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Construction of Optimal Multi-Level Supersaturated Designs

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Publication Date
2003

CONSTRUCTION OF OPTIMAL MULTI-LEVEL SUPERSATURATED DESIGNS

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A supersaturated design is a design whose run size is not large enough for estimating all the main effects. The goodness of multi-level supersaturated designs can be judged by the generalized minimum aberration criterion proposed by Xu and Wu (2001). Optimal supersaturated designs are shown to have a periodic property and general methods for constructing optimal multi-level supersaturated designs are proposed. Inspired by the Addelman-Kempthorne construction of orthogonal arrays, optimal multi-level supersaturated designs are given in an explicit form: columns are labeled with linear or quadratic polynomials and rows are points over a finite field. Additive characters are used to study the properties of resulting designs. Some small optimal supersaturated designs of 3, 4 and 5 levels are listed with their properties.

AMS 2000 subject classifications. Primary 62K15; secondary 62K05, 05B15.

Key words and phrases. Addelman-Kempthorne construction, additive character, generalized minimum aberration, minimum moment aberration, orthogonal array.

1 Introduction

As science and technology have advanced to a higher level, investigators are becoming more interested in and capable of studying large-scale systems. Typically these systems have many factors that can be varied during design and operation. The cost of probing and studying a large-scale system can be prohibitively expensive. Building prototypes are time-consuming and costly. Even the quicker route of using computer modeling can take up many hours of CPU time. To address the challenges posed by this technological trend, research in experimental design has lately focused on the class of supersaturated designs for its run size economy and mathematical novelty. Formally, a supersaturated design (SSD) is a design whose run size is not large enough for estimating all the main effects represented by the columns of the design matrix. The design and analysis rely on the assumption of the effect sparsity principle [Box and Meyer (1986), Wu and Hadama (2000, Section

[1]Supported by NSF Grant DMS-0204009.

[2]Supported by NSF Grant DMS-0072489 and NSA Grant MSPR-00G-091.

3.5)], that is, the number of relatively important effects in a factorial experiment is small. Some practical applications of SSDs can be found in Lin (1993, 1995), Wu (1993) and Nguyen (1996).

The construction of SSD dates back to Satterthwaite (1959) and Booth and Cox (1962). The former suggested the use of random balance designs and the latter proposed an algorithm to construct systematic SSDs. Many methods have been proposed for constructing two-level SSDs in the last decade, e.g., among others, Lin (1993, 1995), Wu (1993), Nguyen (1996), Cheng (1997), Li and Wu (1997), Tang and Wu (1997) and Butler, Mead, Eskridge and Gilmour (2001). There are, however, only a few results on multi-level SSDs. Yamada and Lin (1999) and Yamada, Ikebe, Hashiguchi and Niki (1999) considered the construction of three-level SSDs, and Fang, Lin and Ma (2000) considered the construction of mutli-level SSDs.

A popular criterion in the SSD literature is the $E(s^2)$ criterion [Booth and Cox (1962)], which measures the average correlation among columns. Extensions of $E(s^2)$ criterion to the multi-level case are not unique. One extension is an average χ^2 statistic [Yamada and Lin (1999)], which measures the goodness of a three-level SSD. Both $E(s^2)$ and the average χ^2 statistic are indeed special cases of the *generalized minimum aberration* (GMA) criterion [Xu and Wu (2001)]. The GMA criterion, an extension of the popular *minimum aberration* criterion [Fries and Hunter (1980)], assesses the goodness of general fractional factorial designs including SSDs as special cases. The GMA criterion also covers the minimum generalized aberration criterion [Ma and Fang (2001)] as a special case. For computational and other purposes, Xu (2001) proposed a novel combinatorial criterion, called *minimum moment aberration* criterion, and developed a unified theory for multi-level nonregular designs and SSDs.

This paper studies the construction of optimal multi-level SSDs. Section 2 reviews the optimality criteria such as GMA and minimum moment aberration criteria. Section 3 presents some general optimality results for multi-level SSDs. An improved lower bound is derived and optimal SSDs achieving this lower bound are discussed; optimal multi-level SSDs are shown to be periodic. Inspired by the Addelman-Kempthorne construction of orthogonal arrays, Section 4 describes explicit construction methods that produce optimal multi-level SSDs whose columns are labeled with linear or quadratic polynomials and rows are points over a finite field. Section 5 gives proofs that use additive characters of a finite field. Section 6 lists some small optimal SSDs of 3, 4, and 5 levels and compares them with existing ones.

2 Optimality criteria

Some definitions and notation are necessary in order to review the optimality criteria.

An (N, s^m)-design is an $N \times m$ matrix whose elements are from a set of s symbols $\{0, 1, \ldots, s-1\}$. Two designs are *isomorphic* if one can be obtained from the other through permutations of rows, columns and symbols in each column. A design is balanced if each level appears equally often in any column. An $OA(N, m, s, 2)$ is an *orthogonal array* (OA) of N runs, m columns, s levels and strength 2, in which all possible level combinations appear equally often for any pair of columns. An SSD of N runs, m columns and s levels is denoted as $SSD(N, s^m)$.

