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Implementation of the stratification pattern by Tian and Xu via power coding

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Abstract

Recently, Tian and Xu proposed a stratification pattern for assessing the qualities of stratum orthogonal arrays (SOAs) or generalizations of these (GSOAs). The stratification pattern is directly related to (G)SOA strength. Tian and Xu's presentation relies on a contrast matrix that contains complex elements, unless the number of levels of the GSOA is a power of 2. The complex contrasts can be replaced by a suitable real-valued coding, and this paper introduces power coding for that purpose. The paper explains the ideas behind the stratification pattern and presents its implementation with the help of power coding. As a byproduct of the implementation, dimension by weight tables provide more detailed insights than the stratification pattern alone. As the calculation of stratification patterns can be computationally demanding for moderately large arrays, the implementation permits to specify upper limits for dimension and/or weight, in favor of saving resources.

1 Introduction

He and Tang (2013) introduced so-called "Strong Orthogonal Arrays" (SOAs) and proposed their use for the construction of Latin Hypercube Designs (LHDs) for computer experiments. Grömping (2022a) gave an overview of SOA constructions to date, changing the long version of the acronym to "Stratum Orthogonal Arrays", because SOAs are actually *weak* orthogonal arrays (OAs), typically of OA strength 1 only. This paper also uses the term "Stratum Orthogonal Arrays".

The general idea of SOAs is to provide arrays for computer experimentation with quantitative variables, with many levels for each variable. Such arrays are required to have good space-filling properties, and the introduction of SOAs is one systematic way for guaranteeing space filling by certain stratification properties: He and Tang (2013) proposed SOAs with SOA strength t (see below) for columns with s^t levels each (s a prime or prime power). An OA with OA strength 2 would require s^{2t} equireplicated level combinations for each pair of columns in s^t levels, which is usually prohibitive. SOAs make weaker requests by considering coarsened columns obtained by grouping column levels into strata of adjacent levels: s^{t-1} strata of s adjacent levels each, s^{t-2} strata of s^2 adjacent levels each, and so forth. Balance is then considered for stratum combinations. A classical SOA of strength t for m columns at s^t levels each ensures s^t equireplicated strata for up to t dimensions. For example, for $s = 3$ and $t = 4$, the SOA has $3^4 = 81$ levels (and thus 3^4 equireplicated strata in 1D), 81 strata in 2D (9×9 or 3×27 or 27×3), 81 strata in 3D ($9 \times 3 \times 3$, $3 \times 9 \times 3$, $3 \times 3 \times 9$) and 81 strata in 4D ($3 \times 3 \times 3 \times 3$).
Requesting SOAs of strength t to have s^t levels is restrictive; variations have been considered of strength 3 with only s^2 levels (3−, introduced by Zhou and Tang 2019), strength 2 with 2D stratification properties of strength 3 (2+, introduced by He, Cheng and Tang 2018), strength 2+, but also with s^3 levels (2*, introduced by Li, Liu and Yang 2021); these can readily be extended to other strengths (e.g., strength 3+ or 4−, as considered in Grömping 2022a and Tian and Xu 2022). Tian and Xu (2022) generalized SOAs to GSOAs (G for "general"), by fully separating the strength from the power to which s is taken for obtaining the number of levels.

Tian and Xu's (2022) main contribution is the so-called space-filling pattern – called stratification pattern in this paper – that has a close relationship to the generalized word length pattern of Xu and Wu (2001). In a simulation study, Tian and Xu demonstrated that superior performance on the stratification pattern was related to superior performance in evaluating a benchmark function for space-filling designs, the 8-dimensional borehole function included in the text book by Fang, Li and Sudjianto (2006). Their proposed stratification pattern is therefore worth studying.

Both the papers by Xu and Wu (2001) and by Tian and Xu (2022) based their results on complex coding. For the Xu and Wu (2001) paper, it is well-known that results are unchanged for other types of so-called normalized orthogonal coding. The present paper shows that results by Tian and Xu (2022) can equivalently − and even more conveniently − be obtained using a newly introduced coding for factors in s^ℓ levels: power coding based on power contrasts. Using power coding, this paper presents an implementation of the stratification pattern introduced by Tian and Xu (2022), which is available in R package SOAs (relevant functions: `contr.Power`, `Spattern` and `dim_wt_tab`). The second purpose of this paper is to spread the word on GSOAs and stratification patterns and make them accessible to a less theoretically-minded audience; interspersed examples illustrate more formal definitions in order to support this audience.

The paper proceeds as follows: Section 2 provides notation and basic facts regarding orthogonal arrays (OAs). Section 3 presents general tools around coding in linear models and explains the GWLP as a predecessor and close relative of the stratification pattern, before introducing the power contrasts in Section 3.3. Section 4 introduces Tian and Xu's GSOAs and stratification patterns, and Section 5 explains the implementation of the stratification pattern via the power contrasts in R package SOAs. Section 6 presents examples, and the discussion points to opportunities for further research. The code for all examples is available as supplemental online material[1].

2 Notation and basic facts

$\lfloor\cdot\rfloor$ and $\lceil\cdot\rceil$ denote the floor and ceiling functions. Except in the very narrow context of complex roots of the unity, where it denotes the square root of -1, the letter i is used for indices. 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), $\mathbf{I}_n$ denotes the n-dimensional identity matrix, $\top$ denotes the transpose of a matrix or vector, and $\otimes$ the Kronecker product. Column vectors with single digit integer elements are parsimoniously written as a string of integers, e.g. $2 \cdot \mathbf{1}_5 = 22222$. The $n \times m$ matrix $\mathbf{X}$ is written as

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

Functions and unary or binary operators for scalars are applied to vectors element by element.

2.1 Galois fields

A Galois field $GF(s)$ (see e.g. Appendix A of Hedayat et al. 1999) is a finite field over s elements, where s is a prime or an integer power of a prime. For the purpose of this paper, the elements of Galois fields are denoted as the integers 0 to $s-1$, and they come with addition (neutral element 0) and multiplication (neutral element 1). If s is a prime, modulo arithmetic can be used. For non-prime s, one has to use suitable addition and multiplication tables that fulfill the requirements for a field (see, e.g., Grömping 2022a for the tables for $s = 4, 8, 9$). Addition w.r.t. a Galois field $GF(s)$ will be denoted as $+_s$, multiplication as $\cdot_s$.

2.2 Orthogonal arrays and OA strength

An OA in n runs with m columns and s_i levels in the ith column is denoted as $\mathrm{OA}(n, m, s_1 \times s_2 \times \ldots \times s_m, t)$, where t stands for the strength of the OA (explicitly called OA strength in this paper, in order to set it apart from the different concept of (G)SOA strength): OA strength t means that any tuple of t distinct columns $i_1, \ldots, i_t$ of the OA has $s_{i_1} \cdot \ldots \cdot s_{i_t}$ equireplicated level combinations. An OA in n runs is *saturated*, if the main effects for its columns use $n-1$ degrees of freedom. An OA is symmetric, if $s_1 = s_2 = \cdots = s_m = s$; symmetric OAs are denoted as $\mathrm{OA}(n, m, s, t)$. A symmetric OA in n runs with s a prime or prime power is *regular*, if all its columns can be obtained as linear combinations of a few linearly independent basic columns from $\mathrm{GF}(s)^n$. (This is not an exhaustive definition of regular OAs, but suffices for the purpose of this paper.)

