3 or more columns (and neither a strength 2^* or a strength $3-$ OSOA).

4.1.2. Strength 3 constructions from a strength 2 OA

Strength 3 for the OSOA $\mathbf{D}$ does not require that the OA $\mathbf{V}$ in Equation (12) has OA strength 3: it is sufficient that the matrix $\mathbf{A}$ has OA strength 3. This is for example achieved for $s = 2$, whenever $\mathbf{V}$ is the 0/1 version of a Hadamard matrix without the constant column, or more generally, whenever the foldover method is able to turn a strength 2 OA $\mathbf{V}$ into OA strength 3. Thus, strength 3 OSOAs with 8-level columns in n runs can be obtained for up to $n/2 - 2$ columns from a Hadamard matrix construction (see Section 3.2 of Li et al. 2021).

For $s > 2$, the foldover principle no longer holds. Nevertheless, the matrix $\mathbf{A}$ from Equation (12) can achieve OA strength 3 in some cases, and whether or not that happened can at least be diagnosed post-hoc. If a strength 2 matrix $\mathbf{V}$ is subjected to the Weng (2014) method of column wise level permutations, some matrices $\mathbf{A}$ from Equation (12) may have OA strength 3, others only OA strength 2.

There are three different approaches of richer level permutations than only permuting the columns of $\mathbf{V}$: 1) One can create the matrix $\mathbf{A}$ from a matrix $\mathbf{V_A}$ obtained by using different permutations of the levels of $\mathbf{V}$ than those used for obtaining $\mathbf{B}$ in Equation (12) (permuting the levels of the columns of $\mathbf{A}$ instead of those of the columns of $\mathbf{V}$ would not affect the OA strength of $\mathbf{A}$). 2) Alternatively, one can use a single permutation for $\mathbf{V}$ and can apply Weng's (2014) method to the added values of a slight generalization of Li et al.'s construction of $\mathbf{A}$: The key idea here is to add column-specific constants in the construction of $\mathbf{A}$:

$$\mathbf{A} = \mathbf{B} +_s \mathbf{M}, \quad \mathbf{B} = (\mathbf{V}^\top, \mathbf{V}^\top, \ldots, \mathbf{V}^\top)^\top, \tag{13}$$

where $\mathbf{M}$ is an $n \times m'$ matrix that consists of columns $(\pi_{1\ell}\mathbf{1}_{n/s}^\top, \ldots, \pi_{s\ell}\mathbf{1}_{n/s}^\top)^\top$, $\ell = 1, \ldots, m'$, with $\boldsymbol{\pi}_\ell = (\pi_{1\ell}, \ldots, \pi_{s\ell})^\top$ denoting a permutation of $(0, \ldots, s-1)$. This construction, combined with level permutation applied to the columns of $\mathbf{B}$ and $\mathbf{M}$, is currently implemented in R package SOAs. 3) It would also be possible to combine 1) and 2), i.e., to replace $\mathbf{A}$ in Equation (13) with $\mathbf{A} = (\mathbf{V_A}^\top, \mathbf{V_A}^\top, \ldots, \mathbf{V_A}^\top)^\top +_s \mathbf{M}$ obtained from using a separate tuples of level permutations for the matrices $\mathbf{V_A}$ and $\mathbf{M}$.

If $\mathbf{V}$ already had OA strength 3, all three approaches preserve that strength. If $\mathbf{V}$ has OA strength 2 only, a beneficial pattern of level permutations in $\mathbf{V_A}$ and/or $\mathbf{M}$ can cause the OA strength of $\mathbf{A}$ to become 3. For example, as an OA$(81, 9, 3, 3)$ exists, one can expect that an OSOA$(81, 8, 27, 3)$ should be obtainable by the algorithm: thus, using the first eight 3-level columns from the mixed-level OA$(27, 3^9 9^1, 2)$, optimization of space filling via level permutation indeed yields such an array for some seeds (and can be looped until it succeeds in doing so; R package SOAs succeeded with a seed of 6540 on a Windows 10 system). In the examples that were inspected, the strength 3 OSOAs did not exhibit close to optimal space filling in terms of the ϕ_p value, but rather a value around the upper quartile of ϕ_p values. Thus, higher strength and better space filling in terms of ϕ_p seem to be conflicting targets, but this may very well be dependent on specifics of the situation. This matter has not been explored in depth.

4.2. Shi and Tang's strength 3 SOAs with additional balance properties

Shi and Tang (2020) constructed SOAs from a $2^k \times (2^k - 1)$ saturated regular strength 2 fraction $\mathbf{S}$. The $n \times m'$ matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ ($n = 2^k$) for Equation (4) have columns from that $\mathbf{S}$. Shi and Tang treated 2-level fractions in the $-1/+1$ coding with multiplication that is often used for 2-level fractions. Here, we will use the equivalent $0/1$ encoding with $+_2$. The additional balance properties α, β and γ that were introduced by Shi and Tang were already presented in Section 3.3. Emphasis is on the construction of matrices $\mathbf{A}$ and $\mathbf{B}$. The matrix $\mathbf{C}$ can always be obtained according to Lemma 4.

4.2.1. $5n/16$ *8-level columns with property* α

Shi and Tang's first family of SOAs exists for $n \geq 16$ and is based on the following recursive construction.

Lemma 12. *Let* $\mathbf{A}_k$ *and* $\mathbf{B}_k$ *fulfill all conditions for obtaining an SOA*$(2^k, m, 8, 3)$ *with property* α *through Equation (4). Then the matrices* $\mathbf{A}_{k+2}$ *and* $\mathbf{B}_{k+2}$ *constructed by*

$$\mathbf{A}_{k+2} = \begin{pmatrix} \mathbf{A}_k & \mathbf{A}_k & \mathbf{A}_k & \mathbf{A}_k \\ \mathbf{A}_k & 1 +_2 \mathbf{A}_k & \mathbf{A}_k & 1 +_2 \mathbf{A}_k \\ \mathbf{A}_k & \mathbf{A}_k & 1 +_2 \mathbf{A}_k & 1 +_2 \mathbf{A}_k \\ \mathbf{A}_k & 1 +_2 \mathbf{A}_k & 1 +_2 \mathbf{A}_k & \mathbf{A}_k \end{pmatrix}$$

and

$$\mathbf{B}_{k+2} = \begin{pmatrix} \mathbf{B}_k & \mathbf{B}_k & \mathbf{B}_k & \mathbf{B}_k \\ \mathbf{B}_k & \mathbf{B}_k & 1 +_2 \mathbf{B}_k & 1 +_2 \mathbf{B}_k \\ \mathbf{B}_k & 1 +_2 \mathbf{B}_k & 1 +_2 \mathbf{B}_k & \mathbf{B}_k \\ \mathbf{B}_k & 1 +_2 \mathbf{B}_k & \mathbf{B}_k & 1 +_2 \mathbf{B}_k \end{pmatrix}.$$

fulfill all conditions for obtaining an SOA$(2^{k+2}, 4m, 8, 3)$ *with property* α *through Equation (4).*

Lemma 12 states the recursive construction rule by Shi and Tang in the notation of this paper. Once there are start values for even and for odd k, one can recursively construct all designs for larger values of k. Start values are available for $k = 4$ and $k = 7$, and the case $k = 5$ can be treated separately, so that SOAs with property α are available for $k \geq 4$. Start values are provided in Appendix B.

The recursive construction of Lemma 12 is somewhat inconvenient, and it is not straightforward to state it as a non-recursive general formula. However, it is straightforward to state update rules in terms of Yates matrix column numbers, which simplifies considerations and computations. The construction of Lemma 12 means that the Yates matrix columns from the smaller design remain in place, and further Yates matrix columns are added according to the following proposition.

