

## MINIMAL SECOND ORDER SATURATED DESIGNS AND THEIR APPLICATIONS TO SPACE-FILLING DESIGNS

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*Abstract:* Second order saturated (SOS) designs allow the estimation of a saturated model consisting of main effects and two-factor interactions. Apart from being useful in their own right, SOS designs have recently been applied to the construction of space-filling designs. This paper introduces the notion of minimal SOS designs to facilitate the study of SOS designs, and presents some results on the characterization and construction of minimal SOS designs. Both regular and nonregular minimal SOS designs are considered, and are applied to construct space-filling designs.

*Key words and phrases:* Clear effect, maximal design, nonregular design, space-filling design, strong orthogonal array.

### 1. Introduction

Second order saturated (SOS) designs allow the estimation of saturated models consisting of main effects and two-factor interactions (2fi's). They make the most efficient use of the degrees of freedom by allocating all of them to the estimation of factorial effects of the first two orders, which are the most important orders according to the principle of effect hierarchy. SOS designs were first introduced in Block and Mee (2003), and were also discussed in Chen and Cheng (2004) under the notion of estimation index. Constructions of nonregular SOS designs were explored by Cheng, Mee and Yee (2008). For more details about SOS designs, see Mee (2009, Sec. 7.2) and Cheng (2014, Sec. 11.2).

SOS designs are important in their own right, but become more so owing to their utility in designing computer experiments. It is widely accepted that space-filling designs are appropriate choices for computer experiments (Santner, Williams and Notz (2003)). Among the methods available for constructing

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space-filling designs, that based on orthogonal arrays is very attractive because it provides designs that enjoy some guaranteed space-filling properties in low-dimensional projections. This line of research started with Latin hypercubes, which are orthogonal arrays of strength one, in McKay, Beckman and Conover (1979), and continued with the work of Owen (1992) and Tang (1993). A significant enhancement to the idea is the recent introduction of strong orthogonal arrays (SOAs) by He and Tang (2013), Liu and Liu (2015), and He, Cheng and Tang (2018). SOAs can be used to construct designs that have better space-filling properties than those constructed using ordinary orthogonal arrays. In the process of constructing SOAs using regular  $2^{m-p}$  designs, He, Cheng and Tang (2018) found that all such SOAs can be constructed from SOS designs.

This paper examines applications of regular and nonregular SOS designs to the construction of SOAs by introducing the concept of minimal SOS designs. This concept is useful because, as shown later, all SOS designs can be generated from minimal ones. Furthermore, to produce SOAs that can accommodate more factors, one needs SOS designs with fewer factors. Section 2 reviews some material on SOAs of strength 2+ from He, Cheng and Tang (2018), including how SOS designs can be used to construct SOAs. Section 3 first presents a characterizing result for regular minimal SOS designs using clear effects, and then shows that the four constructions in He, Cheng and Tang (2018) all produce minimal SOS designs. This section imports several results from projective geometry and coding theory, using the equivalence of regular SOS designs to 1-saturating sets and duals of linear codes with covering radius 2. These results allow us to improve the bounds on the maximum number of factors in an SOA of strength 2+ obtained in He, Cheng and Tang (2018). In Section 4, we discuss nonregular SOS designs. We first present extensions of the four constructions of regular SOS designs in He, Cheng and Tang (2018) to nonregular designs, showing that they all give minimal SOS designs. We then show how to use these nonregular minimal SOS designs to construct SOAs of strength 2+. In addition to more flexible run sizes, SOAs constructed from nonregular SOS designs have other advantages, including possibly better three- and higher-dimensional projections. Furthermore, nonregular SOS designs provide more options for constructing SOAs because there are often many more nonisomorphic nonregular designs than regular ones. Section 5 concludes the paper with a discussion.

## 2. Second Order Saturated Designs and Strong Orthogonal Arrays

A major focus of this study is two-level SOS designs. The following definition applies to both regular and nonregular designs.

**Definition 1.** A two-level fractional factorial design with  $n$  runs and  $m$  factors is second order saturated (SOS) if it can be used to estimate all of the  $m$  main effects, together with at least one set of  $n - 1 - m$  2fi's (assuming that all other effects are negligible).

Regular SOS designs were first considered by Block and Mee (2003). Under such a design, one can entertain a model with the largest number of 2fi's. Independently, Chen and Cheng (2004) defined the notion of estimation index. It is well known that each regular design is equivalent to a linear code; then the estimation index is the same as the covering radius of the dual code, and a design is SOS if and only if the estimation index is equal to 2.

Given a design of resolution IV, if one factor is added, the resulting design may have resolution III. A resolution IV design is called maximal if no factor can be added to maintain resolution IV. This concept is useful because all resolution IV designs can be obtained as projections of maximal resolution IV designs. It follows from a geometric result in Bruen, Haddad and Wehlau (1998) that two-level designs of resolution IV are maximal if and only if they have estimation index 2. Therefore, a resolution IV design is maximal if and only if it is SOS. An important byproduct of this result is that every two-level resolution IV design is a projection of a certain SOS design of resolution IV, a fact also observed by Block and Mee (2003). Thus, in addition to being able to entertain the largest number of 2fi's, another important practical value of SOS designs of resolution IV is that they can be used to generate all resolution IV designs of the same run size via projections. For example, there are three 32-run two-level SOS designs of resolution IV: a  $2^{16-11}$ , a  $2^{10-5}$ , and a  $2^{9-4}$ . All other 32-run resolution IV designs can be obtained by deleting factors from one of these three designs.

Unexpectedly and interestingly, SOS designs have a third application: they can be used to construct strong orthogonal arrays. We use  $OA(n, m, s_1 \times \cdots \times s_m, t)$  to denote an orthogonal array of strength  $t$  in  $n$  runs for  $m$  factors, with its  $j$ th factor having  $s_j$  levels,  $0, 1, \dots, s_j - 1$ . If  $s_1 = \cdots = s_m = s$ , the array is denoted as  $OA(n, m, s, t)$  for simplicity. Hedayat, Sloane and Stufken (1999) and Dey and Mukerjee (1999) are two good general references for orthogonal arrays.

An  $n \times m$  matrix with entries from  $\{0, 1, \dots, s^2 - 1\}$  is called an SOA of strength 2+ for  $n$  runs and  $m$  factors at  $s^2$  levels if any subarray of two columns

can be collapsed into an  $OA(n, 2, s^2 \times s, 2)$  and an  $OA(n, 2, s \times s^2, 2)$ . We denote this array by  $SOA(n, m, s^2, 2+)$ . Here, collapsing  $s^2$  levels to  $s$  levels takes place according to  $[a/s]$  for  $a = 0, 1, \dots, s^2 - 1$ , where  $[x]$  denotes the greatest integer not exceeding  $x$ . An  $s$ -level orthogonal array of strength two can be used to construct a Latin hypercube design that contains an equal number of points in each cell of  $s \times s$  grids in all two-dimensional projections. However, a Latin hypercube design constructed from an  $SOA(n, m, s^2, 2+)$  has the better space-filling property that it contains the same number of points in each cell of finer  $s \times s^2$  and  $s^2 \times s$  grids in all two-dimensional projections.