The following lemma provides the so-called Rao-Hamming construction that can be obtained for s-level columns with s a prime or prime power (see e.g. Section 3.4 of Hedayat et al.).

[1] The URL is https://prof.bht-berlin.de/fileadmin/prof/groemp/downloads/SupplSpattern.zip.

Lemma 1 (Rao Hamming construction)**.** *Let s be a prime or prime power, and $n = s^k$, $k \geq 2$.*

(i) The basic vectors $\mathbf{e}_1(k) = (0, 1, \ldots, s-1)^\top \otimes \mathbf{1}_{s^{k-1}}$ to $\mathbf{e}_k(k) = \mathbf{1}_{s^{k-1}} \otimes (0, 1, \ldots, s-1)^\top$ on $GF(s)^n$, together with all their linear combinations with coefficient vectors from $GF(s)^k$ whose first non-zero element is 1, form a regular saturated OA.

(ii) Let $\mathbf{R}(s, k)$ denote the OA of (i). It can be constructed recursively as follows:

- $\mathbf{R}(s, 2) = \mathbf{e}_1(2), \mathbf{e}_2(2), \mathbf{e}_1(2) +_s \mathbf{e}_2(2), \ldots, \mathbf{e}_1(2) +_s (s-1) \cdot_s \mathbf{e}_2(2)$.
- *For $i > 2$, $\mathbf{R}(s, i) = (\mathbf{R}(s, i-1) \otimes \mathbf{1}_s, \mathbf{e}_i(i), \mathbf{e}_i(i) \odot_s \mathbf{R}(s, i-1), \ldots, ((s-1) \cdot_s e_i(i)) \odot_s (\mathbf{R}(s, i-1) \otimes \mathbf{1}_s)$, where $\odot_s$ denotes the element wise multiplication of a column with each column of the subsequent matrix w.r.t. to $GF(s)$.*

(iii) A alternative non-recursive construction of an $OA(s^k, (s^k-1)/(s-1), s, 2)$ is as follows:

- *Create an $s^k \times k$ matrix $\mathbf{E}$ that contains the $\mathbf{e}_j(k), j = 1, \ldots, k$ as its columns.*
- *Create a coefficient matrix $\mathbf{C}$ by transposing the matrix from the previous bullet and removing the all-zero column and all columns whose first non-zero element is different from 1.*
- $\mathbf{EC}$*, with all operations in the matrix multiplication are done w.r.t. $GF(s)$, yields the same $OA(s^k, (s^k-1)/(s-1), s, 2)$ as the recursive process of (ii).*

In words, $\mathbf{e}_1(k)$ to $\mathbf{e}_k(k)$ of Lemma 1 (i) are the slowest changing to fastest changing arrangements of s^{k-1} replicates each of the numbers 0 to $s-1$. Lemma 1 (ii) implies an ordering of the columns of the resulting OA and makes the structure obvious, Lemma 1 (iii) is easier to implement. For some purposes, it is not important whether the columns of the matrix $\mathbf{E}$ in part (iii) of the lemma are coded from slow-changing to fast-changing or from fast-changing to slow-changing. For the power coding introduced in this paper, however, this *is* important.

Example 1. For $s = 3$ and $k = 2$, an $\text{OA}(3^2, (3^2-1)/(3-1), 3, 2) = \text{OA}(9, 4, 3, 2)$ is obtained from the two basic vectors $\mathbf{e}_1(2)$=000111222 and $\mathbf{e}_2(2)$=012012012 and their two linear combinations $\mathbf{e}_1(2) + \mathbf{e}_2(2) = 012120201$ and $\mathbf{e}_1(2) +_3 2 \cdot_3 \mathbf{e}_2(2) = 012201120$. This 9×4 OA can be used as $\mathbf{R}(3, 2)$ in part (ii) of the lemma and can be extended to the 27×13 OA $\mathbf{R}(3, 3)$ as follows: The first four columns consist of three stacked identical copies of $\mathbf{R}(3, 2)$. Column 5 is $\mathbf{e}_3(3) = 012012012012012012012012012$, columns 6 to 9 are the first four columns plus $\mathbf{e}_3(3)$ (modulo 3), and columns 10 to 13 are the first four columns plus $2 \cdot_3 \mathbf{e}_3(3)$ (modulo 3). The matrix $\mathbf{C}$ of part (iii) for the 27×13 OA consists of the columns 100, 010, 110, 120, 001, 101, 011, 111, 121, 102, 012, 112, 122.

2.3 Projections, coarsening, and level expansion

Let $\mathbf{D}$ be an OA with n rows and m columns. Any $n \times d$ sub matrix of $\mathbf{D}$ is called a d-dimensional projection of $\mathbf{D}$. For brevity, dimensionality is denoted as 1D, 2D, …, or generally as dD.

Collapsing the levels $0, \ldots, s^\ell - 1$ of a column in s^ℓ levels into only s^k levels $0, \ldots, s^k - 1$, $k = 1, \ldots, \ell - 1$, can be simply done by applying the formula $x_{s^k} = \lfloor x_{s^\ell}/(s^{\ell-k}) \rfloor$, where x_{s^ℓ} denotes the initial levels. Such coarsening groups the initial s^ℓ levels into s^k strata of adjacent levels.

Conversely, if $n = \lambda \cdot s^\ell$, $\lambda \geq 1$, the columns of an $\text{OA}(n, m, s^k, 1)$ can be expanded from s^k levels to s^ℓ levels by replacing

- the $\lambda \cdot s^{\ell-k}$ instances of the original level 0 with values $0, \ldots, s^{\ell-k} - 1$ (each occurring λ times)
- the $\lambda \cdot s^{\ell-k}$ instances of the original level 1 with values $s^{\ell-k}, \ldots, 2s^{\ell-k} - 1$ (each occurring λ times)
- the $\lambda \cdot s^{\ell-k}$ instances of the original level 2 with values $2s^{\ell-k}, \ldots, 3s^{\ell-k} - 1$ (each occurring λ times)
- …
- the $\lambda \cdot s^{\ell-k}$ instances of the original level $s^k - 1$ with values $(s^k - 1)s^{\ell-k}, \ldots, s^\ell - 1$ (each occurring λ times)

Example 2. The two-column OA (full factorial) with columns 000111222 and 012012012 can, e.g., be expanded to 012345678 and 036147258 or to 012345678 and 048156237. Coarsening the levels will return the ingoing columns in either case.

The example illustrates that expanding levels can be done in different ways; these can lead to results of diverse quality. On the contrary, the coarsening of levels is a simple and unique activity.

3 Model matrices and related tools

As was mentioned before, GSOAs are typically used for experimentation with quantitative variables. However, investigation of their stratification behavior relies on a coding for qualitative factors. This section introduces useful terminology around qualitative coding and the related GWLP, as well as a suitable real-valued coding that can be used for obtaining the stratification pattern by Tian and Xu (2022), which can be seen as a close relative to the GWLP that is able to reflect the stratification behavior of a GSOA.