Proposition 2. *Let* $Y_{\mathbf{A}}$ *and* $Y_{\mathbf{B}}$ *denote the tuples of Yates matrix column numbers of matrices* $\mathbf{A}$ *and* $\mathbf{B}$*, and let* $\mathbf{A}_k$ *and* $\mathbf{B}_k$ *denote the matrices from constructions for* $n = 2^k$*. Then, the matrices for* $n = 2^{k+2}$ *can be obtained with the following Yates matrix tuples:*

$$Y_{\mathbf{A}_{k+2}} = (Y_{\mathbf{A}_k}, Y_{\mathbf{A}_k} + 2^k, Y_{\mathbf{A}_k} + 2^{k+1}, Y_{\mathbf{A}_k} + 2^k + 2^{k+1}),$$
$$Y_{\mathbf{B}_{k+2}} = (Y_{\mathbf{B}_k}, Y_{\mathbf{B}_k} + 2^{k+1}, Y_{\mathbf{B}_k} + 2^k + 2^{k+1}, Y_{\mathbf{B}_k} + 2^k).$$

According to Lemma 10 (i), the matrix $\mathbf{C}$ is irrelevant for obtaining property α. With the start values given in Appendix B, it can be observed that the Yates matrix column numbers from Proposition 2 do not contain multiples of 16 (excluding the single special case $k = 5$). This also holds for $Y_{\mathbf{A}+_2\mathbf{B}}$. According to Lemma 4, it is therefore adequate (though by no means necessary) to choose $\mathbf{C}$ as a matrix with all columns equal to one of those Yates matrix columns. (For $k = 4$, there are no such Yates matrix columns; Appendix B suggests one of many possible solutions for that case.)

Example 9. For $k = 4$, the Shi and Tang family 1 SOA(16, 4, 8, 3) of Table 11 was obtained using the first four elements of the start values from Appendix B, i.e.,

- Yates matrix columns 1, 2, 4 and 8 for $\mathbf{A}$ ($\mathbf{A} = \lfloor \mathbf{D}/2^2 \rfloor$ shows that levels of column 8 were swapped),
- Yates matrix columns 12, 9, 3 and 6 for $\mathbf{B}$ ($\mathbf{B} = \lfloor (\mathbf{D} - 2^2 \cdot \mathbf{A})/2 \rfloor$ shows that the levels of columns 12, 9 and 6 were swapped),
- and Yates matrix columns 2, 1, 1 and 1 for $\mathbf{C}$ ($\mathbf{C} = \mathbf{D} - 2^2 \cdot \mathbf{A} - 2 \cdot \mathbf{B}$ shows that the levels of the second and third column were swapped).

Level permutations yielded a slight improvement of ϕ_p (from 0.169 to 0.148. As the SOA has property α, coarsening its levels to four instead of eight by collapsing neighboring levels yields an OA(16, 4, 4, 2). The SOA does neither have property β nor property γ.

4.2.2. Strength 3+ SOAs in $n/4 - 1$ 8-level columns, or one more column without property γ

Shi and Tang proposed two further SOA families in $n = 2^k$ runs: SOA$(n, n/4, 8, 3)$ with properties α and β (their Family 2) and an SOA$(n, n/4 - 1, 8, 3+)$ (their Family 3). The two constructions are closely related and are therefore presented together.

The starting point is a saturated regular OA$(n/4, n/4 - 1, 2, 2)$ called $\mathbf{X}$ that is based on $k - 2$ basic vectors. Let $\mathbf{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_{n/4-1})$ be a reshuffling of the columns of $\mathbf{X}$ such that

- $\mathbf{x}_\ell$ and $\mathbf{y}_\ell$ are different for $\ell = 1, \ldots, n/4 - 1$
- for $\mathbf{Z} = \mathbf{X} +_2 \mathbf{Y}$, the triple $(\mathbf{x}_\ell, \mathbf{y}_\ell, \mathbf{z}_\ell)$ has strength at least 2 for $\ell = 1, \ldots, n/4 - 1$.

Shi and Tang proved that such a $\mathbf{Y}$ can be found. The start matrices for $k = 2$ and $k = 3$ for the recursive construction are given in Lemma 13 in terms of Yates matrix column numbers, and the subsequent proposition provides the recursive construction:

Lemma 13 (restated from Shi and Tang 2020)**.** *Let $Y_\mathbf{M}$ denote the tuple of Yates matrix column numbers for a matrix $\mathbf{M}$. The start values of the Shi and Tang construction for their Families 2 and 3 are given as follows:*
For $k = 2$, $Y_\mathbf{X} = (1, 2, 3)$, $Y_\mathbf{Y} = (2, 3, 1)$, and $Y_\mathbf{Z} = (3, 1, 2)$.
For $k = 3$, $Y_\mathbf{X} = (1, 2, 3, 4, 5, 6, 7)$, $Y_\mathbf{Y} = (7, 5, 2, 1, 6, 4, 3)$ and $Y_\mathbf{Z} = (6, 7, 1, 5, 3, 2, 4)$.

Proposition 3 (restated from Shi and Tang 2020)**.** *Let $Y_{\mathbf{X}_k}$, $Y_{\mathbf{Y}_k}$ and $Y_{\mathbf{Z}_k}$ denote the tuples of Yates matrix column numbers for $2^k \times (2^k - 1)$ matrices $\mathbf{X}_k$, $\mathbf{Y}_k$ and $\mathbf{Z}_k$, such that $\mathbf{x}_\ell +_2 \mathbf{y}_\ell = \mathbf{z}_\ell$ and $(\mathbf{x}_\ell, \mathbf{y}_\ell, \mathbf{z}_\ell)$ have at least strength 2, $\ell = 1 \ldots, 2^k - 1$. Then, $2^{k+2} \times (2^{k+2} - 1)$ matrices $\mathbf{X}_{k+2}$, $\mathbf{Y}_{k+2}$ and $\mathbf{Z}_{k+2}$ with the same properties can be obtained using the following Yates matrix tuples:*

$$\begin{aligned}
Y_{\mathbf{X}_{k+2}} &= (Y_{\mathbf{X}_k}, 2^k, Y_{\mathbf{X}_k} + 2^k, 2^{k+1}, Y_{\mathbf{X}_k} + 2^{k+1}, 2^k + 2^{k+1}, Y_{\mathbf{X}_k} + 2^k + 2^{k+1}),\\
Y_{\mathbf{Y}_{k+2}} &= (Y_{\mathbf{Y}_k}, 2^{k+1}, Y_{\mathbf{Y}_k} + 2^{k+1}, 2^k + 2^{k+1}, Y_{\mathbf{Y}_k} + 2^k + 2^{k+1}, 2^k, Y_{\mathbf{Y}_k} + 2^k),\\
Y_{\mathbf{Z}_{k+2}} &= (Y_{\mathbf{Z}_k}, 2^k + 2^{k+1}, Y_{\mathbf{Z}_k} + 2^k + 2^{k+1}, 2^k, Y_{\mathbf{Z}_k} + 2^k, 2^{k+1}, Y_{\mathbf{Z}_k} + 2^{k+1}).
\end{aligned}$$

Together with the start tuples from Lemma 13, a construction of $2^k \times (2^k - 1)$ matrices $\mathbf{X}$, $\mathbf{Y}$ and $\mathbf{Z}$ is thus available for all $k \geq 2$.

Example 10. Applying Proposition 3 for obtaining the 16×15 matrices (i.e., $k + 2 = 4$) yields

- Yates matrix columns 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15 for $\mathbf{X}$,
- Yates matrix columns 2,3,1,8,10,11,9,12,14,15,13,4,6,7,5 for $\mathbf{Y}$ and consequently
- Yates matrix columns 3,1,2,12,15,13,14,4,7,5,6,8,11,9,10 for $\mathbf{Z}$.

The saturated $\mathbf{X}$ is always in original Yates order, i.e., $Y_{\mathbf{X}_k} = (1, \dots, 2^k - 1)$. Algorithmically, it suffices to construct the reshuffled $\mathbf{Y}$, since $\mathbf{Z}$ is a direct consequence and is also not needed for the construction (see below).

The following lemma states the construction of the matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ for Equation (4) from the matrices $\mathbf{X}$ and $\mathbf{Y}$.