**Example 1.** Displayed below are an  $SOA(16, 10, 2^2, 2+)$  (left), and a Latin hypercube design constructed from it (right):

$$\left( \begin{array}{cccccccccc} 2 & 2 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 2 & 0 & 0 & 1 & 2 & 2 & 2 \\ 2 & 0 & 2 & 0 & 2 & 1 & 2 & 1 & 2 & 2 \\ 2 & 0 & 0 & 0 & 0 & 3 & 3 & 3 & 0 & 0 \\ 0 & 2 & 2 & 1 & 1 & 2 & 2 & 2 & 1 & 2 \\ 0 & 2 & 0 & 1 & 3 & 0 & 3 & 0 & 3 & 0 \\ 0 & 0 & 2 & 3 & 1 & 1 & 0 & 3 & 3 & 0 \\ 0 & 0 & 0 & 3 & 3 & 3 & 1 & 1 & 1 & 2 \\ 1 & 1 & 1 & 2 & 2 & 2 & 2 & 2 & 2 & 1 \\ 1 & 1 & 3 & 2 & 0 & 0 & 3 & 0 & 0 & 3 \\ 1 & 3 & 1 & 0 & 2 & 1 & 0 & 3 & 0 & 3 \\ 1 & 3 & 3 & 0 & 0 & 3 & 1 & 1 & 2 & 1 \\ 3 & 1 & 1 & 1 & 1 & 2 & 0 & 0 & 3 & 3 \\ 3 & 1 & 3 & 1 & 3 & 0 & 1 & 2 & 1 & 1 \\ 3 & 3 & 1 & 3 & 1 & 1 & 2 & 1 & 1 & 1 \\ 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \end{array} \right), \left( \begin{array}{ccccccccc} 8 & 9 & 10 & 11 & 8 & 10 & 0 & 2 & 3 & 3 \\ 10 & 10 & 1 & 10 & 1 & 3 & 7 & 8 & 9 & 10 \\ 9 & 3 & 11 & 3 & 11 & 7 & 10 & 6 & 11 & 9 \\ 11 & 0 & 0 & 1 & 3 & 12 & 14 & 15 & 2 & 2 \\ 2 & 8 & 8 & 5 & 4 & 11 & 8 & 10 & 6 & 11 \\ 0 & 11 & 2 & 6 & 13 & 2 & 15 & 0 & 15 & 0 \\ 1 & 2 & 9 & 12 & 5 & 4 & 2 & 14 & 12 & 1 \\ 3 & 1 & 3 & 15 & 15 & 14 & 6 & 7 & 7 & 8 \\ 7 & 7 & 4 & 8 & 10 & 9 & 11 & 9 & 10 & 7 \\ 5 & 5 & 14 & 9 & 0 & 0 & 12 & 3 & 1 & 12 \\ 6 & 15 & 6 & 2 & 9 & 5 & 1 & 12 & 0 & 13 \\ 4 & 13 & 13 & 0 & 2 & 15 & 4 & 4 & 8 & 4 \\ 13 & 4 & 5 & 7 & 7 & 8 & 3 & 1 & 13 & 14 \\ 12 & 6 & 15 & 4 & 14 & 1 & 5 & 11 & 5 & 6 \\ 14 & 12 & 7 & 13 & 6 & 6 & 9 & 5 & 4 & 5 \\ 15 & 14 & 12 & 14 & 12 & 13 & 13 & 13 & 14 & 15 \end{array} \right).$$

The SOA has the property that when the entries 0, 1, 2, and 3 in any column are replaced by 0, 0, 1, and 1 respectively, in the  $16 \times 2$  matrix formed by the resulting column and any other original column, all eight ordered pairs of  $\{0, 1\}$  and  $\{0, 1, 2, 3\}$  appear equally often as rows. The Latin hypercube design on the right is obtained from the SOA by replacing the four occurrences of  $i = 0, 1, 2, 3$ , with a permutation of  $4i, 4i + 1, 4i + 2$ , and  $4i + 3$ , respectively. If we divide all entries by 16, and consider each row as a point, then we obtain 16 points in the 10-dimensional unit cube  $[0, 1)^{10}$ . This design exhibits the uniformity

property that there are two points in each cell of  $4 \times 2$  and  $2 \times 4$  grids in all two-dimensional projections. For a design constructed from a two-level orthogonal array of strength two, only stratification in  $2 \times 2$  grids is guaranteed.

He, Cheng and Tang (2018) gave the following result, which provides a complete characterization of SOAs of strength  $2+$ , and also shows how they can be constructed from ordinary orthogonal arrays.

**Lemma 1.** *An SOA( $n, m, s^2, 2+$ ), say  $D$ , exists if and only if there exist two arrays  $A$  and  $B$ , where  $A = (a_1, \dots, a_m)$  is an OA( $n, m, s, 2$ ) and  $B = (b_1, \dots, b_m)$  is an OA( $n, m, s, 1$ ), such that  $(a_j, a_k, b_k)$  is an orthogonal array of strength three for any  $j \neq k$ . The three arrays are linked through  $D = sA + B$ .*

Theorem 1 of He, Cheng and Tang (2018) shows how Lemma 1 can be applied to two-level regular designs. As usual, we use  $C = (c_{ij})_{n \times m}$ , where  $c_{ij} = \pm 1$ , to represent a two-level factorial design of  $n$  runs for  $m$  factors. A regular saturated design  $S$  of  $2^k$  runs for  $2^k - 1$  factors can be obtained by first writing down a full factorial for  $k$  factors, and then adding all possible interaction columns. Then each regular  $2^{m-p}$  design  $C$  with  $p = m - k$  consists of  $m$  columns of  $S$ . The set of columns not in  $C$ , denoted by  $\overline{C} = S \setminus C$ , is called the complementary design of  $C$ . Being regular,  $S$  has the property that  $ab \in S$  for any  $a, b \in S, a \neq b$ , where  $ab$  is the interaction column of  $a$  and  $b$ . If  $C$  is SOS, then the  $2^k - 1$  degrees of freedom of  $S = C \cup \overline{C}$  correspond to the main effects and a set of  $2^k - 1 - m$  2fi's of the  $m$  factors in  $C$ . (Our use of the union symbol technically corresponds to a matrix augmentation; the above  $C \cup \overline{C}$  represents a matrix obtained by combining the column vectors of  $C$  with those of  $\overline{C}$ .) This gives a very simple description of  $C$ : each  $d \in \overline{C}$  can be expressed as  $d = ab$  for some  $a, b \in C$ . Let  $\overline{C}$  be  $(a_1, \dots, a_{m'})$ , where  $m' = 2^k - 1 - m$  and  $a_i = b_i c_i$ , with  $b_i, c_i \in C$ , for all  $i = 1, \dots, m'$ . As shown in the proof of Theorem 1 in He, Cheng and Tang (2018), this implies that  $(a_j, a_k, b_k)$  is an orthogonal array of strength three for any  $j \neq k$ . Thus, Lemma 1 is applicable. Following this lemma, we can construct an SOA( $n, m', 2^2, 2+$ ) by taking  $A = \overline{C} = (a_1, \dots, a_{m'})$  and  $B = (b_1, \dots, b_{m'})$ . Then  $D = A + B/2 + 3/2$  is a desired SOA( $n, m', 2^2, 2+$ ). Note that because, for two-level designs, the two levels in Lemma 1 are represented by 0 and 1, to apply Lemma 1, we first need to transform  $-1$  and  $1$  to 0 and 1, respectively. Thus, instead of  $D = 2A + B$  as stated in Lemma 1, we should use  $D = A + B/2 + 3/2$  here.

**Example 2.** Let  $(x_1, x_2, x_3, x_4)$  be a full  $2^4$  factorial in 16 runs. Then  $C = (x_1, x_2, x_3, x_4, x_1x_2x_3x_4)$  is an SOS design. Note that this design has the defin-

ing relation  $I = 12345$ . It has resolution V, with the five main effects and ten 2fi's distributed in the 15 alias sets, and hence is SOS. From the previous discussion, to construct an SOA using Lemma 1, we can let  $A = \overline{C} = (x_1x_2, x_1x_3, x_1x_4, x_2x_3, x_2x_4, x_3x_4, x_1x_2x_3, x_1x_2x_4, x_1x_3x_4, x_2x_3x_4)$ , and choose an appropriate  $B = (b_1, \dots, b_{10})$ . Denote the  $i$ th column of  $A$  by  $a_i$ ; then for all  $i = 1, \dots, 10$ , any  $b_i$  such that both  $b_i$  and  $a_ib_i$  are columns of  $C$  will do. One choice is  $B = (x_1, x_1, x_1, x_2, x_2, x_3, x_4, x_3, x_2, x_1)$ . Then  $D = A + B/2 + 3/2$  is the SOA(16, 10, 4, 2+) as shown in Example 1.

### 3. Minimal SOS Designs and Results on Regular Factorials

#### 3.1. SOS designs and their minimality

Let  $C$  be an SOS design. Obviously, adding a factor to  $C$  still gives an SOS design. When a factor is deleted from  $C$ , the resulting design can be SOS, but is not necessarily so. If the design obtained by deleting one factor from  $C$  is still SOS, then we can continue the process of deleting a factor from the current SOS design until no factor can be deleted while maintaining an SOS design. At the end, we must obtain an SOS design such that if any factor is removed, the resulting design is no longer SOS.