2.1 Generalized minimum aberration

For an (N, s^m)-design D, consider the following ANOVA model

$$Y = X_0\alpha_0 + X_1\alpha_1 + \cdots + X_m\alpha_m + \varepsilon,$$

where Y is the vector of N observations, α_j is the vector of all j-factor interactions, X_j is the matrix of orthonormal contrast coefficients for α_j, and ε is the vector of independent random errors. For $j = 0, 1, \ldots, m$, Xu and Wu (2001) defined $A_j(D)$, a function of X_j, to measure the aliasing between all j-factor interactions and the general mean. Specifically, if $X_j = [x_{ik}^{(j)}]$, let

$$A_j(D) = N^{-2} \sum_k \left| \sum_{i=1}^{N} x_{ik}^{(j)} \right|^2 .$$

The GMA criterion is to sequentially minimize the generalized wordlength patterns $A_1(D)$, $A_2(D)$, $A_3(D)$, ... Xu and Wu (2001) showed that isomorphic designs have the same generalized wordlength patterns and therefore are not distinguishable under the GMA criterion.

The generalized wordlength patterns have the property that $A_1(D) = 0$ if D is balanced and $A_2(D) = 0$ if D is an OA. For SSDs, $A_2(D) > 0$. The GMA criterion suggests that we shall minimize $A_2(D)$ among balanced designs. Note that $A_2(D)$ measures the overall aliasing between all pairs of columns. Let $R = (r_{ij})$ be the correlation matrix of all the main effects. Then $A_2(D) = \sum_{i<j} r_{ij}^2$. In particular, for a two-level design, $A_2(D)$ is equal to the sum of squares of correlation between all possible pairs of columns.

Let $c_1, \ldots, c_m$ be the columns of D. For each pair of columns c_i and c_j, we can define a *projected* A_2 value as $A_2(c_i, c_j) = A_2(d)$, where d consists of the two columns c_i and c_j. Obviously, the *overall* A_2 value is equal to the sum of the projected A_2 values, i.e., $A_2(D) = \sum_{1 \le i < j \le m} A_2(c_i, c_j)$.

2.2 Minimum moment aberration

For an (N, s^m)-design D and a positive integer t, define the tth power moment to be

$$K_t(D) = [N(N-1)/2]^{-1} \sum_{1 \le i < j \le N} [\delta_{ij}(D)]^t \,,$$

where $\delta_{ij}(D)$ is the number of coincidences between the ith and jth rows. The minimum moment aberration criterion proposed by Xu (2001) is to sequentially minimize the power moments $K_1(D), K_2(D), K_3(D), \ldots$. As the GMA criterion, the minimum moment aberration criterion does not distinguish isomorphic designs.

By applying some fundamental identities in algebraic coding theory, Xu (2001) showed that the power moments are linear combinations of the generalized wordlength patterns and that sequentially minimizing $K_1, K_2, K_3, \ldots$ is equivalent to sequentially minimizing $A_1, A_2, A_3, \ldots$. Therefore, minimum moment aberration is equivalent to GMA, and a design has GMA if and only if it has minimum moment aberration. The following lemma from Xu (2001) shows the connection between A_2 and K_2.

Lemma 1. *For a balanced (N, s^m)-design D,*

(i) $A_1(D) = 0$ and $A_2(D) = [(N-1)s^2 K_2(D) + m^2 s^2 - Nm(m+s-1)]/(2N)$;

(ii) $K_1(D) = m(N-s)/[(N-1)s]$ and $K_2(D) = [2NA_2(D) + Nm(m+s-1) - m^2 s^2]/[(N-1)s^2]$.

Since GMA and minimum moment aberration are equivalent, either criterion can be used as the optimality criterion for SSDs. In this paper we present results in A_2 rather than K_2 because the former is easier to interpret than the latter.

On the other hand, minimum moment aberration is more convenient for studying the overall property while GMA is more convenient for studying projection property. For a design of N runs and m columns, the complexity of computing K_2 is $O(N^2 m)$ while the complexity of computing A_2 is $O(Nm^2)$. Therefore, K_2 is much cheaper to compute than A_2 when m is much larger than N. However, when considering projections (e.g., $m = 2$), A_2 is cheaper to compute than K_2.

2.3 Connection with other optimality criteria

Let $c_1, \ldots, c_m$ be the columns of an (N, s^m)-design D. Define

$$\chi^2(c_i, c_j) = \sum_{a=0}^{s-1} \sum_{b=0}^{s-1} [n_{ab} - N/s^2]^2/(N/s^2),$$

where n_{ab} is the number of times that pair (a, b) appears as a row in columns c_i and c_j. Yamada and Lin (1999) proposed the following two criteria to evaluate the maximum and average dependency of columns:

$$\max \chi^2 = \max_{1 \le i < j \le m} \chi^2(c_i, c_j) \text{ and } \operatorname{ave} \chi^2 = \sum_{1 \le i < j \le m} \chi^2(c_i, c_j)/[m(m-1)/2].$$

Xu (2001) showed that $\operatorname{ave} \chi^2 = NA_2(D)/[m(m-1)/2]$. Therefore, the $\operatorname{ave} \chi^2$ is a special case of the GMA. Finally, for an $(N, 2^m)$-design D, the popular $E(s^2)$ criterion can be defined as $E(s^2) = N^2 A_2(D)/[m(m-1)/2]$.

3 Some optimality results

3.1 An improved lower bound

From the moment inequality $K_2(D) \ge K_1(D)^2$, Xu (2001) derived the following lower bound.

Lemma 2. *For a balanced (N, s^m)-design D, $A_2(D) \ge [m(s-1)(ms-m-N+1)]/[2(N-1)]$.*

Noting that the number of coincidences, $\delta_{ij}(D)$, is an integer, we can improve the moment inequality as $K_2(D) \ge K_1(D)^2 + \eta(1-\eta)$, where $\eta = K_1(D) - \lfloor K_1(D) \rfloor$ is the fraction part of $K_1(D)$ and $\lfloor x \rfloor$ is the largest integer that does not exceed x. Applying the equations in Lemma 1, we obtain an improved lower bound of A_2 as follows.