3.1 Model matrices and effect column groups

For using a qualitative factor with s levels in a linear model, its $s-1$ main effects degrees of freedom are coded in separate model matrix columns, e.g. by dummy coding, polynomial coding or Helmert coding. Xu and Wu (2001) used the afore-mentioned normalized orthogonal coding, which is now formally defined:

Definition 1 (Normalized orthogonal coding)**.** An $s \times (s-1)$ matrix is a *normalized orthogonal contrast matrix* for a factor in s levels, if and only if all its columns have sum zero, are pairwise uncorrelated, and have squared length s.
A model matrix for a factorial model for n runs in m factors is in *normalized orthogonal coding*, if and only if its first column is $\mathbf{1}_n$ (for the intercept), the main effect for each factor is coded with a normalized orthogonal contrast matrix, and the $(s_1-1)\cdot\cdots\cdot(s_d-1)$ d-factor interaction columns for any d factor projection are obtained as the element wise products of all combinations of main effect columns from d distinct factors.

Let $\mathbf{F}$ denote a full factorial design in m columns at $s_1 \times \cdots \times s_m$ levels, which has $N=\prod_{i=1}^m s_i$ rows. For the $N \times N$ full model matrix $\mathbf{M}(\mathbf{F})$ in normalized orthogonal coding, $\mathbf{M}(\mathbf{F})^\top\mathbf{M}(\mathbf{F}) = N\mathbf{I}_N$. The full model matrix in normalized orthogonal coding of an actual design $\mathbf{D}$ consists of a suitable selection from the N rows of $\mathbf{M}(\mathbf{F})$; as it is instrumental in assessing the properties of $\mathbf{D}$, some notation and terminology for it is now defined.

Definition 2 (Full model matrix and effect column groups)**.** Let $\mathbf{D}$ denote an OA with n runs and m columns.

(i) The *full model matrix* for $\mathbf{D}$ can be written as

$$\mathbf{M} = (\mathbf{1}_n, \mathbf{M}_1, \ldots, \mathbf{M}_m), \tag{1}$$

where $\mathbf{M}_1$ holds all columns for main effects and $\mathbf{M}_d$ holds all columns for the $\binom{m}{d}$ d-factor interaction effects, $d=2,\ldots,m$.

(ii) Within $\mathbf{M}_d$, the columns for a specific d-dimensional projection are called an *effect column group*.

Example 3. Tables 1 and 2 show matrices $\mathbf{M}_1$ in normalized orthogonal coding using normalized orthogonal polynomial contrasts for saturated regular OA$(4,3,2,2)$, OA$(8,7,2,2)$, OA$(9,4,3,2)$, and OA$(16,5,4,2)$. For the 2-level OAs, all effect column groups consist of a single column. The effect column groups for the four columns of the 3-level OA consist of two columns each, and those for the five columns of the 4-level OA consist of three columns each. Matrices $\mathbf{M}_2$ can be obtained by taking all pairwise products between columns from different effect column groups, and so forth. The effect column groups of matrix $\mathbf{M}_2$ have single columns for the 2-level OAs, four columns each for the 3-level OA and 9 columns each for the 4-level OA. The extension to $\mathbf{M}_d, d>2$ is obvious.

3.2 The GWLP and generalized minimum aberration

The GWLP is a tool for ranking factorial designs for qualitative factors via generalized minimum aberration (GMA). It is included here for two reasons: Tian and Xu's (2022) proposal for ranking (G)SOAs follows the same spirit as GMA, and the stratification pattern and the GWLP are closely related and consist of the same ingredients.

Once the model matrix $\mathbf{M}$ of Equation (1) is available for the OA, it is straightforward to obtain the GWLP $(A_0, A_1, \ldots, A_m)$. In the notation of this paper, Xu and Wu's (2001) definition of A_d amounts to

$$A_d = \mathbf{1}_n^\top\mathbf{M}_d\mathbf{M}_d^\top\mathbf{1}_n/n^2 = \sum_{\{i_1,\ldots,i_d\}\subseteq\{1,\ldots,m\}} a_{\{i_1,\ldots,i_d\}}, \tag{2}$$

Table 1: The matrices $\mathbf{M}_1$ for saturated regular OA$(4, 3, 2, 2)$, OA$(8, 7, 2, 2)$, and OA$(9, 4, 3, 2)$. Columns with the same column number in the topmost header row form an effect column group.

OA$(4,3,2,2)$		
1	2	3
1	2	3
-1	-1	-1
-1	$+1$	$+1$
$+1$	-1	$+1$
$+1$	$+1$	-1

OA$(8,7,2,2)$						
1	2	3	4	5	6	7
1	2	3	4	5	6	7
-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	$+1$	$+1$	$+1$	$+1$
-1	$+1$	$+1$	-1	-1	$+1$	$+1$
-1	$+1$	$+1$	$+1$	$+1$	-1	-1
$+1$	-1	$+1$	-1	$+1$	-1	$+1$
$+1$	-1	$+1$	$+1$	-1	$+1$	-1
$+1$	$+1$	-1	-1	$+1$	$+1$	-1
$+1$	$+1$	-1	$+1$	-1	-1	$+1$

OA$(9,4,3,2)$							
1		2		3		4	
1	2	3	4	5	6	7	8
$-\sqrt{3/2}$	$\sqrt{1/2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$
$-\sqrt{3/2}$	$\sqrt{1/2}$	0	$-\sqrt{2}$	0	$-\sqrt{2}$	$\sqrt{3/2}$	$\sqrt{1/2}$
$-\sqrt{3/2}$	$\sqrt{1/2}$	$\sqrt{3/2}$	$\sqrt{1/2}$	$\sqrt{3/2}$	$\sqrt{1/2}$	0	$-\sqrt{2}$
0	$-\sqrt{2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$	0	$-\sqrt{2}$	0	$-\sqrt{2}$
0	$-\sqrt{2}$	0	$-\sqrt{2}$	$\sqrt{3/2}$	$\sqrt{1/2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$
0	$-\sqrt{2}$	$\sqrt{3/2}$	$\sqrt{1/2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$	$\sqrt{3/2}$	$\sqrt{1/2}$
$\sqrt{3/2}$	$\sqrt{1/2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$	$\sqrt{3/2}$	$\sqrt{1/2}$	$\sqrt{3/2}$	$\sqrt{1/2}$
$\sqrt{3/2}$	$\sqrt{1/2}$	0	$-\sqrt{2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$	0	$-\sqrt{2}$
$\sqrt{3/2}$	$\sqrt{1/2}$	$\sqrt{3/2}$	$\sqrt{1/2}$	0	$-\sqrt{2}$	$-\sqrt{3/2}$	$\sqrt{1/2}$

Table 2: Matrix $\mathbf{M}_1$ for the saturated regular OA$(16, 5, 4, 2)$. Columns with the same column number in the topmost header row form an effect column group.

1			2			3			4			5		
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$
$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$
$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$
$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$
$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$
$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$
$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$
$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$
$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$
$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$
$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$
$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$
$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$
$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$
$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$
$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$\sqrt{9/5}$	$+1$	$\sqrt{1/5}$	$-\sqrt{9/5}$	$+1$	$-\sqrt{1/5}$	$\sqrt{1/5}$	-1	$-\sqrt{9/5}$	$-\sqrt{1/5}$	-1	$\sqrt{9/5}$

i.e., $n^2 A_d$ is the sum of squared column sums of matrix $\mathbf{M}_d$. A_d can also be broken down into projection specific contributions $a_{\{i_1,\dots,i_d\}}$, where $a_{\{i_1,\dots,i_d\}}$ consists of only the summands belonging to columns from the effect column group for factors $i_1,\dots,i_d$.