Lemma 14 (restated from Shi and Tang 2020)**.** *Let $\mathbf{X}$ and $\mathbf{Y}$ be $2^{k-2} \times (2^{k-2} - 1)$ matrices according to Proposition 3.*

(i) *$2^k \times 2^{k-2}$ matrices for constructing Shi and Tang's Family 2 from Equation (4) are given as*

$$\mathbf{A} = \begin{pmatrix} \mathbf{0}_{n/4} & \mathbf{X} \\ \mathbf{0}_{n/4} & \mathbf{X} \\ \mathbf{1}_{n/4} & 1 +_2 \mathbf{X} \\ \mathbf{1}_{n/4} & 1 +_2 \mathbf{X} \end{pmatrix}, \quad \textit{and} \quad \mathbf{B} = \begin{pmatrix} \mathbf{0}_{n/4} & \mathbf{Y} \\ \mathbf{1}_{n/4} & 1 +_2 \mathbf{Y} \\ \mathbf{0}_{n/4} & \mathbf{Y} \\ \mathbf{1}_{n/4} & 1 +_2 \mathbf{Y} \end{pmatrix}. \tag{14}$$

(ii) *The construction (i) yields an $SOA(n, n/4, 8, 3)$ with properties α and β, if $\mathbf{c}_\ell$ is chosen as a column from the saturated $OA(2^k, 2^k - 1, 2, 2)$ that is unequal to all three of $\mathbf{a}_\ell$, $\mathbf{b}_\ell$ and $\mathbf{a}_\ell +_2 \mathbf{b}_\ell$.*

(iii) *If each first column is omitted, and one of them is used instead for each column of $\mathbf{C}$, the result is an $SOA(n, n/4 - 1, 8, 3+)$ corresponding to Shi and Tang's Family 3.*

The construction of Equation (14) for a design with $n = 2^k$ rows based on $n/4 \times (n/4 - 1)$ matrices $\mathbf{X}$ and $\mathbf{Y}$ and can be stated as follows in Yates matrix notation:

Corollary 1. *The construction of Lemma 14 is equivalent to using the following tuples of Yates matrix columns for constructing the matrices $\mathbf{A}$ and $\mathbf{B}$ (omitting the respective first column for the strength 3+ construction):*

- $Y_{\mathbf{A}} = (n/2, n/2 + Y_{\mathbf{X}}) = (n/2, n/2 + 1, \dots, 3n/4 - 1)$,
- $Y_{\mathbf{B}} = (n/4, n/4 + Y_{\mathbf{Y}})$,
- $Y_{\mathbf{A}+_2\mathbf{B}} = (n/2 + n/4, n/2 + n/4 + Y_{\mathbf{Z}})$.

Proof. The Yates column numbers follow from careful considerations regarding the structure of Yates matrices. □

Example 11. The smallest SOAs for this construction have $n = 16$ runs and are obtained from the start values of Lemma 13 for $k = 2$. The Yates matrix column numbers for the Family 2 construction are

- $Y_{\mathbf{A}} = (8, 9, 10, 11)$ and
- $Y_{\mathbf{B}} = (4, 6, 7, 5)$,

which implies that $Y_{\mathbf{A}+_2\mathbf{B}} = (12, 15, 13, 14)$. Shi and Tang stated that the columns for $\mathbf{C}$ must be chosen different from the three columns in the respective position (cf. Lemma 4), i.e., the first column of $\mathbf{C}$ must not be any of 8, 4, or 12, and so forth. The Family 3 construction omits the first element from each tuple.

The following lemma proposes a choice of columns for $\mathbf{C}$ such that the strength 3+ SOA of Shi and Tang's Family 3 becomes an OSOA, and the strength 3 SOA of Shi and Tang's Family 2 has a single pair of correlated columns only.

Lemma 15 (**C** for orthogonal columns)**.** *The following column choices for matrix* **C** *in the constructions of Shi and Tang's Families 2 and 3 are beneficial for obtaining orthogonal columns:*

(i) *For Family 3, choosing* **C** *as the matrix of the first* $n/4-1$ *Yates columns guarantees that an OSOA*$(n, n/4-1, 8, 3+)$ *is obtained.*
(ii) *For Family 2, choosing* **C** *as a matrix of the first* $n/4-1$ *Yates columns with exactly one column duplicated guarantees that there is only a single column pair with non-zero correlation.*

Proof. The proposed column choices fulfill the assumptions of Lemma 4. (i) follows from Lemma 5. (ii) also follows from that lemma, if one realizes that any $n/4-1$ column sub matrix that does not contain the pair with the same **C** column has orthogonal columns according to the lemma. □

Example 12. Table 11 in Appendix C provides the SOA$(16, 4, 8, 3)$ (Family 2) and the OSOA$(16, 3, 8, 3+)$ (Family 3), which were obtained using the Yates matrix columns given in Example 11 for **A** and **B** and Yates matrix columns 1 to 3 for matrix **C** (with one column repeated for Family 2). Optimization of ϕ_p yielded relevant improvement for the Family 2 design, but not for the Family 3 design (see Table 10). If four columns are needed, Family 2 is preferable to Family 1, because the design has properties α and β, instead of property α only. If only three columns are needed, the Family 3 design is preferable, because it has strength 3+.

Chapter 3 of the Supplemental Material provides details for two slightly larger applications of the construction.

5. SOA constructions with m columns in s^2 levels

This section uses the construction from Lemma 2 with Equation (3). Lemmas 7, 8 and 9 gave conditions for a strength 2+ SOA, an OSOA or a strength 3− SOA. The constructions of this section are based on these lemmas.

5.1. Constructions by Zhou and Tang (2019)

The constructions by Zhou and Tang (2019) are similar to the constructions by Li et al. (2021a), which were of course developed later, but were already presented in the previous section. Basically, the matrices **A** and **B** from the Li et al. constructions are used, and the unnecessary matrix **C** is omitted. Generally, the constructions by Zhou and Tang have the same number of columns or one more column, and yield s^2 levels instead of s^3.

Where Li et al. obtained an OSOA$(n, n/2-2, 8, 3)$ from a doubled Hadamard matrix with $n/2$ rows (special case of Equation (12) with **V** a Hadamard matrix), Zhou and Tang obtained an OSOA$(n, n/2-1, 4, 3-)$.

Where Li et al. obtained an OSOA$(s^k, 2\lfloor(s^{k-1}-1)/(2(s-1))\rfloor, s^3, 2^*)$ from a regular saturated OA in s^{k-1} runs (special case of Equation (12) or (13) with **V** a saturated regular OA), Zhou and Tang obtained an OSOA$(s^k, (s^{k-1}-1)/(s-1), s^2, 2+)$.

Where Li et al. obtained an OSOA$(n, 2\lfloor m/2\rfloor, s^3, 3)$ from an OA$(n/s, m, s, 3)$ or an OSOA$(n, 2\lfloor m/2\rfloor, s^3, t)$ ($t = 2^*$ or $t = 3$) from an OA$(n/s, m, s, 2)$, Zhou and Tang obtained an OSOA$(n, m, s^2, 3-)$ (although they did not claim that strength for their general construction) or an OSOA$(n, m, s^2, 2+)$. For this construction, they used **A** and **B** in switched roles (their Theorem 4), which can be improved upon: Using **A** and **B** from Equations (12) or (13) in Equation (3), it is sometimes possible to achieve a strength 3− OSOA in spite of using a matrix **V** with OA strength 2, e.g. when using an OA$(9, 3, 3, 2)$ in the role of **V**.

Example 13. The OSOA$(16, 7, 4, 3-)$ of Table 12 (subtable ZT) has been obtained using the OA$(8, 7, 2, 2)$ of Table 13 in the role of $\mathbf{V}$. In principle, $\mathbf{B}$ consists of two vertically-stacked identical copies of the OA, whereas matrix $\mathbf{A}$ consists of a copy of the OA stacked with another copy that has reversed levels. In addition, Weng's algorithm for level permutation has been applied, which reduced ϕ_p by about a third (see Table 10). The actual matrices $\mathbf{A}$ and $\mathbf{B}$ after application of level swapping can be easily reverse-engineered as $\mathbf{A} = \lfloor \mathbf{D}/2 \rfloor$ and $\mathbf{B} = \mathbf{D} - 2 \cdot \mathbf{A}$.

5.2. He et al.'s construction of strength 2+ SOAs for regular 2-level fractions

He, Cheng and Tang (2018) provided a construction based on regular 2-level fractions. The columns for both $\mathbf{A}$ and $\mathbf{B}$ are chosen from a saturated regular 2-level array $\mathbf{S}$. The construction relies on the concept of an SOS design $\mathbf{X}$ which is characterized as follows: all columns of $\mathbf{S}$ that do not belong to a main effect of $\mathbf{X}$ contain a two-factor interaction of a pair of columns in $\mathbf{X}$. He et al. (2018) proved that it is necessary and sufficient for strength 2+ that all columns of $\mathbf{A}$ are from the complement $\overline{\mathbf{X}}$ in $\mathbf{S}$ of an SOS design $\mathbf{X}$; suitable columns for $\mathbf{B}$ can then be picked from $\mathbf{X}$. According to Lemma 8, populating $\mathbf{B}$ with distinct columns from $\mathbf{X}$ (if possible) makes $\mathbf{D}$ an OSOA; a pair-matching algorithm for bipartite graphs can help to find distinct columns for $\mathbf{B}$. If $\mathbf{A}$ has OA strength 3, the resulting (O)SOA $\mathbf{D}$ has strength $3-$. However, it is not obvious how to ensure OA strength 3 for $\mathbf{A}$ in a systematic way.