Theorem 1. *For a balanced (N, s^m)-design D,*

$$A_2(D) \ge [m(s-1)(ms-m-N+1)]/[2(N-1)] + (N-1)s^2\eta(1-\eta)/(2N),$$

where $\eta = m(N-s)/((N-1)s) - \lfloor m(N-s)/((N-1)s) \rfloor$.

The lower bound in Lemma 2 is achieved if and only if the number of coincidences, $\delta_{ij}(D)$, is a constant for all $i < j$. The lower bound in Theorem 1 is achieved if and only if the number of coincidences, $\delta_{ij}(D)$, differs by at most one for all $i < j$. The following lemma from Xu (2001) says that such a design is optimal under GMA.

Lemma 3. *If D is balanced and the difference among all $\delta_{ij}(D)$, $i < j$, does not exceed one, then D has minimum moment aberration and GMA.*

3.2 Optimal designs

Many optimal SSDs that achieve the lower bound in Theorem 1 can be derived from saturated OAs. An $OA(N, t, s, 2)$ is saturated if $N - 1 = t(s - 1)$. The following lemma from Mukerjee and Wu (1995) says that the number of coincidences between distinct rows is a constant for a saturated OA.

Lemma 4. *Suppose H is a saturated $OA(N, t, s, 2)$ with $t = (N - 1)/(s - 1)$. Then $\delta_{ij}(H) = (N - s)/[s(s - 1)]$ for any $i < j$.*

Tang and Wu (1997) first proposed to construct optimal two-level SSDs by juxtaposing saturated OAs derived from Hadamard matrices. This method can be extended to construct optimal multi-level SSDs. Suppose $D_1, \ldots, D_k$ are k saturated $OA(N, t, s, 2)$ with $t = (N - 1)/(s - 1)$. Let $D = D_1 \cup \cdots \cup D_k$ be the *column* juxtaposition, which may have duplicated or fully aliased columns. It is evident that $\delta_{ij}(D) = k(N - s)/[s(s - 1)]$ for any $i < j$. Then by Lemma 3, D is an optimal SSD under GMA.

As Tang and Wu (1997) suggested, to construct an SSD with $m = kt - j$ columns, $1 \leq j < t$, we may simply delete the last j columns from D. Though the resulting design may not be optimal, it has an A_2 value very close to the lower bound in Theorem 1.

If one column is removed from or one balanced column is added to D, the resulting design is still optimal. Cheng (1995) showed that for two-level SSDs, removing (and resp. adding) two orthogonal columns from (and resp. to) D also results in an optimal SSD. This is not true for multi-level SSDs in general. For $N = s^2$, we have a stronger result in Lemma 4 that the number of coincidences between any two rows is equal to 1. Then removing (and resp. adding) any number of orthogonal columns from (and resp. to) D also results in an optimal SSD under GMA since the resulting design has the property that the number of coincidences between any two rows differs by at most one. In particular, for any m, the lower bound in Theorem 1 is tight.

Lin (1993) used half fractions of Hadamard matrices to construct two-level SSDs by taking a column as the branching column. This method can be extended to construct multi-level SSDs as follows. Taking any column of saturated $OA(N, t, s, 2)$ as the branching column, we obtain s fractions according to the levels of the branching column. All fractions are balanced after removing the branching column and the number of coincidences between any two rows is a constant. The *row* juxtaposition of any k fractions form an $SSD(kNs^{-1}, s^{t-1})$ of which the number of coincidences between any two rows differs by at most one. By Lemma 3, such a design is optimal under GMA. For $N = s^2$, any subdesign is also optimal since the number of coincidences between any two rows is either 0 or 1.

Since a saturated $OA(s^n, (s^n-1)/(s-1), s, 2)$ exists for any prime power s, we have the following result.

Theorem 2. *Suppose s is a prime power.*

(i) For any n and k, there exists an optimal $SSD(s^n, s^m)$ that achieves the lower bound in Theorem 1, where $m = k(s^n - 1)/(s - 1)$ or $m = k(s^n - 1)/(s - 1) \pm 1$.

(ii) For any n and $k < s$, there exists an optimal $SSD(ks^{n-1}, s^m)$ that achieves the lower bound in Theorem 1, where $m = (s^n - 1)/(s - 1) - 1$.

(iii) For any m, there exists an optimal $SSD(s^2, s^m)$ that achieves the lower bound in Theorem 1.

(iv) For any $m \leq s$ and $k < s$, there exists an optimal $SSD(ks, s^m)$ that achieves the lower bound in Theorem 1.

The above optimal SSDs may contain fully aliased columns. We will study construction methods that produce optimal SSDs without fully aliased columns in the next section.

3.3 Periodicity of optimal supersaturated designs

We show here that A_2-optimal SSDs are periodic when the number of columns is large enough. Chen and Wu (1991) showed a similar periodicity property of maximum resolution and minimum aberration designs.

Given N and s, let $a_2(m) = \min\{A_2(D) : D \text{ is an } SSD(N, s^m)\}$, where designs may have fully aliased columns.