**Definition 2.** An SOS design is said to be minimal if the design resulting from deleting any factor is no longer SOS.

Let  $(x_1, x_2, x_3)$  be a full  $2^3$  factorial in eight runs. Then  $C = (x_1, x_2, x_3, x_1x_2x_3)$  is a minimal SOS design. The SOS design of 16 runs for five factors in Example 2 is also minimal.

The discussion prior to Definition 2 also explains why minimal SOS designs are useful, which we summarize in a lemma.

**Lemma 2.** *Any SOS design is either minimal or can be obtained by adding factors to a minimal SOS design.*

Lemma 2 states that all SOS designs can be constructed if all minimal SOS designs are available. Therefore, studies on SOS designs can be focused on minimal SOS designs. Furthermore, by Theorem 1 of He, Cheng and Tang (2018), using a regular SOS design of  $n$  runs for  $m$  factors, one can construct an  $n$ -run SOA of strength 2+ for  $n - 1 - m$  factors. In order to construct SOAs with more factors, we need SOS designs with fewer factors. Thus, SOS designs with fewer factors are of interest.

The next two subsections are devoted to regular minimal SOS designs. We examine nonregular SOS designs in Section 4.

### 3.2. Characterization and construction of regular minimal SOS designs

A main effect or 2fi is said to be clear if it is not aliased with any other main effect or 2fi. Under the reasonable assumption that interactions of order three or higher are negligible, a clear effect is estimable regardless of other effects. For a detailed discussion on clear effects, refer to Cheng (2014, Chap. 10). The next result provides a complete characterization of a regular SOS design being minimal through clear effects.

**Theorem 1.** *Let  $C = (c_1, \dots, c_m)$  be a regular SOS design, with  $c_j$  denoting its  $j$ th column. Then  $C$  is a minimal SOS design if and only if, for any  $i = 1, \dots, m$ , at least one of the following  $m$  effects is clear: the main effect  $c_i$  and all 2fi's  $c_i c_j$  with  $j \neq i$ .*

Theorem 1 is obvious, and so not really in need of a proof. It simply recognizes the fact that the design given by deleting column  $c_i$  from  $C$  remains SOS if and only if none of  $c_i$  and  $c_i c_j$ , with  $j \neq i$ , are clear. Theorem 1 may be mathematically simple, but it is a very useful result as will be seen throughout the paper.

#### Corollary 1.

- (i) *If an SOS design has resolution IV or higher, then it must be minimal.*
- (ii) *A minimal SOS design of resolution III must have at least one clear 2fi.*
- (iii) *For a minimal SOS design of  $n = 2^k$  runs and  $m$  factors, we must have that  $m \leq n/2$ .*

*Proof.* Part (i) of Corollary 1 is true because all main effects are clear in a resolution IV or higher design. Part (ii) follows because some main effects cannot be clear in a resolution III design, meaning that some 2fi's have to be clear, from Theorem 1. Parts (i) and (ii) state that a minimal SOS design is either of resolution IV or higher, or has some clear 2fi's, both of which imply that  $m \leq n/2$  (Cheng (2014, Corollary 9.6 and Thm. 10.7)). The first result follows from Rao's bound, and the second was originally obtained by Chen and Hedayat (1998). This proves Corollary 1(iii).

He, Cheng and Tang (2018) presented four constructions of regular SOS designs. Using Theorem 1, we show that these SOS designs are actually minimal. Again, let  $S$  be the saturated design based on  $k$  independent factors, which we

denote by  $a_1, \dots, a_{k_1}, b_1, \dots, b_{k_2}$ , where  $k_1 \geq 2$ ,  $k_2 \geq 2$ , and  $k_1 + k_2 = k$ . Consider two subsets  $P$  and  $Q$  of  $S$ , where  $P$  consists of  $a_1, \dots, a_{k_1}$  and their interaction columns, and  $Q$  consists of  $b_1, \dots, b_{k_2}$  and their interaction columns. All four constructions build SOS designs using  $P$  and  $Q$ .

Construction 1:  $C_1 = P \cup Q$ .

Construction 2:  $C_2 = (P \setminus \{a_1\}) \cup (Q \setminus \{b_1\}) \cup \{a_1 b_1\}$ .

Construction 3:  $C_3 = (P \setminus \{a_1\}) \cup (a_1 Q)$ .

Construction 4:  $C_4 = (b_1 P) \cup (a_1 Q \setminus \{a_1 b_1\})$ .

Construction 1 gives a design with  $n = 2^k$  runs and  $2^{k_1} + 2^{k_2} - 2$  factors. Constructions 2–4 all produce designs with the same run size, but with  $2^{k_1} + 2^{k_2} - 3$  factors, where  $k_1 \geq 2$ ,  $k_2 \geq 2$ , and  $k_1 + k_2 = k \geq 4$ .

**Theorem 2.** *Designs  $C_1, C_2, C_3$ , and  $C_4$  given by Constructions 1–4 are all minimal SOS designs.*

*Proof.* That  $C_1, C_2, C_3$ , and  $C_4$  are all SOS is established in He, Cheng and Tang (2018). Design  $C_4$  has resolution IV, and is thus minimal, by Corollary 1(i). For design  $C_1$ , it is obvious that the 2fi  $pq$  is clear for any  $p \in P$  and any  $q \in Q$ , implying that  $C_1$  is minimal, by Theorem 1. Design  $C_2$  is minimal because  $pq$ ,  $a_1 b_1 p$ , and  $a_1 b_1 q$  are all clear for any  $p \in P \setminus \{a_1\}$  and any  $q \in Q \setminus \{b_1\}$ . Design  $C_3$  is minimal because  $pq$  is clear for any  $p \in P \setminus \{a_1\}$  and any  $q \in a_1 Q$ .

By Corollary 1, all SOS designs of resolution IV are minimal. On the other hand, as noted in Section 2, maximal designs of resolution IV are SOS. Therefore, we have the following simple result.

**Corollary 2.** *All maximal resolution IV designs are minimal SOS designs.*

Chen and Cheng (2006) examined the structures and constructions of maximal designs with  $n/4 + 1$  or more factors. In contrast, the minimal SOS designs given by Constructions 1–4 all have fewer than  $n/4 + 1$  factors unless  $k_1 = 2$  or  $k_2 = 2$ . Finally, note that Constructions 1 and 4 were also given in Tang et al. (2002) in their studies of clear 2fi's.

### 3.3 Imports from projective geometry and coding theory

It is well known that constructing a regular  $2^{m-p}$  design amounts to choosing  $m$  points, one point for each factor, from the  $2^{m-p} - 1$  points in an  $(m - p - 1)$ -dimensional projective geometry based on the Galois field  $GF(2) = \{0, 1\}$ . Each



line in this geometry contains three points. Then a 2fi can be identified with the third point on the line determined by the points corresponding to the two factors. A set  $A$  of points is called a 1-saturating set if every point in the complement of  $A$  is on the line determined by a certain pair of points in  $A$ . Thus, it is clear that regular SOS designs are equivalent to 1-saturating sets, and regular minimal SOS designs are equivalent to minimal 1-saturating sets. Regular SOS designs also have a coding theory connection, because the dual codes of linear codes with covering radius 2 are equivalent to 1-saturating sets. In this subsection, we import some results from projective geometry and coding theory.

Davydov, Marcugini and Pambianco (2006) presented several construction methods for minimal 1-saturating sets. Their Constructions  $A$  and  $B$  are equivalent to our Constructions 1 and 2, respectively, in Section 3.2. In design language, we present one of their other methods because it gives SOS designs with fewer factors than our Constructions 1–4 do. As commented in the paragraph following Lemma 2, SOS designs with fewer factors are of interest because they result in SOAs with more factors.