5.2.1. Constructions for SOS designs and upper bound for number of columns

He et al. gave four constructions for an SOS design as follows: For a total of $k \geq 4$ independent columns, let $P = P(\{\mathbf{a}_1, \ldots, \mathbf{a}_{k_1}\})$ denote the set of all effects pertaining to $k_1 \geq 2$ columns (i.e., $2^{k_1} - 1$ elements), $Q = Q(\{\mathbf{b}_1, \ldots, \mathbf{b}_{k_2}\})$ the set of all effects pertaining to the remaining $k_2 = k - k_1 \geq 2$ columns (i.e., $2^{k_2} - 1$ elements). Then, the following column choices yield SOS designs (where $\setminus$ denotes subtraction between sets, and $+_2$ between a column and a set denotes the set of separate sums):

(i) $C_1 = P \cup Q$ ($2^{k_1} + 2^{k_2} - 2$ elements),
(ii) $C_2 = (P \setminus \{\mathbf{a}_1\}) \cup (Q \setminus \{\mathbf{b}_1\}) \cup \{\mathbf{a}_1 +_2 \mathbf{b}_1\}$ ($2^{k_1} + 2^{k_2} - 3$ elements),
(iii) $C_3 = (P \setminus \{\mathbf{a}_1\}) \cup (\mathbf{a}_1 +_2 Q)$ ($2^{k_1} + 2^{k_2} - 3$ elements),
(iv) $C_4 = (\mathbf{b}_1 +_2 P) \cup (\mathbf{a}_1 +_2 (Q \setminus \{\mathbf{b}_1\}))$ ($2^{k_1} + 2^{k_2} - 3$ elements).

The minimum possible number of columns for an SOS design determines the maximum possible number m_k of columns for the SOA from this construction. The minimum number achievable from the above constructions is attained by choosing $k_1 = \lfloor k/2 \rfloor$ which implies $2^{\lfloor k/2 \rfloor} + 2^{k - \lfloor k/2 \rfloor} - 3$ SOS matrix columns for C_2 to C_4. Obviously, m_k is at least $2^k - 1$ minus this number. He et al. stated an upper bound for m_k as $2^k - 1 - M(k)$, with $M(k)$ the maximum number of columns in a strength 4 OA. This upper bound can be slightly tightened by realizing that the number of columns m in an SOS design must fulfill the quadratic inequality $m + m(m-1)/2 \geq 2^k - 1$. It is likely that incorporation of structural requirements would lead to further tightening of the upper bound for m_k.

5.2.2. Implementation of the construction

The implementation of the construction has the following steps:

a) Allocate P and Q with k_1 and k_2 columns, $k_1 + k_2 = k$, $|k_1 - k_2| \leq 1$; this choice of k_1 and k_2 minimizes the number of columns of the SOS design.
b) Define R as one of C_2, C_3 or C_4 (set of remaining columns).
c) Obtain $\mathbf{A}$ as the matrix of the columns from the saturated regular $2^k \times (2^k - 1)$ array $\mathbf{S}$ that are not in R, and define A as the set of the columns of $\mathbf{A}$.
d) If the number m of requested columns is smaller than the maximum possible number of columns, reduce $\mathbf{A}$ and A to m columns / elements, respectively, and augment R by the removed elements of A.

e) For each column $\mathbf{a}_j \in A$, define the set S_j as those columns $\mathbf{c} \in R$ that yield a triple of OA strength 3 when added to any pair $\{\mathbf{a}_\ell, \mathbf{a}_j\} \subset A$, $\ell \neq j$ that involves column $\mathbf{a}_j$.

f) Define a bipartite graph G with the vertices from A (type 1) and R (type 2) and edges between $\mathbf{a}_j$ and all elements of S_j. (There is at least one edge for each element of A.)

g) Create $\mathbf{B}$ from the columns $\mathbf{b}_j \in R$ according to the following matching approach:
   - Match a $\mathbf{b}_j$ to each $\mathbf{a}_j \in A$, using a maximum bipartite matching algorithm on the graph G. *If this step matches all columns of A, $\mathbf{B}$ will have strength 2 and column orthogonality will be achieved.*
   - For any unmatched $\mathbf{a}_j \in A$, assign an arbitrary element of S_j as $\mathbf{b}_j$.

h) Apply the algorithm by Weng (2014) for improving ϕ_p, permuting levels in the columns of $\mathbf{A}$ and $\mathbf{B}$.

i) Return $\mathbf{D} = s\mathbf{A} + \mathbf{B}$ from the optimized permutation pattern.

He et al. (2018) did not specify an explicit algorithm, but simply prescribed to populate $\mathbf{B}$ with columns $\mathbf{b}_j$ that are not eligible for $\mathbf{A}$ and fulfill the criteria for membership in the S_j of Step e). Using Steps d) to to h) in the above implementation allows to obtain orthogonal columns (Steps d) to g)) and improved ϕ_p (Step h)). The creation of the bipartite graph and the subsequent bipartite matching can be slow for large applications. Furthermore, it appears that enforcing orthogonal columns can conflict with achieving small values for ϕ_p. For both reasons, the R package SOAs (Grömping 2022b) allows to suppress steps d) to g); in this case, the first possible column from R is assigned for each column position in matrix $\mathbf{B}$, which is exactly in line with He et al.'s prescription.

Example 14. Table 12 (subtables HCT and HCT orth.) holds two SOA$(16, 7, 4, 2+)$s from this construction (at most 10 columns would be possible), an orthogonal and a non-orthogonal one. The R function `SOAs2plus_regular` used the SOS construction C_2, partitioning the four basic columns into the first two and the last two. Looking at the Yates matrix of Table 13, the first two basic columns are columns **1** and **2**, while the last two basic columns are columns **4** and **8**. C_2 consists of (the effects mapped by) columns **2**, $\mathbf{1} +_2 \mathbf{2} = 3$, **8**, $\mathbf{4} +_2 \mathbf{8} = 12$ and $\mathbf{1} +_2 \mathbf{4} = 5$ of the Yates matrix. Hence, the columns of $\mathbf{A}$ must be chosen from the remaining ten columns of the saturated 2-level OA, i.e., from columns 1, 4, 6, 7, 9 to 11, 13 to 15 of the Yates matrix. $\mathbf{A}$ consists of the first seven of these columns, $\mathbf{B}$ can be populated from the set $R = \{2, 3, 8, 12, 5, 13, 14, 15\}$. For the OSOA, the bipartite pair matching algorithm yields Yates matrix columns 2, 8, 3, 5, 12, 15, 14 in that order; the algorithm that skips Steps d) to g) of the implementation uses the first possible matches which are Yates matrix columns 2, 8, 3, 2, 12, 2, 3. It can be seen from Table 10 that application of the Weng (2014) algorithm reduced ϕ_p by around 20 percent in both cases (slightly more for the OSOA and less for the non-orthogonal SOA); the non-orthogonal SOA has a smaller ϕ_p value.
Note that the regular array used in the HCT algorithm is slow changing first; furthermore, the Weng (2014) optimization swapped level order in some cases. Hence, for direct comparison of the OSOA and SOA shown in Table 12 with in-going matrices, one has to calculate $\mathbf{A} = \lfloor \mathbf{D}/2 \rfloor$ and $\mathbf{B} = \mathbf{D} - 2\mathbf{A}$ from the SOA and has to rearrange the rows in the order (1,9,5,13,3,11,7,15,2,10,6,14,4,12,8,16) either for the Yates matrix or for the SOA.

For $s = 2$, the bipartite matching algorithm introduced in this paper can achieve column orthogonality for at most $n/2 - 1$ columns (like in the example); it has not been checked whether it is always guaranteed to do so. The original proposal by He et al. (2018) without step 4 of the implementation would have limited the number of orthogonal columns to five in Example 14.

5.3. He et al.'s construction of strength $2+$ SOAs for regular s level fractions ($s \geq 3$)

The construction of this section works for primes or prime powers $s \geq 3$ via a saturated regular fraction $\mathbf{S}$ which is an OA$(s^k, (s^k - 1)/(s - 1), s, 2)$, $k \geq 3$ (see Section 2.3.1 for the construction of $\mathbf{S}$). An SOA obtained by this construction has s^k runs with up to $m = (s^k-1)/(s-1) - ((s-1)^k-1)/(s-2)$ columns, e.g. six 9-level columns in 27 runs ($s=3$, $k=3$), eight 16-level columns in 64 runs ($s=4$, $k=3$), 25 9-level columns in 81 runs ($s=3$, $k=4$), or 45 16-level columns in 256 runs ($s=4$, $k=4$). The necessary and sufficient conditions for the existence of an SOA of strength 2+ were given in Lemma 7.