According to Xu and Wu (2001), the A_d (and by a simple argument also the $a_{\{i_1,\dots,i_d\}}$) are invariant to the choice of normalized orthogonal coding for $\mathbf{M}$. It is known that $A_0 = 1$ (for the intercept column), and that the sum of all A_d, $d = 0,\dots,m$, is N/n for OAs with distinct rows. The GWLP is related to the strength of an OA as follows: $A_1 = \dots = A_t = 0$ and $A_{t+1} > 0$ is equivalent to OA strength exactly t (i.e., criteria for OA strength $t+1$ are violated). Xu and Wu proposed to rank OAs by GMA, i.e. to consider an OA $\mathbf{D}_1$ as better than an OA $\mathbf{D}_2$, if the leftmost element for which the GWLPs differ is smaller for $\mathbf{D}_1$ than for $\mathbf{D}_2$.

3.3 Power contrasts and power coding

For the definition of power coding, the saturated regular $\mathrm{OA}(s^\ell, (s^\ell-1)/(s-1), s, 2)$ of Lemma 1 (ii) is an important ingredient.

Definition 3 (Power contrasts, power coding, and effect column micro groups)**.** Consider a column in s^ℓ levels.

(i) The $s^\ell - 1$ contrast columns that are obtained by

- first creating the regular saturated $\mathrm{OA}(s^\ell, (s^\ell-1)/(s-1), s, 2)$ of Lemma 1 (ii)
- and then replacing each of the OA columns with the $s-1$ columns according to the normalized orthogonal polynomial coding for s levels

are called *power contrasts*. They are arranged in an $s^\ell \times (s^\ell - 1)$ matrix.

(ii) The $s^\ell - 1$ columns of the effect column group for a main effect coded with power contrasts can be subdivided into $(s^\ell-1)/(s-1)$ *effect column micro groups* according to the effect column groups for main effects of the underlying saturated OA in s-level factors.

(iii) For a d-factor interaction with all factors coded in power contrasts, an *effect column micro group* consists of all columns that are obtained as product columns of from a single main effect column micro group for each of the factors.

(iv) Coding main effects with power contrasts and interaction effects as products of main effects columns in the usual way is called *power coding* in this paper.

The definition arbitrarily fixes the choice of normalized orthogonal contrasts to polynomial. Results of this paper would not change by using a different normalized orthogonal coding. The $2^m - 1$ effect column groups in the matrix $\mathbf{M}$ of Equation (1) (excluding the intercept) are subdivided into a total of $2^{m\cdot\ell} - 1$ effect column micro groups.

Proposition 1. *Power coding for arrays with all columns in s^ℓ levels is a normalized orthogonal coding in the sense of Definition 1.*

Proof. It suffices to show that power contrasts are normalized orthogonal contrasts. The $s^\ell \times (s^\ell - 1)$ matrix $\mathbf{P}$ of main effect power contrasts for a single column is the full model matrix $\mathbf{M}(\mathbf{F})$ without the intercept column for the full factorial in the s-level basic vectors $\mathbf{e}_1,\dots,\mathbf{e}_\ell$ used in the Rao-Hamming construction of Lemma 1 (ii). Thus, its column sums are zero, and $\mathbf{P}^\top\mathbf{P} = s^\ell \mathbf{I}_{s^\ell - 1}$, as requested in Definition 1. Hence, power coding uses normalized orthogonal contrasts and handles them in the way prescribed in Definition 1 and is thus a normalized orthogonal coding. □

Example 4. The model matrices of Tables 1 and 2 can also serve as power contrasts for factors in 4, 8, 9 or 16 levels. The effect column groups indicated in the tables are the effect column micro groups for the s^ℓ level main effect columns. Note that power contrasts for 16-level columns can be based on $16 = 4^2$, like in the table, or on $16 = 2^4$ in analogy to 4 and 8 levels; in the latter case, each single column would consist of -1/+1 values and would be considered as an effect column micro group of its own.
An effect column group within the model matrix $\mathbf{M}_2$ consists of $(s^\ell - 1)^2$ columns (9, 49, 64, 225 respectively); there are $\binom{m}{2}$ such effect column groups. An effect column *micro* group within $\mathbf{M}_2$ consists of $(s-1)^2$ columns (1 for $s = 2$, 4 for $s = 3$, 9 for $s = 4$), and there are $(s+1)^2$ such effect column micro groups within each effect column group.

Proposition 2. *Consider the matrix of power contrasts for an s^ℓ level column, $\ell = 1, 2, \ldots$, and let u denote the column number.*

(i) $u \in \{1, \ldots, s-1\}$*: Column u is a main effect column for $\mathbf{e}_1(\ell)$ in the Rao-Hamming construction (slowest changing). It has up to s^1 distinct values, with the same value assigned within each of s strata of adjacent levels.*

(ii) For $\ell \geq 2$: $s^{i-1} \leq u \leq s^i - 1$, $i = 2, \ldots, \ell$: Column u is a main effect column for $\mathbf{e}_i(\ell)$ or an interaction column involving $\mathbf{e}_i(\ell)$ and (slower-changing) basic columns $\mathbf{e}_\nu(\ell), \nu < i$, of the Rao-Hamming construction. It has up to s^i distinct values, with the same value assigned within each of s^i strata of adjacent levels.

(iii) The exponent of s in the maximum number of distinct values according to (i) and (ii) can be calculated as $\rho(u) = \lceil \log_s(u+1) \rceil$.

The proof is omitted, because it is straightforward.

The $\rho(u)$ of part (iii) of the proposition are the "weights" of Tian and Xu (2022); $\rho(u)$ is also the minimum number of digits that is needed for representing the column number u as an s-ary number.

Remember that the single weight $\rho(u)$ from Proposition 2 indicates constancy of the main effect model matrix column within $s^{\rho(u)}$ strata of adjacent levels. If a model matrix column in $\mathbf{M}_d$ is a product of d such columns, it relates to crossed strata obtained from the d contributing columns, and the number of crossed strata is, of course, $\prod_{i=1,\ldots,d} s^{\rho(u_i)} = s^{\sum_{i=1,\ldots,d} \rho(u_i)}$. This makes it natural to define the weight of a vector of column numbers as the sum of individual weights:

Definition 4 (Weight for a model matrix column (restated from Tian and Xu 2022))**.** Let $\mathbf{m}$ denote a column in the model matrix portion $\mathbf{M}_d$ from Equation (1) from power coding for an OA with n runs and m columns in s^ℓ levels each.
Let $\mathbf{u} = (u_1, \ldots, u_d)^\top$ denote the vector of column positions within their respective main effect column group for the columns that were multiplied to obtain $\mathbf{m}$.
The weight assigned to the column $\mathbf{m}$ is $\rho(\mathbf{u}) = \sum_{i=1}^{d} \rho(u_i)$, with $\rho(u_i)$ according to Proposition 2 (iii).

Example 5. The weights for the contrasts of Tables 1 and 2 are 122 (4 levels), 1223333 (8 levels), 11222222 (9 levels), and 111222222222222 (16 levels). Would one consider the 16 runs using power contrasts based on $16 = 2^4$, the resulting (different) 16-level power contrasts would have weights 122333344444444.
These apply to main effect column groups, i.e., the $n \times (m \cdot (s^\ell - 1))$ matrix $\mathbf{M}_1$ for an array with m columns in s^ℓ levels each consists of m effect column groups with $s^\ell - 1$ columns each, and the weights within each such group are as stated above. As was mentioned before, these weights are constant within effect column micro groups of $s-1$ columns each.
Columns of $\mathbf{M}_2$ have at least weight 2 (two main effect columns with weight 1 each) and at most weight 2ℓ (two main effect columns with weight ℓ each). Considering the two variants of power contrasts for 16 levels, the maximum weight for the columns of $\mathbf{M}_2$ is thus 4 for the tabulated coding and 8 for the alternative 16-level power contrasts based on $16 = 2^4$. Of course, the meaning of the weight changes with s, because weights were derived as exponents to s.