Recall that our Construction 1 gives a minimal SOS design with  $2^{k_1} + 2^{k_2} - 2$  factors, and Constructions 2–4 produce minimal SOS designs with  $2^{k_1} + 2^{k_2} - 3$  factors, where  $k_1 \geq 2$ ,  $k_2 \geq 2$ , and  $k_1 + k_2 = k \geq 4$ . However, if  $k \geq 7$ , a minimal SOS design with  $2^{k_1} + 2^{k_2} - 4$  factors can be constructed for  $k_1 \geq 3$ ,  $k_2 \geq 4$ , and  $k_1 + k_2 = k$ . This is Construction  $C$  of Davydov, Marcugini and Pambianco (2006), which is presented below.

Let  $S$ ,  $P$ , and  $Q$  be defined as in Section 3.2. Let  $p_1p_2p_3 = q_1q_2q_3 = I$  be two defining words of length three, where  $p_1, p_2, p_3 \in P$ ,  $q_1, q_2, q_3 \in Q$ , and  $I$  is the all-ones column. Take any  $q_4 \in Q \setminus \{q_1, q_2, q_3\}$ . Consider

$$C_5 = (P \setminus \{p_1, p_2, p_3\}) \cup (Q \setminus \{q_1, q_2, q_3, q_4\}) \cup \{p_1q_3, p_2q_3, p_3q_1, p_3q_2, p_3q_4\}.$$

**Lemma 3.** (*Davydov, Marcugini and Pambianco (2006)*) *Design  $C_5$  is a minimal SOS design of  $n = 2^k$  runs with  $2^{k_1} + 2^{k_2} - 4$  factors, where  $k_1 \geq 3$ ,  $k_2 \geq 4$ , and  $k = k_1 + k_2 \geq 7$ .*

However, for  $k \geq 7$ , SOS designs with even fewer factors can be constructed, as given in Theorems 1 and 2 of Gabidulin, Davydov and Tombak (1991) in terms of duals of linear codes with covering radius 2. We summarize their results in a lemma.

**Lemma 4.** (*Gabidulin, Davydov and Tombak (1991)*) *For  $k \geq 7$ , an SOS design of  $n = 2^k$  runs for  $m$  factors can be constructed, where*

$$m = \begin{cases} 5 \times 2^{w-2} - 1 & \text{if } k = 2w - 1, \\ 7 \times 2^{w-2} - 2 & \text{if } k = 2w. \end{cases}$$

To the best of our knowledge, whether or not the SOS designs given in Lemma 4 are minimal has not been established in the literature on coding theory and projective geometry. Here, we provide an affirmative answer to the question.

**Proposition 1.** *The SOS designs in Lemma 4 are minimal.*

The proof is rather lengthy and, thus, is given in the Appendix.

**Example 3.** For  $k = 7$ , and thus  $w = 4$ , the construction in Lemma 4 gives an SOS design with  $n = 2^k = 128$  runs for  $m = 5 \times 2^{w-2} - 1 = 19$  factors. The design matrix is given by taking all linear combinations of the rows of

$$B = \begin{bmatrix} 000 & 1111 & 1111 & 1111 & 1111 \\ 011 & 0011 & 0011 & 0011 & 0000 \\ 101 & 0101 & 0101 & 0101 & 0000 \\ 000 & 0011 & 0101 & 0110 & 0011 \\ 000 & 0110 & 0011 & 0101 & 0101 \\ 000 & 0000 & 0000 & 1111 & 1111 \\ 000 & 0000 & 1111 & 0000 & 1111 \end{bmatrix},$$

with all calculations within  $GF(2) = \{0, 1\}$ . The resulting design can be converted to a version with familiar levels  $\pm 1$  by changing 0 to  $-1$ . According to Proposition 1, this SOS design is minimal. It is of resolution III, having one word of length three, which is given by the first three columns. In comparison, for  $k = 7$  and  $n = 128$ , Construction 1 gives a minimal SOS design with 22 factors, Constructions 2–4 generate minimal SOS designs with 21 factors, and Lemma 3 gives a minimal SOS design with 20 factors. For  $k = 8$ , the construction in Lemma 4 gives an SOS design with 256 runs for 26 factors, which is also minimal, by Proposition 1.

Let  $m_k$  be the largest  $m$  for which an  $SOA(2^k, m, 4, 2+)$  based on regular designs can exist. Using Constructions 2–4, He, Cheng and Tang (2018) obtained a general lower bound on  $m_k$ . Lemma 4 offers an improvement for  $k \geq 7$ .

**Proposition 2.** *We have that, for  $k \geq 7$ ,*

$$m_k \geq \begin{cases} 2^k - 5 \times 2^{w-2} & \text{if } k = 2w - 1, \\ 2^k - 7 \times 2^{w-2} + 1 & \text{if } k = 2w. \end{cases}$$

Table 1. Classification of all regular minimal SOS designs for  $n \leq 64$  and  $n = 128$  with  $m \leq 20$ .

$n$	$m$	III	IV	total
8	4	1	1	2
16	5	0	1	1
16	6	1	0	1
16	8	1	1	2
32	9	1	1	2
32	10	6	1	7
32	11	1	0	1
32	16	1	1	2
64	13	7	1	8
64	14	19	0	19
64	15	14	0	14
64	16	16	0	16
64	17	48	5	53
64	18	108	1	109
64	20	1	1	2
64	32	1	1	2
128	19	5	0	5
128	20	36	0	36

Davydov, Marcugini and Pambianco (2006) provide a complete enumeration of all minimal 1-saturating sets in small geometries. Thus, their Table 1 classifies all regular minimal SOS designs for up to 64 runs and all regular minimal SOS designs with  $m \leq 20$  for 128 runs. We give a summary of their results in Table 1 for the benefit of design researchers.

For given  $n$  and  $m$ , the last column of Table 1 gives the number of all regular minimal SOS designs; the third and fourth columns give the numbers of minimal SOS designs of resolution III and IV, respectively. For example, with  $n = 64$  runs and  $m = 13$  factors, there are exactly seven minimal SOS designs of resolution III, one minimal SOS design of resolution IV, and eight minimal SOS designs in total.

Using the search results in Table 2 of Davydov, Marcugini and Pambianco (2006), we obtain lower and upper bounds on  $m'_k$ , the size of the smallest regular minimal SOS design for  $7 \leq k \leq 10$ . These bounds on  $m'_k$  are then used to obtain upper and lower bounds on  $m_k$ , the greatest  $m$  such that an SOA( $2^k, m, 4, 2+$ ) based on regular designs exists, because  $m'_k + m_k = 2^k - 1$ . Our Table 2 updates and expands Table 1 of He, Cheng and Tang (2018). For completeness, we include information on both  $m'_k$  and  $m_k$  in Table 2. For  $4 \leq k \leq 7$ , the  $m'_k$  and  $m_k$  values

Table 2. The smallest number  $m'_k$  of factors for a regular minimal SOS design, and the largest number  $m_k$  of factors for an SOA of strength 2+ based on regular designs.

$k$	$n = 2^k$	$m'_k$	$m_k$
4	16	5	10
5	32	9	22
6	64	13	50
7	128	19	108
8	256	[25, 26]	[229, 230]
9	512	[34, 39]	[472, 477]
10	1,024	[47, 51]	[972, 976]

are exact. For  $8 \leq k \leq 10$ , Table 2 gives the best known lower and upper bounds (e.g.,  $25 \leq m'_8 \leq 26$  and  $229 \leq m_8 \leq 230$ ).

## 4. Nonregular Minimal SOS Designs and Their Applications

### 4.1. Characterization and construction

Orthogonal arrays were introduced in Section 2. Throughout this subsection, the two levels in an  $OA(n, m, 2, t)$  are denoted by  $\pm 1$ , rather than 0 and 1. An  $OA(n, m, 2, 2)$  is said to be a nonregular design if it is not regular. For a review of nonregular designs, see Xu, Phoa and Wong (2009). Prior to Sun and Wu (1993), nonregular designs were referred to as irregular (e.g., Addelman (1961)). Hadamard matrices provide rich sources of nonregular designs, although not every nonregular design can be imbedded into a Hadamard matrix; see Sun, Li and Ye (2008) and Bulutoglu and Kaziska (2009) for details. A main effect or 2fi is called clear in a nonregular design if it is orthogonal to all other main effects and 2fi's (Tang (2006)).