The following coarse implementation steps can be followed for an implementation that guarantees orthogonality (through a strength 2 matrix $\mathbf{B}$, according to Lemma 8), whenever that is compatible with strength 2+ for the requested number of runs and columns. The details are very similar to Section 5.2.2 and are therefore omitted.

a) The matrix $\mathbf{A}$ is populated with m of the $(s^k-1)/(s-1) - ((s-1)^k-1)/(s-2)$ linear combinations of at least two of the k basic columns (contained in $\mathbf{S}$) whose first non-zero coefficient is 1 (holds for all columns of $\mathbf{S}$) and whose further coefficients include at least one element $s-1$. The set of the columns of $\mathbf{A}$ is denoted as A.
b) The set of the remaining columns of $\mathbf{S}$ is denoted as R.
c) Consider the elements of A and R as the two types of vertices in a bipartite graph G. Like in Section 5.2, a set $S_j \subseteq R$ of permissible columns is identified for each $\mathbf{a}_j \in A$: the elements of S_j must yield a triple of OA strength 3 with any pair $(\mathbf{a}_\ell, \mathbf{a}_j), j \neq \ell$ (cf. Lemma 7). The graph G has edges between $\mathbf{a}_j$ and all elements of S_j.
d) The columns $\mathbf{b}_j \in R$ of the matrix $\mathbf{B}$ are then chosen by a bipartite pair matching algorithm. Where no perfect match can be found, an arbitrary element of S_j can be chosen for $\mathbf{b}_j$.
e) Optimization of permutations in columns of $\mathbf{A}$ and $\mathbf{B}$ improves the space filling behavior (using the Weng 2014 algorithm).
f) The SOA$(s^k, m, s^2, 2+)$ is obtained as $\mathbf{D} = s\mathbf{A} + \mathbf{B}$ from the optimized permutation pattern.

Improvements versus the construction proposed in He et al. (2018) lie in using all columns not *used* for $\mathbf{A}$ in Step a) (instead of only the columns not eligible for $\mathbf{A}$), in the bipartite matching algorithm of Steps c) and d), and in using level permutations for improving space-filling in Step e). The bipartite matching algorithm achieves orthogonal columns in many relevant settings. For example, for $n = 81$ runs the construction permits up to 25 9-level columns; for up to 20 columns, an OSOA is obtained. All 8 16-level columns in 64 runs can be made orthogonal, while up to 42 (of the 45 possible) 16-level columns in 256 runs can be made orthogonal. For $n = 125$ or $n = 625$ runs in 25-level columns, column orthogonality is achieved for the maximum possible number of columns (10 or 71 columns, respectively). Like for $s = 2$, the bipartite matching can be suppressed, sacrificing orthogonality for the benefit of a potential speed gain and a potentially smaller ϕ_p value.

6. Overview of sizes, strengths and constructions

Aspects in the choice of a suitable (O)SOA are

- the affordable run size n
- the required number of columns m
- the required number of levels per column s^r
- and the required balance properties, reflected by the strength or column orthogonality.

Of course, the larger the strength, the larger the run size requirements for the same number of levels. The R package SOAs (Grömping 2022b) provides two guidance functions (`guide_SOAs` and `guide_SOAs_from_OA`) that help users find suitable SOAs for their application, including a suggestion for (modifiable) construction code.

Table 4 lists the different constructions that are covered in this paper. Tables 5, 6 and 7 give the maximum numbers of columns for the different constructions for some n and $s = 2$ to $s = 4$. For $s = 3$ and $s = 4$,

Table 4: Overview of the construction methods of this paper.

Eq.	levels	input	s	n	maximum number of columns	t	OSOA	Source
(3)	s^2	$\mathrm{OA}(n, m, s, 2)$	s	n	m	2	no	HT 2013
(4)	s^3	$\mathrm{OA}(n, m, s, 3)$	s	n	$m-1$	3	no	HT 2013
(2)	s^4	$\mathrm{OA}(n, m, s, 4)$	s	n	$\lfloor m/2 \rfloor$	4	no	HT 2013
(2)	s^5	$\mathrm{OA}(n, m, s, 5)$	s	n	$\lfloor (m-1)/2 \rfloor$	5	no	HT 2013
(3)	s^2	$\mathrm{OA}(n, m, s, 2)$	s	n	$2\lfloor m/2 \rfloor$	2	yes	LL 2015
(4)	s^3	$\mathrm{OA}(n, m, s, 3)$	s	n	$2\lfloor m/4 \rfloor$ or $2\lfloor m/4 \rfloor + 1$	3	yes	LL 2015
(2)	s^4	$\mathrm{OA}(n, m, s, 4)$	s	n	$2\lfloor m/4 \rfloor$	4	yes	LL 2015
(3)	4	2, k, (m)	2	2^k	$2^k - 2^{\lfloor k/2 \rfloor} - 2^{k-\lfloor k/2 \rfloor} + 2$	2+	no or yes	HCT 2018
(3)	s^2	s, k, (m)	$p^q \neq 2$	s^k	$\frac{s^k-1}{s-1} - \frac{(s-1)^k-1}{s-2}$	2+	no or yes	HCT 2018
(4)	s^3	$\mathrm{OA}(n/s, m, s, 2)$	s	n	$2 \cdot \lfloor m/2 \rfloor$	2^* or 3	yes	LLY 2021a
(4)	s^3	$\mathrm{OA}(n/s, m, s, 3)$	s	n	$2 \cdot \lfloor m/2 \rfloor$	3	yes	LLY 2021a
(4)	8	m and/or n	2	$8 \cdot \left\lceil \frac{m+2}{4} \right\rceil$	$n/2 - 2$	3	yes	LLY 2021a
(4)	s^3	s, k, (m)	$p^q \neq 2$	s^k	$2 \cdot \left\lfloor \frac{s^{k-1}-1}{2(s-1)} \right\rfloor$	2^* or 3	yes	LLY 2021a
(3)	s^2	$\mathrm{OA}(n/s, m, s, 2)$	s	n	m	2+ or 3−	yes	ZT 2019
(3)	4	m and/or n	2	$8 \cdot \left\lceil \frac{m+1}{4} \right\rceil$	$n/2 - 1$	3−	yes	ZT 2019
(3)	s^2	s, k, (m)	$p^q \neq 2$	$s^k \geq s^3$	$\frac{s^{k-1}-1}{s-1}$	2+ or 3−	yes	ZT 2019
(4)	8	n, (m)	2	2^k, ≥ 16	$5n/16$	3	no	ST 2020
(4)	8	n, (m)	2	2^k, ≥ 16	$n/4$	3	no	ST 2020
(4)	8	n, (m)	2	2^k, ≥ 16	$n/4 - 1$	3+	yes	ST 2020

Notes:
HT=He and Tang (2013), LL=Liu and Liu (2015), HCT=He, Cheng and Tang (2018), LLY=Li, Liu and Yang (2021a), ZT=Zhou and Tang (2019), ST=Shi and Tang (2020).
p^q indicates a prime or prime power; where this is restricted to $\neq 2$, $s = 2$ is treated as another special case.
The LL construction yields 3-orthogonal columns for strengths 3 and 4 (and for strength 2 constructions based on an $\mathrm{OA}(n, m, s, 3)$, i.e., a strength 3 $\mathbf{V}$, if Conjecture 1 holds true).
The HCT construction achieves orthogonal columns under some circumstances. For *very* few columns, it may be possible to achieve strength 3− (not practically relevant). The stated number of columns is achievable with the SOS matrix constructions provided in Section 5.2.1; it may be possible to find constructions for more columns.
Where it matters, the entries for the LLY and ZT constructions assume that $\mathbf{A}$ is constructed according to Equation (13). One could also use an $\mathrm{OA}(n/s, m, s, 3)$ in the ZT approach and achieve strength 3−; that table row has been omitted because it does not seem too practically relevant. Where the strength column lists two alternatives, the higher strength is not achievable for numbers of columns close to the maximum.
The ST constructions enable additional balance properties, even where strength 3+ is not achieved; the construction of the matrix $\mathbf{C}$ is assumed to follow this paper. The $n = 2^5$ case for the first construction allows only $m = 9 < 5n/16$ columns.

the maximum sizes of the relevant OAs underlying the constructions have been taken from the MinT database (Schmid, Schürer and others). The OAs are available in R package DoE.base (Grömping 2022a). The tables show that the strength 2+ SOAs by He, Cheng and Tang have a lot more columns than the strength 3− ($s = 2$) or 2+ ($s > 2$) OSOAs by Zhou and Tang, i.e., column orthogonality comes at a cost for this strength. For the strength 3 (O)SOAs, the numbers of columns obtainable with and without orthogonality are almost identical. Here, Li, Liu and Yang have increased the number of columns obtainable with s^3 levels by dropping the 3D projection properties (strength 2^*). On the other end, the OSOAs by Liu and Liu (2015) are available for smaller numbers of columns only; this is the price for their attractive feature of 3-orthogonality, which is beneficial for the estimation of second order linear models, so that their construction is worth being studied. For 2-level factors, Shi and Tang constructed strength 3+ SOAs that have the 2D and 3D balance properties of strength 4 SOAs. As the number of columns that can be accommodated in a strength 4 SOA is very small (e.g. 7 columns in 729 runs for $s = 3$), strength 3+ is quite attractive. Unfortunately, there are so far no strength 3+ constructions for $s > 2$.