Proposition 3. *Let $\mathbf{M}$ be a full model matrix according to Equation* (1) *based on power coding, with column weights according to Definition 4. All columns in the same effect column micro group have the same weight.*

Proof. Proposition 2 implies that all columns within the same effect column micro group for $\mathbf{M}_1$ have the same weights. An effect column micro group for $\mathbf{M}_d$ combines one effect column micro group from $\mathbf{M}_1$ for each of the d variables from the dD projection, which implies that exactly one combination weight is obtained. □

The proposition is important, because it implies that column groups defined by weights comprise entire effect column micro groups only, which will make it possible to prove that power coding can be used in place of Tian and Xu's complex coding.

4 GSOAs and the stratification pattern

As was mentioned before, in an OA of OA strength at least two with columns in s^ℓ levels, each 2D projection would consist of equireplicated copies of all conceivable $s^{2\ell}$ distinct level combinations. (G)SOAs typically have OA strength 1 only (and need not even have that strength). For evaluating their behavior in d dimensions, one considers coarsened columns, as was explained in the introduction for classical SOAs. As was mentioned before, Tian and Xu (2022) proposed GSOAs that consider s^ℓ levels in combination with strength t, where ℓ and t need not coincide. These are now defined.

Definition 5 (SOA and GSOA)**.** An array in $n = \lambda s^\ell$ runs with m columns at s^ℓ levels each is a GSOA(n, m, s^ℓ, t), $t \le m$, if and only if all possible stratifications into $s^t = s^{u_1} \cdot \ldots \cdot s^{u_t}$ strata, u_i integers with $0 \le u_i \le \ell$ and $u_1 + \ldots + u_t = t$, are equireplicated.
If $t = \ell$, the GSOA is an SOA.

Note that the definition of GSOAs does not guarantee the existence of s^t strata in lower dimensions: for $\ell < t$, 1D (and perhaps even 2D) stratification is equireplicated (implied by balance in equireplication in higher dimensions), but may yield fewer than s^t strata (see also Example 10). For $\ell > t$, a GSOA with s^ℓ levels of strength t can, e.g., be obtained by expanding the levels of an SOA(n, m, s^t, t), assuming that s^ℓ divides n.

Example 6. A GSOA$(81, 4, 81, 3)$ has been created from an SOA$(81, 4, 27, 3)$ by expanding the levels of each column to 81 (assigning the three possible choices for each original level in random order). (The ingoing SOA was obtained by the Li et al. (2021) construction from the OA$(27, 4, 3, 3)$ that is available in R package DoE.base (Grömping 2018) as `L27.3.4`.) This GSOA will be revisited in Examples 7 and 8 for illustrating the stratification pattern and its interpretation.

Tian and Xu (2022) introduced the stratification pattern (the space-filling pattern of their article) as a tool to assess a (G)SOAs strength and stratification behavior, in the same spirit as the GWLP assesses an OAs strength and balance properties. The ingredients for obtaining the stratification pattern are normalized squared column sums of the model matrix of Equation (1). For the GWLP of Xu and Wu (2001), these were summed separately for each dimension of the projection, i.e., there is a sum for each d, $d = 0, 1, \ldots, m$. For the stratification pattern, they are summed separately by the column weights instead.

Definition 6 (Stratification pattern)**.** Let $\mathbf{M}$ denote the model matrix in power contrast coding for an OA with n runs and m columns at s^ℓ levels each. Let $\mathbf{m}$ denote a column in $\mathbf{M}_d, d = 1, \ldots, m$, and let $\mathbf{u}(\mathbf{m}) = (u_1, \ldots, u_d)^\top$ denote the vector of column positions within their main effect column group for the columns that were multiplied to obtain $\mathbf{m}$.

The elements of the stratification pattern $(S_1, \ldots, S_{m\cdot\ell})$ are

$$S_j = \sum_{d=\max(1,\lceil j/\ell \rceil)}^{\min(m,j)} \sum_{\substack{\mathbf{m} \text{ a column of } \mathbf{M}_d \\ \text{and } \rho(\mathbf{u}(\mathbf{m})) = j}} (\mathbf{1}_n^\top \mathbf{m})^2 / n^2. \tag{3}$$

Example 7. Table 3 shows the stratification pattern for up to weight 12 (bottom row), split up by contributions from different dimensions, for the GSOA$(81, 4, 81, 3)$ of Example 6. There are four rows for 1D to 4D ($m = 4$), and there are 16 columns (only 12 shown) for weights $j = 1, \ldots, m \cdot \ell$. The right margin shows the GWLP - which also includes the hidden columns (easy to verify with function `GWLP` of R package DoE.base). The boundaries for d in Definition 6 start at 1 for $j = 1, \ldots, 4$, at 2 for $j = 5, \ldots, 8$,

Table 3: Dimension by weight table of contributions to GWLP and stratification pattern from the GSOA$(81, 4, 81, 3)$. Row label: dimension. Column label: weight. Bottom margin: stratification pattern (first 12 elements).

	1	2	3	4	5	6	7	8	9	10	11	12		GWLP
1	0	0	0	0	.	.	.	.	.	.	.	.	last	0
2	.	0	0	20	32	80	96	252	.	.	.	.	four	480
3	.	.	0	0	8	112	368	1248	2808	5184	7776	7776	columns	25280
4	.	.	.	0	8	20	104	504	1872	6372	17280	40176	not	505680
Sum	0	0	0	20	48	212	568	2004	4680	11556	25056	47952	shown	531440

and so forth, and go up to j for $j = 1, 2, 3$ and up to 4 for all larger j. The "." in the table indicate impossible combinations of d and j.

Tian and Xu (2022) used a definition comparable to Definition 6, but with a normalized orthogonal coding based on the sth roots of the unity instead of the power coding. It is now shown that use of power coding is equivalent to Tian and Xu's coding as far as obtaining stratification patterns is concerned.

Proposition 4. *The stratification pattern of Definition 6 is equivalent to Tian and Xu's space-filling pattern.*

Proof. Tian and Xu (2022) coded the model matrix columns according to normalized orthogonal coding using a contrast matrix constructed from powers of the complex number $\xi = \exp^{2\pi i/s}$. The contrast matrix has rows for the levels $x = 0, \dots, s^\ell - 1$ and columns for the index value $u = 1, \dots, s^\ell - 1$, and the entry for the combination of row x with column u is obtained as $\chi_u(x) = \xi^{\langle u,x \rangle}$, with $\langle \bullet, \bullet \rangle$ denoting a reversed scalar product based on s-ary representations of x and u. Careful study shows that the columns of Tian and Xu's contrasts also fulfill the properties of Proposition 2. Define s-level contrasts $\chi_1(x)$ $(s = 2)$ or $\chi_1(x), \chi_1(x)^2, \dots, \chi_1(x)^{s-1}$ $(s > 2)$, arranged in a row each for $x = 0$ to $x = s - 1$. This is a normalized orthogonal contrast matrix for s-level columns and can be used instead of the normalized orthogonal polynomial coding in the power contrasts of Definition 3. Because of well-known invariance results for sums of squared column sums for entire effect column micro groups, the modified power coding with the above contrasts yields the same stratification pattern as the original power coding of Definition 3. Furthermore, it can be verified that the above construction yields Tian and Xu's contrast matrix for s^ℓ levels, but with different column order *within columns of the same weight* $\rho(u)$. As changing the column order within columns of the same weight does not impact the stratification pattern, the stratification pattern obtained in this paper coincides with the space-filling pattern introduced by Tian and Xu. □

The proposition implies that Tian and Xu's theoretical results apply to the stratification pattern obtained from power coding.