Lemma 5. *Suppose H is a saturated $OA(N, t, s, 2)$ with $t = (N - 1)/(s - 1)$ and D is a balanced (N, s^m)-design. Let $D \cup H$ be the column juxtaposition of D and H. Then $A_2(D \cup H) = A_2(D) + m(s - 1)$.*

Proof. By Lemma 4, $\delta_{ij}(D \cup H) = \delta_{ij}(D) + \delta_{ij}(H) = \delta_{ij}(D) + (N - s)/[s(s - 1)]$. Then $K_2(D \cup H) = K_2(D) + 2(N - s)/[s(s - 1)]K_1(D) + (N - s)^2/[s(s - 1)]^2$. Applying Lemma 1, with some straightforward algebra, we get $A_2(D \cup H) = A_2(D) + m(s - 1)$. □

When $N = s^2$, Theorem 2(iii) implies that $a_2(m+s+1) = a_2(m) + m(s-1)$ for any $m \geq 1$. The following result shows that for certain N, $a_2(m)$ is periodic when m is large enough.

Theorem 3. *Suppose a saturated $OA(N, t, s, 2)$ exists with $t = (N-1)/(s-1)$. Then there exists a positive integer m_0 such that for $m \geq m_0$, $a_2(m+t) = a_2(m) + m(s-1)$.*

Proof. Let $b(m) = a_2(m) - (s-1)m(m-t)/(2t)$. Lemma 2 implies that $b(m) \geq 0$. From Lemma 5, $a_2(m+t) \leq a_2(m) + m(s-1)$; therefore, $b(m+t) \leq b(m)$. Note that $N^2 a_2(m)$ is an integer, so does $N^2 b(m)$. Therefore, for any $1 \leq r \leq t$, $N^2 b(kt+r)$ is a decreasing integer sequence in k and has a lower bound. There must exist a positive integer $k_0 = k_0(r)$ such that for $k \geq k_0$, $N^2 b(kt+r) = N^2 b(k_0 t + r)$. Let $m_0 = \max\{(k_0(r)+1)t : 1 \leq r \leq t\}$, then for any $m \geq m_0$, $b(m+t) = b(m)$, or equivalently, $a_2(m+t) = a_2(m) + m(s-1)$. $\square$

4 Construction

The construction methods are applicable to any prime power. Throughout this section, we assume $s > 2$ is a prime power. Let F_s be a Galois field of s elements. For clarity, all proofs are given in the next section.

4.1 Half Addelman-Kempthorne orthogonal arrays

Addelman and Kempthorne (1961) described a method for constructing $OA(2s^n, 2(s^n-1)/(s-1)-1, s, 2)$ for any prime power s and any n. Such arrays can be naturally decomposed into two arrays of s^n runs. Each array is an $SSD(s^n, s^m)$ with $m = 2(s^n-1)/(s-1)-1$. We now describe how to construct an SSD in general.

In the construction the columns of an array are labeled with linear or quadratic polynomials in n variables $X_1, \ldots, X_n$ and the rows are labeled with points from F_s^n. Let $f_1(X_1, \ldots, X_n)$ and $f_2(X_1, \ldots, X_n)$ be two functions, linear or nonlinear. They correspond to two columns of length s^n when evaluated at F_s^n. The two functions (or columns) are *fully aliased* if the pair has only s level combinations, each combination occurring s^{n-1} times; and *orthogonal* if the pair has s^2 distinct level combinations, each combination occurring s^{n-2} times. A pair of fully aliased columns has projected $A_2 = s-1$ and a pair of orthogonal columns has projected $A_2 = 0$.

Following Addelman and Kempthorne (1961), $f_1(X_1, \ldots, X_n)$ and $f_2(X_1, \ldots, X_n)$ are said to be *semi-orthogonal* to each other if (i) for s odd, the pair has $(s+1)s/2$ distinct level combinations,

s combinations occurring s^{n-2} times and $s(s-1)/2$ combinations occurring $2s^{n-2}$ times and (ii) for s even, the pair has $s^2/2$ distinct level combinations each occurring $2s^{n-2}$ times. A pair of semi-orthogonal columns has projected $A_2 = (s-1)/s$ for s odd and projected $A_2 = 1$ for s even. This result can be easily verified from the connection between the ave χ^2 statistic and A_2 described in Section 2.3.

Let $L(X_1, \ldots, X_n)$ be the set of all nonzero linear functions of $X_1, \ldots, X_n$, i.e.,

$$L(X_1, \ldots, X_n) = \{c_1X_1 + \cdots + c_nX_n : c_i \in F_s, \text{ not all } c_i \text{ are zero}\}.$$

Every function in $L(X_1, \ldots, X_n)$ corresponds to a balanced column. Two functions f_1 and f_2 in $L(X_1, \ldots, X_n)$ are *dependent* if there is a nonzero constant $c \in F_s$ such that $f_1 = cf_2$; otherwise, they are *independent*. Clearly, dependent linear functions correspond to the same column up to level permutation and thus they are fully aliased while independent linear functions correspond to orthogonal columns. A set of $(s^n-1)/(s-1)$ independent linear functions generate an $OA(s^n, (s^n-1)/(s-1), s, 2)$. The traditional convention is to assume the first nonzero element being 1 for each column. For convenience, we assume the *last* nonzero element being 1 for each column. In particular, let $H(X_1, \ldots, X_n)$ be the set of all nonzero linear functions of $X_1, \ldots, X_n$ such that the *last* nonzero coefficient is 1. When evaluated at F_s^n, $H(X_1, \ldots, X_n)$ is a saturated $OA(s^n, (s^n-1)/(s-1), s, 2)$. This is indeed the regular fractional factorial design and the construction is called the Rao-Hamming construction by Hedayat, Sloane and Stufken (1999, Section 3.4).