Table 5 is limited to regular fractions or arrays based on (selected) Hadamard matrices. Where strong non-regular OAs exist, more columns may be possible for the He and Tang construction. Known such cases are strength 4 SOAs with 7 columns in 16 levels from an OA$(128, 15, 2, 4)$, or 9 columns in 16 levels from an OA$(256, 19, 2, 4)$; both these OAs can be found in Mee 2009 and are available in R package DoE.base. If more non-regular arrays are found, more such cases will arise.

Table 5: Achievable column numbers for (O)SOAs from regular 2-level fractional factorials or Hadamard matrices.

	4 levels			8 levels					16 levels
n	HT, 2	HCT, 2+	ZT, 3−	HT, 3	LLY, 3	ST, 3	ST, 3+	LL, 3	HT, 4
16	15	10	7	7	6	5	3	4	
24	23		12	11	10			6	
32	31	22	15	15	14	10	7	8	
40	39		20	19	18			10	
48	47		24	23	22			12	
56	55		28	27	26			14	
64	63	50	31	31	30	20	15	16	4
80	79		40	39	38			20	
96	95		48	47	46			24	
128	127	106	63	63	62	40	31	32	5
256	255	226	127	127	126	80	63	64	8
512	511	466	255	255	254	160	127	128	11
1024	1023	962	511	511	510	320	255	256	16

Note:
HT=He and Tang 2013, HCT=He, Cheng and Tang 2018, LL=Liu and Liu 2015, LLY=Li, Liu and Yang 2021a, ST=Shi and Tang 2020, ZT=Zhou and Tang 2019.
Only a selection of Hadamard-based sizes have been included.

7. Discussion

SOAs and OSOAs of practical importance exist in many varieties: one can obtain LHDs by e.g. constructing an OSOA$(729, 10, 729, 2^*)$ from an OA$(81, 10, 9, 2)$, or an OSOA$(512, 8, 512, 2^*)$ from an OA$(64, 9, 8, 2)$. A 3-orthogonal OSOA$(512, 4, 512, 3)$ by the Liu and Liu (2015) construction, obtained from an OA$(512, 9, 8, 3)$, is a very good choice for inspecting four factors in detail. The classical computer experimentation with relatively few quantitative factors will benefit from such LHD-like (O)SOAs. (O)SOAs that are not LHDs themselves can be used for creating LHDs by level expansion; it has not been investigated to what extent this brings an advantage over direct expansion from an OA.

Table 6: Achievable column numbers for (O)SOAs from 3-level fractional factorials.

	9 levels			27 levels				81 levels
n	HT, 2	HCT, 2+	ZT, 2+	LL, 2*	HT, 3	LLY, 3	LL, 3	HT, 4
81	40	25	13	12	9	10	4	
243	121	90	40	40	19	20	10	5
729	364	301	121	120	55	56	28	7
2187	1093	966	364	364	111	112	56	13
6561	3280	3025	1093	1092	247	248	124	20

Note:
HT=He and Tang 2013, HCT=He, Cheng and Tang 2018, LL=Liu and Liu 2015, LLY=Li, Liu and Yang 2021a, ZT=Zhou and Tang 2019.

Table 7: Achievable column numbers for (O)SOAs from 4-level fractional factorials.

	16 levels			64 levels				256 levels
n	HT, 2	HCT, 2+	ZT, 2+	LL, 2*	HT, 3	LLY, 3	LL, 3	HT, 4
256	85	45	21	20	16	16	8	
1024	341	220	85	84	40	40	20	5
4096	1365	1001	341	340	125	126	62	10

Note:
HT=He and Tang 2013, HCT=He, Cheng and Tang 2018, LL=Liu and Liu 2015, LLY=Li, Liu and Yang 2021a, ZT=Zhou and Tang 2019.

If quantitative experimental variables are easy to realize at different levels, it may be attractive to use designs that offer the chance to learn something about the functional form of the response surface by providing more levels than the usual orthogonal arrays, even if one does not use LHDs. (O)SOAs can ensure that, while at the same time preserving attractive projection properties over coarser grids. Many questions remain open with respect to practical usefulness of the various types of (O)SOAs, relative to other types of arrays like level-expanded OAs or LHDs.

Exploration of responses for many quantitative experimental variables can be supported by (O)SOAs with smaller numbers of levels, e.g. 4, 8, 9, 16 or 27 levels. For up to $n/4-1$ 8-level columns, strength 3+ OSOAs may be attractive because of their stratification properties and their column orthogonality; the latter can be guaranteed by a modification proposed in this paper. The strength 3+ property has so far only been implemented for $s=2$, i.e., for 8-level columns. Extending strength 3+ (O)SOAs to $s>2$ would be a very attractive invention, because one can expect to obtain more columns (in s^3 levels) than with strength 3 OAs or strength 4 SOAs (which would have s^4 level columns). Strength 3 or stronger OSOAs by Liu and Liu (2015) need a large number of runs relative to the number of columns; they are nevertheless attractive because their columns are 3-orthogonal. Where OAs with OA strength $t \geq 2$ exist for the number of levels and columns under consideration, these may be preferable to SOAs (see also Section 3.5).

Because of their stratification properties, (O)SOAs with columns with moderate or large numbers of levels for quantitative experimental variables can also be used for obtaining insights at coarser discretized versions of the experimental variables. This might also be useful for using selected SOA columns for qualitative factors with fewer levels, while using most columns for quantitative experimental variables, e.g. in linear models with low order polynomials.

He and Tang (2014) pointed out the existence of some SOAs without providing explicit constructions; these have not been included. Furthermore, this paper did not discuss sliced SOAs (Liu and Liu 2015), nearly strong OSOAs (Li, Liu and Yang 2021b) or group SOAs (Liu, Liu and Yang 2021). Like in most of the SOA literature, the mixed level case was also completely ignored; He, Cheng and Tang (2018) are among the few authors who devoted a small part of their paper to that case.

The SOA construction by He, Cheng and Tang (2018) permits particularly large numbers of columns with s^2 levels to be accommodated with SOA strength 2+. Jiang, Wang and Wang (2021) presented a construction based on Addelman and Kempthorne (1961) OAs whose number of runs is twice an odd prime power. Their construction yields welcome additions to the possible run sizes for strength 2+ SOAs in s^2 levels: the HCT construction needs s^k runs for some k, while Jiang, Wang and Wang (2021) need $2s^k$ runs and would, e.g., permit 9, 43 or 165 9-level columns in 54 runs, 162 or 486 runs, as compared to the 25 or 90 columns in 81 or 243 runs shown in Table 6. The construction works with ingredients of the Addelman and Kempthorne construction, and it is not obvious how to use a ready-made Addelman and Kempthorne array for obtaining the construction from that array. It will hopefully be possible to translate the construction into a rule for the columns to pick for **A** and **B** from an Addelman and Kempthorne array.

This discussion closes with another appeal to replace the misleading expression “strong orthogonal arrays” with the more adequate “stratum orthogonal arrays”, since the OA strength of an SOA with SOA strength 4 may easily be 1 only.

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Appendix A: Galois field addition and multiplication tables

As pointed out in Section 2.2, Galois field elements for $GF(s)$ are denoted as $0, \ldots, s-1$ in this paper. Tables 8 and 9 show the rules for Galois field addition and multiplication that are used in this paper.