Lemma 2 (Tian and Xu)**.** *Consider a GSOA with n runs and m columns in s^ℓ levels each, and let $(S_1, \dots, S_{m\cdot\ell})$ denote its stratification pattern.*

(i) The GSOA has stratification strength t, if and only if $S_1 = \cdots = S_t = 0$.
(ii) If the GSOA has distinct rows, $\sum_{j=1}^{m\cdot\ell} S_j = N/n - 1$.

The sum of the elements is (of course) the same as for the GWLP elements, except for omitting the 0th element that is normally included in the GWLP but not in the stratification pattern.

Example 8. We see from Table 3 that the GSOA has strength 3, and that strength 4 is violated because there are two-dimensional projections for which 3^4 equireplicated strata are not achieved; S_4 is inherited from the SOA$(81, 4, 27, 3)$ from which the GSOA was created (2D stratification with weight 4 can of course not involve any single column with 81 levels).
The sum of all pattern entries (including those from hidden columns 13 to 16) is $81^4/81 - 1$, i.e., one less than the sum of *all* GWLP elements (for the GWLP, including $A_0 = 1$ increases that sum by 1). The stratification pattern for the underlying SOA$(81, 4, 27, 3)$ is (0, 0, 0, 20, 32, 140, 232, 616, 1056, 1440, 1728, 1296) and has sum $27^4/81 - 1 = 6560$; additional contributions from level expansion start for weight 5 and increase with increasing weight.

Tian and Xu (2022) proposed the use of a GMA like criterion for stratification patterns; this is now defined as "minimum stratification aberration":

Definition 7 (Stratification aberration and MSA)**.** Let an array $\mathbf{D}$ with n runs and m columns in s^ℓ levels each have the stratification pattern $S(\mathbf{D}) = (S_1, S_2, \dots, S_{m\cdot\ell})$.

(i) Let $\mathbf{D}_1$ and $\mathbf{D}_2$ be two arrays with n runs and m columns in s^ℓ levels each. $\mathbf{D}_1$ has better *stratification aberration* than $\mathbf{D}_2$, if and only if the leftmost element for which $S(\mathbf{D}_1)$ and $S(\mathbf{D}_2)$ differ is smaller for $\mathbf{D}_1$ than for $\mathbf{D}_2$.
(ii) $\mathbf{D}$ has *minimum stratification aberration (MSA)* among all arrays with the same n,m, s^ℓ, if there is no array that has better stratification aberration.

The definition (of course) implies that arrays with larger strength are always better than arrays with smaller strength. Note that the definition restricts comparison to arrays with comparable properties (n,m,s^ℓ). In particular, naïve comparisons between arrays with different numbers of levels may be misleading. Furthermore, where s and ℓ can not be uniquely derived from context, one has to state them with the reported stratification pattern; for example, $s = 9$ with $\ell = 2$ instead of $s = 3$ with $\ell = 4$ would have been possible in Example 7, and would have yielded a very different stratification pattern with $S_2 > 0$. Section 6 provides an explicit example (Example 12).

5 Implementation of the stratification pattern

In the R package SOAs (Grömping 2022b), the power contrasts are implemented in function `contr.Power`, function `Spattern` calculates the stratification pattern, and function `dim_wt_tab` allows to extract and display a dimension by weight table, like in Table 3, from a pattern created by function `Spattern`.

This section presents the algorithm used for implementing the stratification pattern and gives an impression of its run times. As calculations can be resource intensive for moderate or large arrays, and one is often only interested in

- low-dimensional projections (i.e., small d),
- weights j that are not much larger than t or ℓ,

the algorithm permits the use of user-specified upper limits for the dimension ($d_{\max} \leq m$) and the weight ($j_{\max} \leq m\ell$). Per default, $j_{\max} = 4$, and $d_{\max} = j_{\max}$; both can of course be modified. The algorithm then proceeds as follows:

1. Create the main effects model matrix $\mathbf{M}_1$ with $m \cdot (s^\ell - 1)$ columns using power contrasts for s^ℓ levels.
2. Obtain the list of all 1D to $d_{\max}$D projections (list of $d_{\max}$ matrices, the columns of which hold the factor IDs of factors in the projection).
3. Loop over dimensions $d = 1, \ldots, d_{\max}$:
   i. If $j_{\max} - d + 1 < \ell$, restrict the columns to be considered from $\mathbf{M}_1$ to those with weights up to $j_{\max} - d + 1$ (because columns with larger weights cannot contribute to a dD interaction column with weight at most $j_{\max}$).
   ii. Obtain the vector of weights for the columns of a single d-factor interaction matrix (invariant to the specific dD projection, using the reduced columns of $\mathbf{M}_1$ in the construction); create a second vector that only holds weights up to $j_{\max}$.
   iii. Initialize the vector of dD contributions to the stratification pattern with missing values.
   iv. Select the dth element of the list obtained in Step 2.
   v. Loop over the $\binom{m}{d}$ dD projections (columns of the matrix selected in iv.):
      a. determine the d-tuples of column numbers for $\mathbf{M}_1$ columns to be multiplied for obtaining the effect column group (neglecting columns excluded in i.),
      b. remove tuples corresponding to weights larger than $j_{\max}$, using the weights vector from ii.,
      c. loop over the remaining tuples:
      register the weight j (using the reduced weights vector from ii.), calculate the product column and add the square of its column sum to the jth element of the vector of dD contributions (initializing it with this value, if it is still missing).
4. Sum the vectors of dD contributions, $d = 1, \ldots, d_{\max}$, into the stratification pattern; keep the table of separate dD contributions as an attribute of the returned object.

If a stratification pattern has been calculated with an upper limit $d_{\max} < m$ on dimension, it must be interpreted w.r.t. that restriction for weights $j = d_{\max} + 1, \ldots, m\ell$, whereas an upper limit on the weight has no impact on pattern entries for weights up to $j_{\max}$.