Our general discussion on SOS designs and their minimality in Section 3.1 applies to nonregular and regular designs. Theorem 1 in Section 3 gives a complete characterization of a regular SOS design being minimal. A similar result holds for nonregular designs.

**Theorem 3.** *Let  $C = (c_1, \dots, c_m)$  be an SOS design, regular or nonregular. Then  $C$  is minimal if, for any  $i = 1, \dots, m$ , at least one of the  $m$  effects  $c_i$  and  $c_i c_j$  with  $j \neq i$  is clear.*

Similarly to Theorem 1, Theorem 3 states that the condition of existence of certain clear effects is still sufficient for a nonregular SOS design to be minimal. Unlike Theorem 1, the necessity part cannot hold, in general, for nonregular

designs. To illustrate this, consider the following example. There are exactly two nonequivalent  $OA(12, 5, 2, 2)$ s (Sun, Li and Ye (2008)). Using a computer, we can easily check that one is SOS and the other is not. The one that is SOS must also be minimal because there are not enough degrees of freedom for an  $OA(12, 4, 2, 2)$  to be SOS. On the other hand, an  $OA(12, 5, 2, 2)$  cannot have a clear effect, because otherwise the run size would be a multiple of 8 (Tang (2006)). Proposition 1 of Tang (2006) relates to the existence of a clear 2fi; the same argument applies to a clear main effect.

**Corollary 3.** *If an  $OA(n, m, 2, 3)$  is SOS, then it must be minimal.*

This result follows from Theorem 3, because all main effects are clear in an orthogonal array of strength three. Cheng, Mee and Yee (2008) introduced some constructions of SOS  $OA(n, m, 2, 3)$ s, which are all minimal according to Corollary 3. These minimal SOS designs have relatively large numbers of factors; for example, their first construction gives  $m = n/4 + 1$ . When constructing SOAs, it is desirable to obtain minimal SOS designs with fewer factors, which we discuss next.

It turns out that the four constructions in Section 3 can all be adapted to the setting of nonregular designs. Let  $H_{n_1} = (1_{n_1}, a_1, \dots, a_{n_1-1})$  and  $H_{n_2} = (1_{n_2}, b_1, \dots, b_{n_2-1})$  be two Hadamard matrices of orders  $n_1 \geq 4$  and  $n_2 \geq 4$ , respectively, where  $1_{n_1}$  is a column vector of  $n_1$  ones. Let  $p_i = a_i \otimes 1_{n_2}$  for  $i = 1, \dots, n_1 - 1$ , and  $q_j = 1_{n_1} \otimes b_j$  for  $j = 1, \dots, n_2 - 1$ . Furthermore, let  $P = \{p_1, \dots, p_{n_1-1}\}$  and  $Q = \{q_1, \dots, q_{n_2-1}\}$ . Consider the following constructions:

$$\text{Construction(i)} : C_1 = P \cup Q.$$

$$\text{Construction(ii)} : C_2 = (P \setminus \{p_1\}) \cup (Q \setminus \{q_1\}) \cup \{p_1 q_1\}.$$

$$\text{Construction(iii)} : C_3 = (P \setminus \{p_1\}) \cup (p_1 Q).$$

$$\text{Construction(iv)} : C_4 = (q_1 P) \cup (p_1 Q \setminus \{p_1 q_1\}).$$

All four designs have  $n_1 n_2$  runs. Design  $C_1$  has  $n_1 + n_2 - 2$  factors, and designs  $C_2, C_3$ , and  $C_4$  have  $n_1 + n_2 - 3$  factors.

**Theorem 4.** *Designs  $C_1, C_2, C_3$ , and  $C_4$ , given above, are minimal SOS designs.*

*Proof.* For brevity, we give proofs for Constructions (i) and (ii) only. The proofs for Constructions (iii) and (iv) use similar ideas, but are more tedious and complicated.

First, consider design  $C_1 = P \cup Q$  from Construction (i). The Hadamard matrix  $H_{n_1} \otimes H_{n_2}$  then consists of  $1_{n_1 n_2}$ , all main effect columns in  $P$ , all main effect columns in  $Q$ , and all interaction columns  $pq$ , where  $p \in P$  and  $q \in Q$ . Therefore the design  $C_1 = P \cup Q$  is SOS. Because any 2fi  $pq$  with  $p \in P$  and  $q \in Q$  is obviously clear, design  $C_1$  is minimal, by Theorem 3.

Now, consider design  $C_2$  from Construction (ii). We first decompose the set of  $n_1 n_2$  columns in the Hadamard matrix  $H_{n_1} \otimes H_{n_2}$  into a union of six disjoint subsets, as given by

$$H_{n_1} \otimes H_{n_2} = R_0 \cup R_1 \cup R_2 \cup R_3 \cup R_4 \cup R_5,$$

where  $R_0 = \{1_{n_1 n_2}\}$ ,  $R_1 = P$ ,  $R_2 = Q$ ,  $R_3 = p_1 Q$ ,  $R_4 = q_1 P \setminus \{p_1 q_1\}$ , and  $R_5 = \{p_i q_j \mid i = 2, \dots, n_1 - 1; j = 2, \dots, n_2 - 1\}$ . To prove that design  $C_2 = (P \setminus \{p_1\}) \cup (Q \setminus \{q_1\}) \cup \{p_1 q_1\}$  is SOS, we need to show that for each  $R_j$ , where  $j = 1, \dots, 5$ , we can choose a set of linearly independent main effects or 2fi's from design  $C_2$  such that they span the same linear subspace as that spanned by the columns of  $R_j$ . Because every column in  $R_5$  is a 2fi of design  $C_2$ , the job is done for  $R_5$ . Now, consider  $R_1 = P$ . If we can find a 2fi  $p_i p_j$  of design  $C_2$ , where  $2 \leq i < j \leq n_1 - 1$ , such that it is not orthogonal to  $p_1$ , then the main effects  $p_2, \dots, p_{n_1-1}$  of  $C_2$  plus this 2fi  $p_i p_j$  are linearly independent and, thus, span the linear subspace spanned by  $R_1 = P$ . Such a 2fi must exist; otherwise  $p_2, \dots, p_{n_1-1}, p_1 p_2, \dots, p_1 p_{n_1-1}$  are mutually orthogonal within the linear subspace spanned by  $P$ , which is a contradiction. The same argument works for  $R_2 = Q$ . We now turn our attention to  $R_3 = p_1 Q$ . Because the column vectors  $p_1 q_1, p_1 q_1 q_2, \dots, p_1 q_1 q_{n_2-1}$  are mutually orthogonal and all belong to  $L(R_3)$ , the linear subspace spanned by the columns of  $R_3 = p_1 Q$ , they therefore span  $L(R_3)$ . However,  $p_1 q_1$  is a main effect of design  $C_2$ , and  $p_1 q_1 q_j$  for  $j \geq 2$  is a 2fi between factor  $p_1 q_1$  and factor  $q_j$  of design  $C_2$ . This takes care of  $R_3$ . The same argument with a minor modification also works for  $R_4$ . We have thus proved that design  $C_2$  is SOS. That  $C_2$  is minimal follows from the fact that the 2fi of factor  $p_i$  and factor  $q_j$  is clear, for all  $i \geq 2$  and  $j \geq 2$ , and that the main effect  $p_1 q_1$  is also clear.

In the next subsection, we examine how to use the designs given by Constructions (i)–(iv) to construct SOAs of strength  $2+$ .

Small orthogonal arrays have been completely enumerated by Sun, Li and Ye (2008) and Schoen, Eendebak and Nguyen (2010). Using these results, we conduct a complete search of  $OA(n, m, 2, t)$ s that are minimal SOS designs for

Table 3. Classification of all  $OA(n, m, 2, t)$ s that are minimal SOS designs for  $t = 2$  with  $n = 12, 16$ , and  $20$ , and for  $t = 3$  with  $n = 16, 24, 32$ , and  $40$ , where  $N_{\text{all}}$ ,  $N_{\text{SOS}}$ , and  $N_{\text{minsos}}$  denote the number of all nonisomorphic designs, number of SOS designs, and number of minimal SOS designs, respectively.