Table 8: Addition tables for GF(4), GF(8) and GF(9)

	0	1	2	3
0	0	1	2	3
1	1	0	3	2
2	2	3	0	1
3	3	2	1	0

	0	1	2	3	4	5	6	7
0	0	1	2	3	4	5	6	7
1	1	0	3	2	5	4	7	6
2	2	3	0	1	6	7	4	5
3	3	2	1	0	7	6	5	4
4	4	5	6	7	0	1	2	3
5	5	4	7	6	1	0	3	2
6	6	7	4	5	2	3	0	1
7	7	6	5	4	3	2	1	0

	0	1	2	3	4	5	6	7	8
0	0	1	2	3	4	5	6	7	8
1	1	2	0	4	5	3	7	8	6
2	2	0	1	5	3	4	8	6	7
3	3	4	5	6	7	8	0	1	2
4	4	5	3	7	8	6	1	2	0
5	5	3	4	8	6	7	2	0	1
6	6	7	8	0	1	2	3	4	5
7	7	8	6	1	2	0	4	5	3
8	8	6	7	2	0	1	5	3	4

Table 9: Multiplication tables for GF(4), GF(8) and GF(9)

	0	1	2	3
0	0	0	0	0
1	0	1	2	3
2	0	2	3	1
3	0	3	1	2

	0	1	2	3	4	5	6	7
0	0	0	0	0	0	0	0	0
1	0	1	2	3	4	5	6	7
2	0	2	4	6	5	7	1	3
3	0	3	6	5	1	2	7	4
4	0	4	5	1	7	3	2	6
5	0	5	7	2	3	6	4	1
6	0	6	1	7	2	4	3	5
7	0	7	3	4	6	1	5	2

	0	1	2	3	4	5	6	7	8
0	0	0	0	0	0	0	0	0	0
1	0	1	2	3	4	5	6	7	8
2	0	2	1	6	8	7	3	5	4
3	0	3	6	7	1	4	5	8	2
4	0	4	8	1	5	6	2	3	7
5	0	5	7	4	6	2	8	1	3
6	0	6	3	5	2	8	7	4	1
7	0	7	5	8	3	1	4	2	6
8	0	8	4	2	7	3	1	6	5

Appendix B: Start values and example constructions for Shi and Tang Family 1

$n = 2^k$ *for even* $k \geq 4$

The start values are $Y_{\mathbf{A}} = (1, 2, 4, 8, 15)$ and $Y_{\mathbf{B}} = (12, 9, 3, 6, 5)$. This implies $Y_{\mathbf{A}+_2\mathbf{B}} = (13, 11, 7, 14, 10)$. There are many possibilities for $Y_{\mathbf{C}}$, e.g. 2, 1, 1, 1, 1, since one only has to avoid choosing $\mathbf{c}_\ell$ coincident with $\mathbf{a}_\ell$, $\mathbf{b}_\ell$ or $\mathbf{a}_\ell +_2 \mathbf{b}_\ell$.

$n = 2^k$ *for odd* $k \geq 7$

The start values are
$Y_{\mathbf{A}}$=(1, 2, 4, 8, 15, 17, 18, 20, 24, 31, 33, 34, 36, 40, 47, 49, 50, 52, 56, 63, 65, 66, 68, 72, 79, 81, 82, 84, 88, 95, 97, 98, 100, 104, 111, 113, 114, 116, 120, 127),
$Y_{\mathbf{B}}$=(42, 37, 25, 3, 117, 74, 41, 10, 14, 102, 92, 69, 23, 6, 83, 90, 73, 71, 21, 86, 54, 28, 7, 5, 57, 61, 44, 26, 19, 53, 60, 12, 9, 13, 58, 55, 62, 35, 27, 38).
Note that the 28th entry for **B** was corrected from 22 to 26 versus Table 1 of Shi and Tang (or from $\mathbf{e}_2\mathbf{e}_3\mathbf{e}_5$ to $\mathbf{e}_2\mathbf{e}_4\mathbf{e}_5$ in their notation).
$Y_{\mathbf{A}}$ and $Y_{\mathbf{B}}$ imply $Y_{\mathbf{A}+_2\mathbf{B}}$=(43, 39, 29, 11, 122, 91, 59, 30, 22, 121, 125, 103, 51, 46, 124, 107, 123, 115, 45, 105, 119, 94, 67, 77, 118, 108, 126, 78, 75, 106, 93, 110, 109, 101, 85, 70, 76, 87, 99, 89).
Columns of **C** can be most conveniently chosen from the multiples of 16 that do not occur in any of the matrices.

Table 10: Properties of the example 16 run SOAs of Tables 11 and 12

Construction	levels	m	maximum m	ϕ_p	unoptimized ϕ_p	strength	orthogonal	3-orthogonal
HT	8	4	7	0.1340	0.1714	3	no	no
LL	8	4	4	0.1737	0.2606	3	yes	yes
LLY	8	4	4	0.1737	0.2606	3	yes	yes
ST, fam. 1	8	4	5	0.1481	0.1690	3	no	no
ST, fam. 2	8	4	4	0.1489	0.2000	3	no	no
ST, fam. 3	8	3	3	0.2606	0.2627	3+	yes	no
HT	4	7	15	0.2056	0.2056	2	no	no
LL	4	7	14	0.2102	0.2102	2	yes	yes
ZT	4	7	7	0.1762	0.2672	3−	yes	no
HCT orth.	4	7	10	0.2000	0.2570	2+	yes	no
HCT non-orth.	4	7	10	0.1721	0.2028	2+	no	no

Note:
The table shows properties of example designs and should not be generalized to imply properties of construction methods.
The maximum number of columns may require a different input design.
HT=He and Tang 2013, HCT=He, Cheng and Tang 2018, LL=Liu and Liu 2015, LLY=Li, Liu and Yang 2021a, ST=Shi and Tang 2020, ZT=Zhou and Tang 2019.
Optimization for 8-level (O)SOAs was done with three rounds and three repeated starts,
optimization for 4-level (O)SOAs was done with the default of package SOAs (three rounds/repeats would not have made a difference).
ST fam. 3 has three columns only; hence, its ϕ_p is not comparable to the other 8-level SOAs.
The 8-level OSOAs obtained with LL or LLY are identical, except for row order.
The maximum m may require to use a weaker OA with more columns for OA-based 4-level (O)SOAs.

Special case $k = 5$ ($n = 32$)

The maximum number of columns in an SOA$(2^5, m, 8, 3)$ with property α is $m = 9 < 10 = 5 \cdot 2^{5-4}$. This maximal SOA is e.g. obtained with **A** chosen as the GMA design 9-4.1 (Yates columns 1, 2, 4, 8, 16, 7, 11, 19, 29) and **B** consisting of Yates columns 24, 20, 9, 6, 5, 27, 17, 12, 3. Then $\mathbf{A} +_2 \mathbf{B}$ consists of Yates columns 25, 22, 13, 14, 21, 28, 26, 31, 30. For **C**, one can use e.g. Yates column 10 or 15 for all columns.

Appendix C: 16 run SOAs from all constructions

Table 10 shows the 16 run SOAs that are constructed in this paper, with a few of their properties.

Table 11 shows all 16 run SOAs with four 8-level columns (exception: only three columns for Shi and Tang's Family 3) from strength 3 constructions next to each other, Table 12 does the same for all 16 run SOAs with seven 4-level columns.

Table 13 shows the OAs that have been used for the OA-based constructions.

Note: The `LLY` and `ZT` OSOAs were obtained using the OAs from Table 13. Comparable OSOAs can also be obtained instead using the R functions `OSOAs_hadamard` or `OSOAs_regular`.