Run time has not been extensively studied. For an SOA$(125, 6, 25, 2)$, run times with unlimited weights were dominated by the number of contributions from $d_{\max}$-factor interactions that contribute to the stratification pattern for the highest-dimensional projection, which can be calculated as $\binom{m}{d_{\max}} \cdot 24^{d_{\max}}$ (considering $d_{\max} = 2, \ldots, 5$, with run times of 2, 49, 1078, 10888 seconds). For a GSOA$(125, 6, 125, 2)$, the $\binom{m}{d}$ portion of the number of contributions remains unchanged, but the number of columns increases by the factor $(124/24)^d$, i.e., one would expect run times (with unlimited weights) to increase to approximately 41, 6772, 768290, 40085929 seconds=0, 1.9, 213.4, 11135 hours=0, 0.1, 8.9, 464 days, possibly with some additional increase for overhead. Actual durations were about 45 and 7748 seconds for $d_{\max} = 2$ and 3. Though low dimensional projections are the most important ones, it is clearly desirable to substantially reduce the maximum weight $j_{\max}$ in order to make calculations feasible. According to Proposition 2, for a matrix of power contrasts for s^ℓ levels, the number of columns with small weight is relatively low, so that limiting the weight has a very beneficial effect on run times, and a much stronger effect than limiting the dimension. For the 125 run with 25 levels example, there are only a total of 63 interaction effects of all dimensions to be considered, so that the potential from reducing $d_{\max}$ is limited. If $j_{\max}=4$ (implying $d_{\max}=4$, because weights for larger dimensions are larger than 4), calculation of the stratification pattern was completed in about 6 seconds. Run times for $j_{\max}=5$ (implying $d_{\max}=5$) and $j_{\max}=6$ (and $d_{\max}=m=6$) were about 38 seconds or 228 seconds, respectively, which was much faster than when restricting dimension only. For the 125-level case, times were slower, but not dramatically so, because most of the additional interaction columns have relatively large weights: restriction to maximum weights 4, 5 or 6 ran in approximately 8, 73 or 846 seconds, respectively. Besides the larger effect on run time, limiting the weight and thereby only implicitly limiting dimension has the benefit that $S_1,\dots,S_{j_{\max}}$ are not reduced by omitting relevant projections. Note, however, that limiting dimension will have a larger effect for arrays with a large number of columns.

6 Examples

All calculations have been done with R, and the code is available online. Besides the stratification pattern, the ϕ_p criterion (Morris and Mitchell 1995) is used for the assessment of space-filling:

$$\phi_p(\mathbf{X}) = \left(\sum_{\{i,j\}\subset\{1,\dots,n\},i\neq j} d(\mathbf{x}^{(i)},\mathbf{x}^{(j)})^{-p}\right)^{1/p}. \tag{4}$$

For large p, the ϕ_p criterion can mimic the maximin distance criterion well, and the R package SOAs uses the criterion with $p=50$ for optimization of space filling within constructions, via level permutations in construction matrices. Small values of ϕ_p imply better space-filling. The ϕ_p value is a good supplement to the stratification pattern, because it captures a different aspect of space-filling: comparing stratification patterns between arrays with different numbers of levels for each column, e.g., the GSOA$(81,4,81,3)$ of Example 7 and the SOA$(81,4,27,3)$ from which it was created, is of limited use, because the different numbers of levels per column between the arrays are not directly reflected in the pattern as an advantage for the array with more levels, but rather as a disadvantage because the sum of pattern entries is larger for the array with more levels ($(S_1,\dots,S_6)=(0,0,0,20,32,140)$ for the SOA, as compared to the pattern of Table 3). The ϕ_p values do capture the fineness / coarseness of columns: $\phi_p=0.175$ for the SOA and $\phi_p=0.06$ for the GSOA, i.e. expanding the levels substantially reduces (=improves) the ϕ_p value.

Example 9. Sun, Wang and Xu (2019) provided four different arrays with three 25-level columns in 25 runs. Their stratification patterns have $m\ell=3\cdot 2$ elements and are given in Table 4. The sum of pattern elements is $25^3/25-1=624$. The fourth array is the only one that achieves SOA strength 2. This example demonstrates that the power contrast based calculation of the stratification pattern does indeed yield the same results as the construction in Tian and Xu (2022) (their Example 4 provides S_1 to S_4 for each of these arrays).

Example 10. This example treats the extreme case $\ell=1$: The stratification pattern for the OA$(81,8,3,4)$, available in R package DoE.base as `L81.3.8`, is (0, 0, 0, 22.42, 23.51, 18.96, 9.88, 5.23). As $\ell=1$, the stratification pattern has exactly $m=8$ elements, and its elements for $j=1,\dots,m$ coincide with the corresponding GWLP elements, as was already noted by Tian and Xu 2022 for OAs with $\ell=1$. $S_1=S_2=S_3=0$ means that the stratification strength is 3, which implies *up to* $s^3=27$ strata for 1D, 2D and 3D. Of course, there are only three strata in 1D and only nine strata in 2D, because more is simply not possible. This is an extreme example that underlines what a zero in the stratification pattern

Table 4: Stratification patterns of the four 25-level arrays of Sun et al. (2019)

	S_1	S_2	S_3	S_4	S_5	S_6
D_1	0	0.64	26.08	85.92	191.36	320
D_2	0	1.84	22.48	89.52	190.16	320
D_3	0	0.96	25.12	86.88	191.04	320
D_4	0	0.00	28.00	84.00	192.00	320

means: $S_j = 0$ if and only if all existing stratifications with up to s^j strata are equireplicated, and $S_j = 0$ does *not* imply that s^j strata exist in all dimensions up to j.

Example 11. Tian and Xu (2022) conducted an exhaustive search of subsets of columns from Shi and Tang's (2020) construction for up to 9 8-level columns in 32 runs. Among other things, they found 4-column subsets that have stratification strength 4. One of these and several expansions to GSOAs are now inspected. The expansions were obtained by expanding the four observations with the same level (each of 0 to 7) into either

- balanced 16-level: two copies each of corresponding adjacent levels from 0 to 15,
- unbalanced 16-level: one and three copies of adjacent levels from 0 to 15 (deciding at random, which of the levels occurs more frequently; of course, one would avoid using an intentionally unbalanced expansion for an actual experiment),
- balanced 32-level: corresponding adjacent levels from 0 to 31.

Table 5 provides a breakdown into dimensions for the elements of the stratification pattern for the SOA and the three GSOAs. Expanding the levels ensures that stratification into $2^4 = 16$ strata is possible in all dimensions up to 4. The balanced allocations provide strength 4 GSOAs. The unbalanced allocation, on the other hand, yields strength 3 only, because there is a 1D violation of equireplication for 16 strata (and also a 1 in the GWLP for 1D, i.e., the unbalanced GSOA does not have OA strength 1). Note that level expansion substantially reduces ϕ_p from 0.343 for the SOA over 0.143 for the balanced 16-level GSOA to 0.073 for the 32-level GSOA, whereas the stratification patterns do not reflect the improvement. The unbalanced GSOA, even though of stratification strength 3 only, also has a better ϕ_p than the SOA (0.2), but a worse one than the balanced 16-level GSOA. If feasible, the 32-level GSOA should presumably be preferred to the 16-level one, even though this cannot be inferred from the stratification pattern.