The key idea of the Addelman-Kempthorne construction is to use quadratic functions in addition to linear functions. Let

$$Q_1^*(X_1, \ldots, X_n) = \{X_1^2 + aX_1 + h : a \in F_s, h \in H(X_2, \ldots, X_n)\} \tag{1}$$

and $Q_1(X_1, \ldots, X_n) = \{X_1\} \cup Q_1^*(X_1, \ldots, X_n)$.

$H(X_1, \ldots, X_n)$ has $(s^n-1)/(s-1)$ columns and $Q_i^*(X_1, \ldots, X_n)$ has $(s^n-1)/(s-1)-1$ columns. The column juxtaposition of $H(X_1, \ldots, X_n)$ and $Q_1^*(X_1, \ldots, X_n)$ forms an $SSD(s^n, s^m)$ with $m = 2(s^n-1)/(s-1)-1$, which is a half of an Addelman-Kempthorne OA.

Example 1. Consider $s = 3$ and $n = 2$. The functions are

$$\begin{aligned}
H(X_1, X_2) &= \{X_1, X_2, X_1 + X_2, 2X_1 + X_2\}, \\
Q_1^*(X_1, X_2) &= \{X_1^2 + X_2, X_1^2 + X_1 + X_2, X_1^2 + 2X_1 + X_2\}, \\
Q_1(X_1, X_2) &= \{X_1, X_1^2 + X_2, X_1^2 + X_1 + X_2, X_1^2 + 2X_1 + X_2\}.
\end{aligned}$$

$H(X_1, X_2)$ is an $OA(9, 4, 3, 2)$ when the functions are evaluated at F_3^2; so does $Q_1(X_1, X_2)$. They are isomorphic [indeed there is only one unique $OA(9, 4, 3, 2)$ up to isomorphism]. The column juxtaposition of $H(X_1, X_2)$ and $Q_1^*(X_1, X_2)$ forms an $SSD(9, 3^7)$, which is isomorphic to the first (and last) 9 rows of the commonly used $OA(18, 7, 3, 2)$ (e.g., Table 7C.2 of Wu and Hamada (2000)). This SSD has an overall $A_2 = 6$ and achieves the lower bound in Theorem 1. Furthermore, there are no fully aliased columns. Each column of $Q_1^*(X_1, X_2)$ is semi-orthogonal to three columns of $H(X_1, X_2)$ with projected $A_2 = 2/3$.

In general, we have the following results.

Lemma 6. *When evaluated at F_s^n, $Q_1(X_1, \ldots, X_n)$ is an $OA(s^n, (s^n - 1)/(s - 1), s, 2)$.*

Theorem 4. *The column juxtaposition of $H(X_1, \ldots, X_n)$ and $Q_1^*(X_1, \ldots, X_n)$ forms an optimal $SSD(s^n, s^m)$ with $m = 2(s^n - 1)/(s - 1) - 1$. Column X_1 is orthogonal to all other columns. It has an overall $A_2 = s^n - s$ and achieves the lower bound in Theorem 1. Furthermore, it has no fully aliased columns for $s > 2$.*

(i) For s odd, the possible projected A_2 values are 0 and $(s - 1)/s$. There are $s(s^n - s)/(s - 1)$ pairs of semi-orthogonal columns with projected $A_2 = (s - 1)/s$.

(ii) For s even, the possible projected A_2 values are 0 and 1. There are $s^n - s$ pairs of semi-orthogonal columns with projected $A_2 = 1$.

Both $Q_1(X_1, \ldots, X_n)$ and $H(X_1, \ldots, X_n)$ are saturated OAs of the same parameters. It is of interest to know whether they are isomorphic. Example 1 shows that they are isomorphic for $n = 2$ and $s = 3$. This is true as long as $n = 2$. When $n > 2$ and $s > 2$, they are not isomorphic. The following corollary summarizes the result.

Corollary 1. *(i) For $n = 2$, $Q_1(X_1, X_2)$ is isomorphic to the regular design $H(X_1, X_2)$.*

(ii) For $n > 2$ and $s > 2$, $Q_1(X_1, \ldots, X_n)$ is not isomorphic to $H(X_1, \ldots, X_n)$.

Corollary 1(ii) implies that $Q_1(X_1, \ldots, X_n)$ is a nonregular design for $n > 2$ and $s > 2$.

4.2 Juxtaposition of saturated orthogonal arrays

As a by-product of the half Addelman-Kempthorne construction, we have constructed a saturated OA, $Q_1(X_1, \ldots, X_n)$, besides the regular OA, $H(X_1, \ldots, X_n)$. For any $h \in H(X_1, \ldots, X_n)$, we can construct a saturated OA, $Q_h(X_1, \ldots, X_n)$, as follows. Let $h = c_1X_1 + \cdots + c_nX_n$ and k be the last position that $c_i \neq 0$, then $c_k = 1$ and $c_i = 0$ for all $i > k$. Let $Y_1 = h$, $Y_i = X_{i-1}$ for $2 \leq i \leq k$, and $Y_i = X_i$ for $k < i \leq n$. It is clear that $H(X_1, \ldots, X_n)$ is equivalent to $H(Y_1, \ldots, Y_n)$ up to row and column permutations. Define $Q_h^*(X_1, \ldots, X_n) = Q_1^*(Y_1, \ldots, Y_n)$ as in (1) by replacing X_i with Y_i and $Q_h(X_1, \ldots, X_n) = Q_1(Y_1, \ldots, Y_n)$.

Since there are $(s^n - 1)/(s - 1)$ columns in $H(X_1, \ldots, X_n)$, we obtain $(s^n - 1)/(s - 1)$ saturated $OA(s^n, (s^n - 1)/(s - 1), s, 2)$. Although they are all isomorphic, we can obtain many optimal multi-level SSDs by juxtaposing them.