R code for obtaining the (O)SOAs of this appendix (assuming that R package SOAs is loaded):

```
V8 <- (desnum(oa.design(ID=L8.2.7, randomize=FALSE))+1)/2
V16 <- L16.2.8.8.1[,-9] - 1

set.seed(3209)
HT8 <- SOAs(V16, m=4, noptim.rounds=3, noptim.repeats=3)
LiuLiu8 <- OSOAs_LiuLiu(V16, t=3, noptim.rounds=3, noptim.repeats=3)
LLY <- OSOAs(V8, el=3, noptim.rounds=3, noptim.repeats=3)
STfam1 <- SOAs_8level(16, m=4, noptim.rounds = 3, noptim.repeats = 3, constr="ShiTang_alpha")
```

Table 11: (O)SOAs with 4 8-level columns in 16 runs

HT				LL				LLY				ST, fam. 1				ST, fam. 2				ST, fam. 3		
X_1	X_2	X_3	X_4	X_1	X_2	X_3	X_4	X_1	X_2	X_3	X_4	X_1	X_2	X_3	X_4	X_1	X_2	X_3	X_4	X_1	X_2	X_3
4	5	0	3	2	1	4	0	6	2	2	1	2	3	1	6	4	0	3	7	5	4	4
6	7	2	1	2	1	3	7	6	2	5	6	6	0	2	7	5	5	1	0	0	6	3
4	4	5	7	6	2	0	3	7	4	3	7	3	7	3	4	5	2	4	2	7	3	1
6	6	7	5	6	2	7	4	7	4	4	0	7	4	0	5	4	7	6	5	2	1	6
5	1	1	7	0	3	6	2	0	3	3	7	0	3	5	4	6	2	1	5	7	6	6
7	3	3	5	0	3	1	5	0	3	4	0	4	0	6	5	7	7	3	2	2	4	1
5	0	4	3	4	0	2	1	1	5	2	1	1	7	7	6	7	0	6	0	5	1	3
7	2	6	1	4	0	5	6	1	5	5	6	5	4	4	7	6	5	4	7	0	3	4
0	5	1	6	3	7	2	1	3	7	7	4	0	1	1	2	0	4	7	3	1	0	0
2	7	3	4	3	7	5	6	3	7	0	3	4	2	2	3	1	1	5	4	4	2	7
0	4	4	2	7	4	6	2	2	1	6	2	1	5	3	0	1	6	0	6	3	7	5
2	6	6	0	7	4	1	5	2	1	1	5	5	6	0	1	0	3	2	1	6	5	2
1	1	0	2	1	5	0	3	5	6	6	2	2	1	5	0	2	6	5	1	3	2	2
3	3	2	0	1	5	7	4	5	6	1	5	6	2	6	1	3	3	7	6	6	0	5
1	0	5	6	5	6	4	0	4	0	7	4	3	5	7	2	3	4	2	4	1	5	7
3	2	7	4	5	6	3	7	4	0	0	3	7	6	4	3	2	1	0	3	4	7	0

Note:
ST fam. 3 has three columns only, because more are not possible.

Table 12: (O)SOAs with 7 4-level columns in 16 runs (header denotes X_1 to X_7 as 1 to 7 for saving space)

HT							LL							ZT							HCT orth.							HCT non-orth.						
1	2	3	4	5	6	7	1	2	3	4	5	6	7	1	2	3	4	5	6	7	1	2	3	4	5	6	7	1	2	3	4	5	6	7
2	1	0	0	1	3	3	1	3	0	1	0	1	0	0	1	3	2	1	1	0	3	1	0	2	2	2	3	0	2	0	1	0	2	0
2	1	0	1	2	0	1	1	3	0	1	3	2	3	0	1	0	1	2	1	3	3	0	0	2	1	1	0	0	3	0	1	3	0	2
2	0	3	2	1	2	1	1	3	3	2	0	1	3	0	2	3	1	1	2	3	3	3	2	1	3	3	2	0	0	2	3	1	2	0
2	0	3	3	2	1	3	1	3	3	2	3	2	0	0	2	0	2	2	2	0	3	2	2	1	0	0	1	0	1	2	3	2	0	2
3	3	1	2	0	1	3	3	2	2	0	2	0	2	3	1	3	1	2	2	0	2	1	3	0	2	1	0	1	2	3	2	0	1	3
3	3	1	3	3	2	1	3	2	2	0	1	3	1	3	1	0	2	1	2	3	2	0	3	0	1	2	3	1	3	3	2	3	3	1
3	2	2	0	0	0	1	3	2	1	3	2	0	1	3	2	3	2	2	1	3	2	3	1	3	3	0	1	1	0	1	0	1	1	3
3	2	2	1	3	3	3	3	2	1	3	1	3	2	3	2	0	1	1	1	0	2	2	1	3	0	3	2	1	1	1	0	2	3	1
0	1	1	2	0	0	0	0	1	2	0	2	0	1	2	3	1	0	3	3	2	1	1	1	1	0	3	1	2	2	1	3	2	2	3
0	1	1	3	3	3	2	0	1	2	0	1	3	2	2	3	2	3	0	3	1	1	0	1	1	3	0	2	2	3	1	3	1	0	1
0	0	2	0	0	1	2	0	1	1	3	2	0	2	2	0	1	3	3	0	1	1	3	3	2	1	2	0	2	0	3	1	3	2	3
0	0	2	1	3	2	0	0	1	1	3	1	3	1	2	0	2	0	0	0	2	1	2	3	2	2	1	3	2	1	3	1	0	0	1
1	3	0	0	1	2	0	2	0	0	1	0	1	3	1	3	1	3	0	0	2	0	1	2	3	0	0	2	3	2	2	0	2	1	0
1	3	0	1	2	1	2	2	0	0	1	3	2	0	1	3	2	0	3	0	1	0	0	2	3	3	3	1	3	3	2	0	1	3	2
1	2	3	2	1	3	2	2	0	3	2	0	1	0	1	0	1	0	0	3	1	0	3	0	0	1	1	3	3	0	0	2	3	1	0
1	2	3	3	2	0	0	2	0	3	2	3	2	3	1	0	2	3	3	3	2	0	2	0	0	2	2	0	3	1	0	2	0	3	2

Table 13: The OAs that were used as input for the constructions of the SOAs of this appendix. The Yates matrix shows the basic columns in bold face. The rows of the Yates matrix can be reordered so that the first basic column changes slowest rather than fastest by arranging the rows in the order 1, 9, 5, 13, 3, 11, 7, 15, 2, 10, 6, 14, 4, 12, 8, 16.

OA(8, 7, 2, 2)

1	2	3	4	5	6	7
0	0	0	0	0	0	0
0	0	1	1	1	0	1
0	1	0	1	0	1	1
0	1	1	0	1	1	0
1	0	0	1	1	1	0
1	0	1	0	0	1	1
1	1	0	0	1	0	1
1	1	1	1	0	0	0

OA(16, 8, 2, 3)

1	2	3	4	5	6	7	8
0	0	0	0	0	0	0	0
0	0	0	0	1	1	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
0	1	0	1	1	0	1	0
0	1	1	0	0	1	1	0
0	1	1	0	1	0	0	1
1	0	0	1	0	1	1	0
1	0	0	1	1	0	0	1
1	0	1	0	0	1	0	1
1	0	1	0	1	0	1	0
1	1	0	0	0	0	1	1
1	1	0	0	1	1	0	0
1	1	1	1	0	0	0	0
1	1	1	1	1	1	1	1

Yates matrix

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	**0**	0	**0**	0	0	0	**0**	0	0	0	0	0	0	0
1	**0**	1	**0**	1	0	1	**0**	1	0	1	0	1	0	1
0	**1**	1	**0**	0	1	1	**0**	0	1	1	0	0	1	1
1	**1**	0	**0**	1	1	0	**0**	1	1	0	0	1	1	0
0	**0**	0	**1**	1	1	1	**0**	0	0	0	1	1	1	1
1	**0**	1	**1**	0	1	0	**0**	1	0	1	1	0	1	0
0	**1**	1	**1**	1	0	0	**0**	0	1	1	1	1	0	0
1	**1**	0	**1**	0	0	1	**0**	1	1	0	1	0	0	1
0	**0**	0	**0**	0	0	0	**1**	1	1	1	1	1	1	1
1	**0**	1	**0**	1	0	1	**1**	0	1	0	1	0	1	0
0	**1**	1	**0**	0	1	1	**1**	1	0	0	1	1	0	0
1	**1**	0	**0**	1	1	0	**1**	0	0	1	1	0	0	1
0	**0**	0	**1**	1	1	1	**1**	1	1	1	0	0	0	0
1	**0**	1	**1**	0	1	0	**1**	0	1	0	0	1	0	1
0	**1**	1	**1**	1	0	0	**1**	1	0	0	0	0	1	1
1	**1**	0	**1**	0	0	1	**1**	0	0	1	0	1	1	0

```
STfam2 <- SOAs_8level(16, m=4, noptim.rounds=3, noptim.repeats=3)
STfam3 <- SOAs_8level(16, m=3, noptim.rounds=3, noptim.repeats=3)

set.seed(3209)
HT4 <- SOAs(V16, t=2, m=7)
LiuLiu4 <- OSOAs_LiuLiu(V16, t=2, m=7)
ZT <- OSOAs(V8, el=2)
HCT <- SOAs2plus_regular(2, 4, m=7)
HCTf <- SOAs2plus_regular(2, 4, m=7, orth=FALSE)
```