Example 12. An SOA with 5 16 level columns in 64 runs has been obtained using the construction by Zhou and Tang (2019). This example is interesting for two reasons: Level permutations for optimizing ϕ_p (conducted per default by R package SOAs) modify the stratification pattern, and the contrasts for the 16 levels can be taken as power contrasts from 2^4 levels or from 4^2 levels. ϕ_p optimization by level permutations brought an initial unoptimized $\phi_{p;\text{unoptimized}} = 0.256$ down to $\phi_{p;\text{optimized}} = 0.105$ (like in Example 11, it can be expected that level expansion to 32 or 64 levels, i.e., obtaining a GSOA, would further improve (=decrease) ϕ_p; this has not been done here). The stratification pattern has 20 elements for the 2^4 perspective or 10 elements for the 4^2 perspective, respectively. Table 6 shows the first six elements for both: In the 4^2 perspective, the SOA has SOA strength 2 (i.e., $4^2 = 16$ strata are guaranteed for all 1D and 2D projections); the construction yields strength 2+, which is in line with the entry for dimension 2 and weight 3 being zero. In the 2^4 perspective, the array has strength 3, as $S_4 = 1.75$ is the first non-zero element (all dimensions considered); this was achieved by searching for a level permutation that preserves this strength, most level permutations would reduce the strength to 2, by causing a small non-zero S_3. Strength 4 is not attained, because not all $2 \times 2 \times 4$ or $2 \times 4 \times 2$ or $4 \times 2 \times 2$ stratifications yield 16 strata. In 2D, the array even attains 64 equireplicated strata of the form 16×4 or 4×16 (as the entry for 2D and weight 3 is zero in the 4^2 perspective, the 2+ by Zhou and Tang). In the 2^4 perspective, 64 strata are not guaranteed, because 8×8 stratifications are not all equireplicated; at least, there are 32 equireplicated strata (i.e. 16×2, 8×4, 4×8, 2×16).

Example 12 illustrates that the stratification pattern

- depends on the choice of s and ℓ, implying that also the strength depends on this choice,
- can depend on level permutations for improving ϕ_p at least for some constructions,
- yields a somewhat crude story, when considered without dimensionality breakdown,
- allows refined understanding by looking at the underlying dimension by weight table.

7 Discussion

The GSOAs by Tian and Xu (2022) are a natural extension of SOAs. They resolve the unfortunate forced link between stratification strength and number of levels that existed in SOAs and was previously overcome by defining exceptions via qualifiers such as $+$, $-$ or *. Their use for computer experimentation benefits from favorable space-filling properties, and the stratification pattern (called space-filling pattern by Tian and Xu 2022) captures the stratification aspect of space-filling. The stratification pattern is a relative of the long-standing GWLP (Xu and Wu 2001): both sum the same squared sums of model matrix

Table 5: Dimension by weight tables of contributions to GWLP and stratification pattern for an SOA$(32, 4, 8, 4-)$ (top), two GSOAs with 16 level columns derived thereof (second: strength 4, third: strength 3), and a strength 4 GSOA with 32 level columns (bottom). Column headers: weights. Row labels: dimensions. Bottom margin: stratification pattern (first three zero elements omitted for 32 run GSOA).

	1	2	3	4	5	6	7	8	9	10	11	12	GWLP
1	0	0	0	.	.	.	.	.	.	.	.	.	0
2	.	0	0	0	2	6	.	.	.	.	.	.	8
3	.	.	0	0	7	10	11	8	8	.	.	.	44
4	.	.	.	0	0	3	0	8	20	20	16	8	75
Sum	0	0	0	0	9	19	11	16	28	20	16	8	127

	1	2	3	4	5	6	7	8	9	10	11	12		GWLP
1	0	0	0	0	.	.	.	.	.	.	.	.	last	0
2	.	0	0	0	4	14	10	14	.	.	.	.	four	42
3	.	.	0	0	7	15	21	45	84	92	96	64	columns	424
4	.	.	.	0	0	3	1	14	45	82	164	248	not shown	1581
Sum	0	0	0	0	11	32	32	73	129	174	260	312		2047

	1	2	3	4	5	6	7	8	9	10	11	12		GWLP
1	0	0	0	1	.	.	.	.	.	.	.	.	last	1
2	.	0	0	0	5	12	12	12.5	.	.	.	.	four	41.5
3	.	.	0	0	7	13	23	44	80	95	96	64	columns	422
4	.	.	.	0	0	3	1	14	44	87.5	161	248	not shown	1582.5
Sum	0	0	0	1	12	28	36	70.5	124	182.5	257	312		2047

	4	5	6	7	8	9	10	11	12		GWLP
1	0	0	.	.	.	.	.	.	.	last	0
2	0	5.75	21.5	25.75	35.5	49	48.5	.	.	eight	186
3	0	7	12.75	28.25	63.25	154.75	289	478	639	columns	3720
4	0	0	3	1.5	15.25	59	133.75	318	681.5	not shown	28861
Sum	0	12.75	37.25	55.5	114	262.75	471.25	796	1320.5		32767

Table 6: Dimension by weight tables (weights up to 6) for stratification patterns of an SOA$(64, 5, 16, 2)$ (left), which is also a GSOA$(64, 5, 16, 3)$ (right). Row labels: dimensions. Column labels: weights. Bottom margins: stratification patterns.

	s=4, ℓ=2						s=2, ℓ=4					
	1	2	3	4	5	6	1	2	3	4	5	6
1	0	0	.	.	.	.	0	0	0	0	.	.
2	.	0	0	30	.	.	.	0	0	0	0	5
3	.	.	6.5	70.5	199.5	263.5	.	.	0	1.75	6.25	17.25
4	.	.	.	3.5	93	600	.	.	.	0	0.5	2.5
5	.	.	.	.	5	76.5	.	.	.	.	0	0.25
Sum	0	0	6.5	104	297.5	940	0	0	0	1.75	6.75	25

columns, but group the sums by different criteria (dimension for the GWLP, weight for the stratification pattern).

The stratification pattern has been implemented in the R package SOAs, using the newly-introduced power coding of Definition 3. Dimension by weight tabulation of the summands of the stratification pattern is a by-product of the implementation and contributes to an improved understanding of an array's stratification behavior. Due to being based on coding for qualitative factors, obtaining stratification patterns is very resource intensive for arrays with large numbers of levels; an upper limit for the weights (and thus implicitly for the projection dimensions considered) per default keeps computing resources in check. There may be the potential that future implementations by the group of Honguan Xu are faster for situations that are particularly difficult for the model-matrix based approach taken in this paper; this hope is based on the relation between function `GWLP` on the one hand and function `length2` to `length5` on the other hand for obtaining GWLP elements in R package DoE.base. `GWLP` follows Hongquan Xu's approach using Krawtchouk polynomials, whereas the `length*` functions follow the model matrix approach of this paper; these functions complement each other: `GWLP` is faster for arrays that have many columns, the `length*` functions are faster for arrays that have many rows.

Space-filling behavior is a multifaceted phenomenon, and there are further aspects to consider in addition to stratification behavior. For example, using the discrepancy metric ϕ_p (smaller=better, see Equation (4)) in conjunction with the stratification pattern might be a good idea. For computer experiments with quantitative variables, it can be sensible to expand the levels of an SOA to obtain a GSOA with more levels, ideally an LHD. For assessing the properties of such an expanded array, it is proposed to obtain the stratification pattern for the underlying SOA, and to assess improved space-filling of the GSOA via other criteria, e.g., the ϕ_p criterion (see Example 11). In this way, run time for obtaining the space-filling pattern can be kept as low as possible, without loosing relevant information.

So far, the constructions implemented in the R package SOAs permit improvements by level permutation w.r.t. the ϕ_p criterion, using an algorithm proposed by Weng (2014). The ϕ_p criterion can be cheaply calculated, and Weng's algorithm keeps searches over level permutations manageable. Improvements w.r.t. the stratification pattern would also be desirable, and level permutations have been observed to have an impact on the stratification pattern for some constructions (e.g., Example 12), but not for many others. For achieving favorable stratification patterns, improved incorporation of stratification aspects into the development of construction algorithms may be a more promising way than resource-intensive optimization via level permutation. The stratification pattern may help to instigate research in that direction.

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