Example 2. Consider $s = 3$ and $n = 2$. $H(X_1, X_2) = \{X_1, X_2, X_1 + X_2, 2X_1 + X_2\}$. For each $h \in H(X_1, X_2)$, we can define $Q_h(X_1, X_2)$ as follows.

$$
\begin{aligned}
Q_{X_1}(X_1, X_2) &= \{X_1, X_1^2 + X_2, X_1^2 + X_1 + X_2, X_1^2 + 2X_1 + X_2\}, \\
Q_{X_2}(X_1, X_2) &= \{X_2, X_2^2 + X_1, X_2^2 + X_2 + X_1, X_2^2 + 2X_2 + X_1\}, \\
Q_{X_1+X_2}(X_1, X_2) &= \{X_1 + X_2, (X_1 + X_2)^2 + X_1, (X_1 + X_2)^2 + 2X_1 + X_2, (X_1 + X_2)^2 + 2X_2\}, \\
Q_{2X_1+X_2}(X_1, X_2) &= \{2X_1 + X_2, (2X_1 + X_2)^2 + X_1, (2X_1 + X_2)^2 + X_2, (2X_1 + X_2)^2 + 2X_1 + 2X_2\}.
\end{aligned}
$$

Each $Q_h(X_1, X_2)$ is a saturated $OA(9, 4, 3, 2)$ and they are all isomorphic. The column juxtaposition of all four $Q_h(X_1, X_2)$ has 16 columns: 4 linear and 12 quadratic. All linear columns are orthogonal to each other. Each linear column is orthogonal to 3 quadratic columns, and semi-orthogonal to other 9 quadratic columns. Each quadratic column is orthogonal to 1 linear column, semi-orthogonal to other 3 linear columns, orthogonal to 2 quadratic columns, and partially aliased (projected $A_2 = 4/9$) with other 9 quadratic columns. The 16 columns together form an optimal $SSD(9, 3^{16})$ with an overall $A_2 = 48$. The 12 quadratic columns together form an optimal $SSD(9, 3^{12})$ with an overall $A_2 = 24$. For the latter design, each column is partially aliased with 9 columns with projected $A_2 = 4/9$.

Theorem 5. *Let h_1, h_2 be two distinct functions in $H(X_1, \ldots, X_n)$. The column juxtaposition of $Q_{h_1}(X_1, \ldots, X_n)$ and $Q_{h_2}(X_1, \ldots, X_n)$ forms an optimal $SSD(s^n, s^m)$ with $m = 2(s^n - 1)/(s - 1)$. It has an overall $A_2 = s^n - 1$ and is optimal under GMA. Furthermore, there are no fully aliased columns if s is odd or $s > 4$.*

(i) For s odd, the possible projected A_2 values are 0, $(s - 1)/s$, $(s - 1)^2/s^2$, and $(s - 1)/s^2$. There are $2s$ pairs with projected $A_2 = (s - 1)/s$, s^2 pairs with projected $A_2 = (s - 1)^2/s^2$, and $s^2(s^n - s^2)/(s - 1)$ pairs with projected $A_2 = (s - 1)/s^2$.

(ii) For s even, the possible projected A_2 values are $0, 1, 2$ and 3.

(iii) For $s = 4$, the possible projected A_2 values are $0, 1$ and 3. There are one pair of fully aliased columns with projected $A_2 = 3$ and $4^n - 4$ pairs of partially aliased columns with projected $A_2 = 1$.

Theorem 5 states that the column juxtaposition of $Q_{h_1}(X_1, \ldots, X_n)$ and $Q_{h_2}(X_1, \ldots, X_n)$ has the same projected A_2 values and frequencies. It is of interest to note that they can have different geometric structures and be non-isomorphic to each other. For example, when $n = 3$ and $s = 3$, the column juxtaposition of Q_{X_1} and Q_{X_2} is not isomorphic to the column juxtaposition of Q_{X_1} and Q_{X_3}.

Extending Theorem 5, we have the following result.

Theorem 6. *For $1 < k \le (s^n - 1)/(s - 1)$, let $h_1, \ldots, h_k$ be k distinct functions in $H(X_1, \ldots, X_n)$. The column juxtaposition of $Q_{h_i}(X_1, \ldots, X_n)$, $i = 1, \ldots, k$, forms an optimal $SSD(s^n, s^m)$ with $m = k(s^n - 1)/(s - 1)$. It has an overall $A_2 = \binom{k}{2}(s^n - 1)$ and is optimal under GMA. Furthermore, there are no fully aliased columns if s is odd or $s > 4$.*

(i) For s odd, the possible projected A_2 values are 0, $(s - 1)/s$, $(s - 1)^2/s^2$, and $(s - 1)/s^2$. There are $\binom{k}{2}2s$ pairs with projected $A_2 = (s - 1)/s$, $\binom{k}{2}s^2$ pairs with projected $A_2 = (s - 1)^2/s^2$, and $\binom{k}{2}s^2(s^n - s^2)/(s - 1)$ pairs with projected $A_2 = (s - 1)/s^2$.

(ii) For s even, the possible projected A_2 values are $0, 1, 2$ and 3.

(iii) For $s = 4$, the possible projected A_2 values are $0, 1$ and 3. There are $\binom{k}{2}$ pairs of fully aliased columns with projected $A_2 = 3$ and $\binom{k}{2}(4^n - 4)$ pairs of partially aliased columns with projected $A_2 = 1$.