$t$	$(n, m)$	$N_{\text{all}}$	$N_{\text{SOS}}$	$N_{\text{minsos}}$
2	(12, 5)	2	1	1
2	(16, 5)	11	3	3
2	(16, 6)	27	14	2
2	(16, 8)	80	80	2
2	(20, 6)	75	15	15
2	(20, 7)	474	339	22
2	(20, 9)	2,477	2,466	1
3	(16, 5)	2	1	1
3	(16, 8)	1	1	1
3	(24, 12)	1	1	1
3	(32, 9)	34	6	6
3	(32, 10)	32	1	1
3	(32, 16)	5	5	5
3	(40, 20)	3	3	3

$t = 2$  with  $n = 12, 16$ , and  $20$ , and for  $t = 3$  with  $n = 16, 24, 32$ , and  $40$ . Table 3 presents a summary of all minimal SOS designs for these parameters. For a given strength  $t$  and pair  $(n, m)$ , the last column of Table 3 gives the number  $N_{\text{minsos}}$  of  $OA(n, m, 2, t)$ s that are minimal SOS designs. For comparison, we also include in Table 3 the number  $N_{\text{all}}$  of all nonisomorphic designs and the number  $N_{\text{SOS}}$  of all SOS designs. For example, there are 474 nonisomorphic  $OA(20, 7, 2, 2)$ s, of which 339 arrays are SOS. Among the 339 SOS designs, 22 are minimal. Furthermore, Table 3 shows that there exist exactly three  $OA(16, 5, 2, 2)$ s that are minimal SOS designs. Comparing these results with those shown in Table 1, we conclude that one of these minimal SOS designs is regular, and the other two are nonregular.

#### 4.2. Applications to strong orthogonal arrays

In this subsection, we consider the problem of constructing  $SOA(n, m, 4, 2+)$ s. According to Lemma 1, we first need to find two arrays  $A$  and  $B$ , where  $A = (a_1, \dots, a_m)$  is an  $OA(n, m, 2, 2)$  and  $B = (b_1, \dots, b_m)$  is an  $OA(n, m, 2, 1)$ , such that  $(a_j, a_k, b_k)$  has strength three for any  $j \neq k$ . Then, as noted in the paragraph following Lemma 1, we obtain an  $SOA(n, m, 4, 2+)$  using  $D = A + B/2 + 3/2$ .

He, Cheng and Tang (2018) examined how to obtain  $A$  and  $B$  if their columns are selected from a saturated regular design. We now consider obtaining  $A$  and

$B$  by choosing their columns from a saturated orthogonal array, which can be nonregular.

**Theorem 5.** *Let  $S$  be an  $OA(n, n-1, 2, 2)$ . To construct an  $SOA(n, m, 4, 2+)$  using  $D = A + B/2 + 3/2$  with the columns of  $A$  and  $B$  selected from  $S$ , it is necessary and sufficient that, for any column  $a \in A$ , there exists a column  $b \in S \setminus A$  such that  $ab$  is orthogonal to all columns in  $A$ .*

Theorem 5 extends Theorem 1 of He, Cheng and Tang (2018), and includes the latter as a special case, because one can easily see that the condition for array  $A$  in Theorem 5 is equivalent to  $S \setminus A$  being SOS if  $S$  is a regular saturated design. We omit the proof for Theorem 5 because it is very similar to that for Theorem 1 of He, Cheng and Tang (2018).

Theorem 5 is actually constructive. Suppose that  $A = (a_1, \dots, a_m)$  satisfies the required condition in Theorem 5, meaning that, for any  $a_i$ , there exists a column in  $S \setminus A$ , say  $b_i$ , such that  $a_i b_i$  is orthogonal to all  $a_j$ . Then we simply take  $B = (b_1, \dots, b_m)$ .

**Remark 1.** When  $S$  is a nonregular saturated design, the condition for array  $A$  in Theorem 5 may not be equivalent to  $S \setminus A$  being SOS. Further discussion on this issue will be given in Section 5. It is therefore not true that every nonregular SOS design can be used to construct an  $SOA(n, m, 4, 2+)$ . On the other hand, as shown below, almost all SOS designs given by Constructions (i)–(iv) allow the construction of SOAs.

All minimal SOS designs obtained by Constructions (i)–(iii) can be used to construct  $SOA(n, m, 4, 2+)$ s. The minimal SOS designs obtained by Construction (iv) can also be used, provided that one of  $H_{n_1}$  and  $H_{n_2}$  is regular. Details are given as follows. Note that  $S = H_{n_1} \otimes H_{n_2} \setminus \{1_{n_1 n_2}\}$ .

Construction (i). Let  $A_1 = S \setminus C_1$ . All columns in  $A_1$  have the form  $pq$ , where  $p \in P$  and  $q \in Q$ . For any  $a = pq \in A_1$ , we take  $b = p$ .

Construction (ii). Let  $A_2 = S \setminus C_2$ . For  $a = p_i q_j \in A_2$ , where  $i, j \geq 2$ , we take  $b = p_i$ . For  $a = p_1$ , take  $b = p_2$ . For  $a = q_1$ , take  $b = q_2$ . For  $a = p_1 q_j$ , where  $j \geq 2$ , take  $b = p_1 q_1$ . For  $a = q_1 p_i$ , where  $i \geq 2$ , take  $b = p_1 q_1$ .

Construction (iii). Let  $A_3 = S \setminus C_3$ . For  $a = p_i q_j$ , where  $i \geq 2, j \geq 1$ , we take  $b = p_1 q_j$ . For  $a = p_1$ , take  $b = p_2$ . For  $a = q_j$ , where  $j \geq 1$ , take  $b = p_1 q_{j'}$ , where  $j' \neq j$ .



Construction (iv). Assume  $H_{n_1}$  is regular. Let  $A_4 = S \setminus C_4$ . For  $a = p_i$ , take  $b = p_{i'}q_1$ , where  $i' \neq i$ . For  $a = q_j$ , take  $b = p_1q_{j'}$ , where  $j' \neq j$ . For  $a = p_iq_j$ , where  $i \geq 2$  and  $j \geq 2$ , take  $b = p_{i'}q_1$ , where  $p_{i'} = p_1p_i$ , which is possible because  $H_{n_1}$  is regular.

We can verify routinely that  $A_1, A_2, A_3$ , and  $A_4$  satisfy the condition in Theorem 5. The above also shows how to obtain the corresponding  $B_1, B_2, B_3$ , and  $B_4$ . Using  $D = A + B/2 + 3/2$ , we can then obtain  $D_1, D_2, D_3$ , and  $D_4$ . We summarize these developments in the following theorem.

**Theorem 6.** *Design  $D_1$  is an  $SOA(n_1n_2, m, 4, 2+)$  with  $m = n_1n_2 - n_1 - n_2 + 1$ , and designs  $D_2, D_3$ , and  $D_4$  are all  $SOA(n_1n_2, m, 4, 2+)$ s with  $m = n_1n_2 - n_1 - n_2 + 2$ .*

**Example 4.** Take  $n_1 = 4$  and  $n_2 = 12$ . Then  $D_1$  is an  $SOA(48, 33, 4, 2+)$ , and  $D_2, D_3$ , and  $D_4$  are  $SOA(48, 34, 4, 2+)$ s. If we take  $n_1 = n_2 = 12$ , then  $D_1$  is an  $SOA(144, 121, 4, 2+)$ , and  $D_2$  and  $D_3$  are both  $SOA(144, 122, 4, 2+)$ s. Such run sizes cannot be attained using regular SOS designs. Note that  $D_4$  is not available for  $n_1 = n_2 = 12$  because  $H_{n_1}$  and  $H_{n_2}$  are both nonregular.

SOAs constructed from regular and nonregular designs differ in terms of their three-dimensional space-filling properties. The distribution of the design points in the eight cells when projected onto three dimensions and viewed on a  $2 \times 2 \times 2$  grid is determined by the three corresponding columns of the array  $A$  in Lemma 1. This array of three columns has only two possible structures for regular  $A$ , but a lot more for nonregular  $A$ .