When $k = (s^n - 1)/(s - 1)$, the above SSD has $[(s^n - 1)/(s - 1)]^2$ columns, among which $(s^n - 1)/(s - 1)$ columns are linear from $H(X_1, \ldots, X_n)$ and the rest are quadratic. All quadratic functions form another class of SSDs. This SSD does not have semi-orthogonal columns, which have projected $A_2 = (s - 1)/s$ for s odd.

Theorem 7. *Suppose s is odd. For $1 < k \le (s^n - 1)/(s - 1)$, let $h_1, \ldots, h_k$ be k distinct functions in $H(X_1, \ldots, X_n)$. The column juxtaposition of $Q^*_{h_i}(X_1, \ldots, X_n)$, $i = 1, \ldots, k$, forms an $SSD(s^n, s^m)$ with $m = k(s^n - s)/(s - 1)$. There are no fully aliased columns and the possible projected A_2 values are 0, $(s - 1)^2/s^2$ and $(s - 1)/s^2$. There are $\binom{k}{2}s^2$ pairs with projected $A_2 = (s - 1)^2/s^2$, and*

$\binom{k}{2}s^2(s^n-s^2)/(s-1)$ *pairs with projected* $A_2=(s-1)/s^2$. *It has an overall* $A_2=\binom{k}{2}(s^n-2s+1)$ *and is optimal under GMA if* $k=(s^n-1)/(s-1)-1$ *or* $(s^n-1)/(s-1)$.

Corollary 2. *For s odd, the column juxtaposition of $Q_h^*(X_1,X_2)$, $h\in H(X_1,X_2)$, forms an optimal $SSD(s^2,s^{(s+1)s})$. It has an overall $A_2=(s+1)s(s-1)^2/2$ and is optimal under GMA. Each column is orthogonal to $s-1$ columns and partially aliased with other s^2 columns with projected $A_2=(s-1)^2/s^2$.*

4.3 Fractions of saturated orthogonal arrays

First consider fractions of $H(X_1,\ldots,X_n)$. Without loss of generality, taking X_1 as the branching column, we obtain s fractions according to the levels of X_1. Each fraction has s^{n-1} runs and $(s^n-1)/(s-1)$ columns: column X_1 has one level only and all other columns have s levels. The row juxtaposition of any k fractions forms an optimal SSD after removing the column X_1.

Theorem 8. *Take any column of $H(X_1,\ldots,X_n)$ as a branching column. For $k<s$, the row juxtaposition of any k fractions forms an optimal $SSD(ks^{n-1},s^m)$ with $m=(s^n-s)/(s-1)$ after removing the branching column. It has an overall $A_2=(s^n-s)(s-k)/(2k)$ and is optimal under GMA. Furthermore, all possible projected A_2 values are 0 and $(s-k)/k$. There are $(s^n-s)/2$ pairs of nonorthogonal columns with projected $A_2=(s-k)/k$. In particular, there are no fully aliased columns for $1<k<s$.*

Next consider fractions of $Q_1(X_1,\ldots,X_n)$. If X_1 is used as the branching column, the row juxtaposition of the fractions has the same property as that of $H(X_1,\ldots,X_n)$. In the following theorem, we take $X_1^2+X_2$ as the branching column.

Theorem 9. *Take column $X_1^2+X_2$ of $Q_1(X_1,\ldots,X_n)$ as a branching column. The row juxtaposition of any k fractions forms an optimal $SSD(ks^{n-1},s^m)$ with $m=(s^n-s)/(s-1)$ after removing the branching column. It has an overall $A_2=(s^n-s)(s-k)/(2k)$ and is optimal under GMA. Furthermore, there are no fully aliased columns for $1<k<s$.*

(i) For s odd, there are $s(s^n-s^2+s-1)/2$ pairs of nonorthogonal columns, $s(s-1)/2$ pairs with projected $A_2=(s-k)/k$ and $s(s^n-s^2)/2$ pairs with projected $A_2=(s-k)/(ks)$.

(ii) For s even, there are at most $(s-1)(s^n-s^2+s)/2$ pairs of nonorthogonal columns, $s(s-1)/2$ pairs with projected $A_2=(s-k)/k$ and at most $(s-1)(s^n-s^2)/2$ pairs with projected $A_2\le 1$.

(iii) For $s = 4$ and $k = 2$, there are $(4^n - 4)/2$ pairs of nonorthogonal columns with projected $A_2 = 1$; for $s = 4$ and $k = 3$, there are 6 pairs of nonorthogonal columns with projected $A_2 = 1/3$ and $3(4^n - 16)/2$ pairs with projected $A_2 = 1/9$.

By branching other columns, we can obtain different SSDs as illustrated below.

Example 3. Consider $n = 3$ and $s = 3$. The columns of $Q_1(X_1, X_2, X_3)$ are

$$X_1, X_1^2 + X_2, X_1^2 + X_1 + X_2, X_1^2 + 2X_1 + X_2, X_1^2 + X_3, X_1^2 + X_1 + X_3,$$
$$X_1^2 + 2X_1 + X_3, X_1^2 + X_2 + X_3, X_1^2 + X_1 + X_2 + X_3, X_1^2 + 2X_1 + X_2 + X_3,$$
$$X_1^2 + 2X_2 + X_3, X_1^2 + X_1 + 2X_2 + X_3, X_1^2 + 2X_1 + 2X_2 + X_3.$$

Depending on the branching column, we obtain one of three types of optimal $SSD(18, 3^{12})$. The frequencies of projected A_2 values are:

A_2	0	1/6	1/2
type 1	54	0	12
type 2	36	27	3
type 3	42	18	6

We obtain a type 1 SSD if X_1 is used as the branching column, a type 2 SSD if $X_1^2 + aX_1 + X_2$ is used as the branching column, and a type 3 SSD if $X_1^2 + aX_1 + bX_2 + X_3$ is used as the branching column, where $a, b \in F_3$. A type 2 design is preferred in general because it has the smallest number of maximum projected A_2.