**Example 5.** Hall (1961) identified five nonisomorphic Hadamard matrices of order 16, denoted by  $H_I, H_{II}, H_{III}, H_{IV}$ , and  $H_V$ , respectively, where only  $H_I$  is regular. Denote a submatrix consisting of the  $j_1, j_2, \dots, j_m$ th columns of  $H_i$  by  $H_i(j_1, j_2, \dots, j_m)$ , where  $i = I, II, III, IV, V$ . Then it can be verified that  $C_1 = H_I(7, 11, 12, 13, 14, 15)$ ,  $C_2 = H_I(6, 7, 9, 11, 13, 14)$ , and  $C_3 = H_{II}(1, 2, 3, 7, 11, 15)$  are all SOS. Furthermore, their complementary designs  $A_1 = H_I(1, 2, 3, 4, 5, 6, 8, 9, 10)$ ,  $A_2 = H_I(1, 2, 3, 4, 5, 8, 10, 12, 15)$ , and  $A_3 = H_{II}(4, 5, 6, 8, 9, 10, 12, 13, 14)$  all satisfy the condition of Theorem 5. One can construct  $SOA(16, 9, 4, 2+)$ s  $D_i = A_i + B_i/2 + 3/2$ , for  $i = 1, 2, 3$ , by choosing  $B_1 = H_I(12, 12, 12, 11, 11, 11, 7, 7, 7)$ ,  $B_2 = H_I(6, 9, 13, 9, 11, 6, 7, 7, 6)$ , and  $B_3 = H_{II}(3, 2, 1, 3, 2, 1, 3, 2, 1)$ . Because  $A_1$  has seven defining words of length three, for  $D_1$ , there are seven three-dimensional projections in which there are points in only four of the eight cells in a  $2 \times 2 \times 2$  grid. For  $D_2$ , there are six such three-dimensional projections. Because of the

nonregular structure of  $A_3$ , for all three-dimensional projections of  $D_3$ , there is at least one point in each cell. The numbers of four-dimensional projections in which only eight of the sixteen cells in a  $2 \times 2 \times 2 \times 2$  grid are occupied are 51, 45, and 9 for  $D_1, D_2$ , and  $D_3$ , respectively. This comparison shows that  $D_3$ , which is constructed from a nonregular SOS design, has better coverage than  $D_1$  and  $D_2$ , which are constructed from regular SOS designs.

## 5. Discussion

This study conducts a comprehensive investigation of SOS designs and their minimality, focusing on their usefulness in constructing strong orthogonal arrays. In both regular and nonregular cases, we establish characterizing results for SOS designs to be minimal, and provide some construction results for minimal SOS designs. In the case of regular designs, results from projective geometry and coding theory allow us to construct SOAs of strength  $2+$  with more factors (see Proposition 2 and Table 2) than those in He, Cheng and Tang (2018). The nonregular counterparts of the four constructions in He, Cheng and Tang (2018) allow us to construct four families of SOAs of strength  $2+$ .

In the case of regular designs, Grynkiewicz and Lev (2010) studied the structures and sizes of large 1-saturating sets. Although we are more concerned with SOS designs with small numbers of factors, one of their results is relevant here. They show that while the largest minimal SOS design has  $m = n/2$ , the second largest minimal SOS design must have  $m = 5n/16$ , provided that  $n$  is sufficiently large. From Table 1, we see that this is already true for  $n = 64$ . The results in Table 2 of Davydov, Marcugini and Pambianco (2006) confirm the statement.

An important unresolved problem is whether the constructions in Lemmas 3 and 4 can be adapted to nonregular designs. Because the construction for the design in Lemma 4 relies heavily on the regular structure, it does not seem possible to generalize this to nonregular settings. However, in Lemma 3, as long as both  $H_{n_1}$  and  $H_{n_2}$  contain a defining word of length three, there is a nonregular counterpart for the construction. The questions then are whether the resulting design is minimal SOS, and whether it can be used to construct an SOA of strength  $2+$ . We leave these questions to future research.

The construction of SOAs in Theorems 5 and 6 raises an intriguing question, which is at least of technical interest: what is the relationship between the condition in Theorem 5 and the property of being SOS? We know that they are equivalent in the case of regular designs. In the nonregular case, the following

result sheds some light on the issue.

**Lemma 5.** *Let  $C$ , an  $OA(n, m, 2, 2)$ , be an orthogonal SOS design, meaning that there exists a set  $A$  of  $n - 1 - m$  mutually orthogonal 2fi's that are also orthogonal to the main effects. Then array  $A$  satisfies the condition in Theorem 5.*

The proof is straightforward by taking  $S = A \cup C$ , which is an  $OA(n, n - 1, 2, 2)$ . Lemma 5 seems to suggest that the condition in Theorem 5 is stronger than being SOS. A proof or a counterexample is worth seeking.

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## Appendix

### A. Proof of Proposition 1

The constructions were given in Theorems 1 and 2 of Gabidulin, Davydov and Tombak (1991). Our notation in this appendix is different from the main body of our paper. Instead, we use the notation in Gabidulin, Davydov and Tombak (1991). This is just to make presentation easier. Let  $e_0 = 0, e_1, \dots, e_B$  be the elements of  $GF(2^b)$ , where  $B = 2^b - 1$ . Further let  $(e_i)^b$  denote the column vector that is the binary  $b$ -bit representation of  $e_i$ . Define two matrices  $E^b$  and  $F^{2b}(e_j)$  as follows

$$E^b = \begin{bmatrix} (e_0)^b & (e_1)^b & \cdots & (e_B)^b \end{bmatrix},$$

$$F^{2b}(e_j) = \begin{bmatrix} (e_0)^b & (e_1)^b & \cdots & (e_B)^b \\ (e_0)^b & (e_1^{-1}e_j)^b & \cdots & (e_B^{-1}e_j)^b \end{bmatrix}.$$

Let  $E_0^b$  be  $E^b$  with the first column deleted. We use  $P^b(e_i)$  to denote a matrix with the same column  $(e_i)^b$  repeated where the number of repetitions is determined by context.

**Lemma A.** *(Gabidulin, Davydov and Tombak (1991, Thm. 1)) Let the parity*

check matrix of a code be

$$B^{2m-1} = [N \ D \ Q \ M \ G],$$

where  $2m - 1 = r \geq 7$  and matrices  $N, D, Q, M$  and  $G$  are, respectively, given by

$$\begin{bmatrix} 0 \ \cdots \ 0 \\ E_0^{m-2} \\ P^m(e_0) \end{bmatrix}, \begin{bmatrix} 1 \ \cdots \ 1 \\ F^{2(m-2)}(w_1) \\ 0 \ \cdots \ 0 \\ 0 \ \cdots \ 0 \end{bmatrix}, \begin{bmatrix} 1 \ \cdots \ 1 \\ F^{2(m-2)}(w_2) \\ 0 \ \cdots \ 0 \\ 1 \ \cdots \ 1 \end{bmatrix}, \begin{bmatrix} 1 \ \cdots \ 1 \\ F^{2(m-2)}(w_3) \\ 1 \ \cdots \ 1 \\ 0 \ \cdots \ 0 \end{bmatrix}, \begin{bmatrix} 1 \ \cdots \ 1 \\ P^{m-2}(e_0) \\ E^{m-2} \\ 1 \ \cdots \ 1 \\ 1 \ \cdots \ 1 \end{bmatrix},$$

where  $w_1, w_2, w_3 \in GF(2^{m-2})$ ;  $w_1, w_2 \neq 0$ ,  $w_1 \neq w_2$ ,  $w_1 + w_2 = w_3$ . Then this code has covering radius  $R = 2$ .

Let  $C$  be the design generated by taking linear combinations of the rows of  $B^{2m-1}$  with coefficients from  $GF(2) = \{0, 1\}$ . According to Lemma A, design  $C$  is SOS as the code has covering radius  $R = 2$ .

**Proposition 1a.** *The array  $C$ , generated by  $B^{2m-1}$ , is a minimal SOS design.*

*Proof.* We already know that  $C$  is SOS. To show its minimality, we use our Theorem 1 in Section 3. As design  $C$  has entries from  $GF(2) = \{0, 1\}$ , a main effect column  $c_i$  is clear if  $c_i \neq c_j$  and  $c_i \neq c_j + c_k$  for any other columns  $c_j$  and  $c_k$ , and a 2fi  $c_i c_j$  is clear if  $c_i + c_j \neq c_k$  and  $c_i + c_j \neq c_k + c_l$  for any other columns  $c_k$  and  $c_l$ . Equivalently, one can verify these properties for the columns of  $B^{2m-1}$ . We will prove that each column in  $[D, Q, M, G]$  is clear, and each column in  $N$  has a clear 2fi.

Suppose that a column  $\vec{d}$  in  $D$  is not clear. Then there must exist two other columns  $x$  and  $y$  in  $B^{2m-1}$  such that  $\vec{d} = x + y$ , where  $x \neq \vec{d}$  and  $y \neq \vec{d}$ . By examining the first row and last two rows of  $B^{2m-1}$ , we see that  $\vec{d} = x + y$  is possible only if  $x$  is a column in  $N$  and  $y$  a column in  $D$ . Suppose that neither  $\vec{d}$  nor  $y$  is the first column of  $D$ . Since  $\vec{d}$ ,  $x$  and  $y$  have form

$$\vec{d} = \begin{bmatrix} 1 \\ (e_i)^{m-2} \\ (e_i^{-1}w_1)^{m-2} \\ 0 \\ 0 \end{bmatrix}, \quad x = \begin{bmatrix} 0 \\ (e_j)^{m-2} \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ (e_k)^{m-2} \\ (e_k^{-1}w_1)^{m-2} \\ 0 \\ 0 \end{bmatrix},$$

it is impossible to have  $\vec{d} = x + y$  unless  $(e_i^{-1}w_1)^{m-2} = (e_k^{-1}w_1)^{m-2}$ . But  $(e_i^{-1}w_1)^{m-2} = (e_k^{-1}w_1)^{m-2}$  implies  $e_i = e_k$ , which leads to  $\vec{d} = y$ . This is a contradiction. It is also obvious that  $\vec{d} = x + y$  cannot hold if one of  $\vec{d}$  and  $y$  is the first column of  $D$ . Therefore,  $\vec{d}$  must be clear. Similarly, one can prove that any column in  $Q, M$  or  $G$  is also clear.

For any column  $\vec{n}$  of  $N$ , we will show that  $\vec{n} + \vec{d}$  is clear where  $\vec{d}$  is any except the first column of  $D$ . Since  $\vec{d}$  is clear, we only need to prove  $\vec{n} + \vec{d} \neq x + y$  for any other two columns  $x, y$  in  $B^{2m-1}$ . Again by examining the first row and the last two rows of  $B^{2m-1}$ , the only possible scenario for  $\vec{n} + \vec{d} = x + y$  is that  $x$  is a column of  $N$  and  $y$  a column of  $D$ . An argument very similar to that in the last paragraph shows that if  $\vec{n} + \vec{d} = x + y$ , then we must have  $\vec{n} = x$  and  $\vec{d} = y$ . This shows that  $\vec{n} + \vec{d}$  is clear, and thus each column in  $N$  has a clear 2fi. The proof is completed.

Let  $D_1$  and  $B_1^{2m-1}$  be the matrices of  $D$  and  $B^{2m-1}$  with their first column  $(1, 0, \dots, 0)^T$  deleted, respectively.

**Lemma B.** (*Gabidulin, Davydov and Tombak (1991, Thm. 2)*) *Let the parity check matrix of a code be*

$$T^{2m} = [Z \ Y],$$

where  $2m = r \geq 8$  and

$$Z = \begin{bmatrix} 0 & \dots & 0 \\ B_1^{2m-1} \end{bmatrix}, \quad Y = \begin{bmatrix} 1 & \dots & 1 \\ E^{m-1} \\ P^m(e_i) \end{bmatrix},$$

where  $i \in \{0, \dots, 2^m - 1\}$ . Then the code has covering radius  $R = 2$ .

Let  $N^*, D_1^*, Q^*, M^*$  and  $G^*$  denote the matrices of  $N, D_1, Q, M$  and  $G$  with an added head row  $(0, \dots, 0)$ . Partition  $Y$  into  $Y = [Y_1, Y_2]$  such that the second row of  $Y_1$  is the all-zeros row, and the second row of  $Y_2$  is the all-ones row. Then  $T^{2m}$  can be partitioned into seven submatrices as  $T^{2m} = [N^*, D_1^*, Q^*, M^*, G^*, Y_1, Y_2]$  with  $N^*, D_1^*, Q^*, M^*, G^*, Y_1, Y_2$  given, respectively,

by

$$\begin{bmatrix} 0 \cdots 0 \\ 0 \cdots 0 \\ E_0^{m-2} \\ P^m(e_0) \end{bmatrix}, \begin{bmatrix} 0 \cdots 0 \\ 1 \cdots 1 \\ F_0^{2(m-2)}(w_1) \\ 0 \cdots 0 \\ 0 \cdots 0 \end{bmatrix}, \begin{bmatrix} 0 \cdots 0 \\ 1 \cdots 1 \\ F^{2(m-2)}(w_2) \\ 0 \cdots 0 \\ 1 \cdots 1 \end{bmatrix}, \begin{bmatrix} 0 \cdots 0 \\ 1 \cdots 1 \\ F^{2(m-2)}(w_3) \\ 1 \cdots 1 \\ 0 \cdots 0 \end{bmatrix},$$

$$\begin{bmatrix} 0 \cdots 0 \\ 1 \cdots 1 \\ P^{m-2}(e_0) \\ E^{m-2} \\ 1 \cdots 1 \\ 1 \cdots 1 \end{bmatrix}, \begin{bmatrix} 1 \cdots 1 \\ 0 \cdots 0 \\ E^{m-2} \\ P^m(e_i) \end{bmatrix}, \begin{bmatrix} 1 \cdots 1 \\ 1 \cdots 1 \\ E^{m-2} \\ P^m(e_i) \end{bmatrix},$$

where  $F_0^{2(m-2)}(w_1)$  is obtained from  $F^{2(m-2)}(w_1)$  by deleting its first column which consists of all zeros.

**Proposition 1b.** *The array  $C'$ , generated by  $T^{2m}$ , is a minimal SOS design.*

*Proof.* We are going to prove that each column in  $[D_1^*, Q^*, M^*, G^*]$  is clear and each column in  $[N^*, Y_1, Y_2]$  has a clear 2fi.

Since any column of  $D$  is clear in  $B^{2m-1}$  (from the proof of Proposition 1a), we have that if a column  $\vec{d}$  in  $D_1^*$  has  $\vec{d} = x_1 + x_2$  for two other columns  $x_1, x_2$  from  $T^{2m}$ , then at least one of  $x_1$  and  $x_2$  must come from  $Y$ . Examining the first two rows of  $T^{2m}$ , we see that the only possible case is that  $x_1$  is from  $Y_1$  and  $x_2$  is from  $Y_2$ . Now if we take a look at the  $(m + 1)$ th to  $(2m - 2)$ th rows of  $D_1^*, Y_1$  and  $Y_2$ , we see that it is impossible for  $\vec{d} = x_1 + x_2$  to hold. This is because the  $(m + 1)$ th to  $(2m - 2)$ th entries of  $x_1 + x_2$  are all zeros whereas the corresponding entries of  $\vec{d}$  are those of  $(e_i^{-1}w_1)^{m-2}$ , which cannot be all zeros. We have thus established that any column  $\vec{d}$  in  $D_1^*$  is clear. According to the entries in the first and the last two rows of  $T^{2m}$ , one can prove that each column in  $[Q^*, M^*, G^*]$  is also clear.

In a manner almost identical to that of showing a column in  $D_1^*$  is clear as given above, we can show that the 2fi  $\vec{n} + \vec{d}$  is clear for any column  $\vec{n}$  from  $N^*$  and any column  $\vec{d}$  from  $D_1^*$ .

For any column  $\vec{y}$  from  $Y_1$  or  $Y_2$ , and any column  $\vec{d}$  from  $D_1^*$ , we can show that  $\vec{y} + \vec{d}$  is clear. The arguments are, though a bit more involved, also very similar to the above. We omit the details. This completes the proof.

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