5 Some proofs

Additional notation and lemmas are needed for the proofs. Let F_s^* be the set of nonzero elements in F_s. An additive *character* of F_s is an homomorphism mapping $\chi : F_s \to \mathbb{C}$ such that for any $x, y \in F_s$, $|\chi(x)| = 1$ and $\chi(x+y) = \chi(x)\chi(y)$. Clearly $\chi(0) = 1$ since $\chi(0) = \chi(0)\chi(0)$. A character is called *trivial* if $\chi(x) = 1$ for all x; otherwise, it is *nontrivial.* A nontrivial additive character has the property that $\sum_{x \in F_s} \chi(ax) = s$ if $a = 0$ and equals 0 otherwise.

Let χ be a nontrivial additive character. For $u \in F_s$, the function $\chi_u(x) = \chi(ux)$ defines a character of F_s. Then χ_0 is a trivial character and all other characters χ_u are nontrivial. It is important to note that $\{\chi_u, u \in F_s^*\}$ forms a set of orthonormal contrasts defined in Xu and Wu (2001), that is, $\sum_{x \in F_s} \chi_u(x)\overline{\chi_v(x)} = s$ if $u = v$ and equals 0 otherwise. As a result, we can use additive characters to compute the generalized wordlength pattern. In particular, for a column $x = (x_1, \dots, x_N)^T$, the orthonormal contrast coefficient matrix is $(\chi_u(x_i))$ where $u \in F_s^*$ and $i = 1, \dots, N$. Then the projected A_2 value of a pair of columns $x = (x_1, \dots, x_N)^T$ and $y = (y_1, \dots, y_N)^T$ is

$$A_2(x, y) = N^{-2} \sum_{u_1 \in F_s^*} \sum_{u_2 \in F_s^*} \left| \sum_{i=1}^{N} \chi(u_1 x_i + u_2 y_i) \right|^2 . \tag{2}$$

Let $s = p^r$ where p is a prime. Define a mapping $Tr : F_s \to F_p$, called the *trace*, as follows: $Tr(x) = x + x^p + x^{p^2} + \cdots + x^{p^{r-1}}$ for any $x \in F_s$. Let

$$\chi(x) = e^{2\pi i Tr(x)/p} \text{ for any } x \in F_s. \tag{3}$$

This is a nontrivial additive character and called the *canonical* additive character of F_s.

An element $c \in F_s$ is called a *quadratic residue* if there exists $a \in F_s$ such that $c = a^2$.

Lemma 7. *For s odd, let $b \in F_s$ and $c \in F_s^*$.*

(i) If c is a quadratic residue, the number of solutions of $x_1^2 - cx_2^2 = b$ in F_s^2 is equal to $2s - 1$ for $b = 0$ and $s - 1$ for $b \neq 0$.

(ii) If c is not a quadratic residue, the number of solutions of $x_1^2 - cx_2^2 = b$ in F_s^2 is equal to 1 for $b = 0$ and $s + 1$ for $b \neq 0$.

Proof. It follows from Lemma 6.24 of Lidl and Niederreiter (1997). □

Lemma 8. *For s odd, let $a \in F_s^*$, $b, c \in F_s$, and χ be a nontrivial additive character. Then $\left|\sum_{x \in F_s} \chi(ax^2 + bx + c)\right|^2 = s$.*

Proof. Note that $\chi(ax^2 + bx + c) = \chi(a(x + b_0)^2 + c_0) = \chi(a(x + b_0)^2)\chi(c_0)$, where $b_0 = b/(a + a)$ and $c_0 = c - ab_0^2$. Then $\left|\sum_{x \in F_s} \chi(ax^2 + bx + c)\right|^2 = \left|\sum_{x \in F_s} \chi(a(x + b_0)^2)\right|^2 = \left|\sum_{x \in F_s} \chi(ax^2)\right|^2$. On the other hand,

$$\left| \sum_{x \in F_s} \chi(ax^2) \right|^2 = \sum_{x \in F_s} \chi(ax^2) \sum_{y \in F_s} \chi(-ay^2) = \sum_{x \in F_s} \sum_{y \in F_s} \chi(a(x^2 - y^2)).$$

By Lemma 7(i), $x^2 - y^2$ has s levels, level 0 occurring $(2s - 1)$ times and other $s - 1$ levels occurring $(s - 1)$ times. Therefore, $\sum_{x \in F_s} \sum_{y \in F_s} \chi(a(x^2 - y^2)) = s + (s - 1) \sum_{z \in F_s} \chi(az) = s$ since $a \neq 0$. □

The following lemma is from Lidl and Niederreiter (1997, Corollary 5.35).

Lemma 9. *For s even, let $a, b \in F_s$ and χ be the canonical additive character of F_s defined in* (3)*. Then $\sum_{x\in F_s} \chi(ax^2 + bx) = s$ if $a = b^2$ and equals 0 otherwise.*

Lemma 10. *Let G be a subset of F_s, $|G| = k$ and χ be a nontrivial additive character. Then $\sum_{u\in F_s^*} \left|\sum_{x\in G} \chi(ux)\right|^2 = (s - k)k$.*

Proof.

$$\left|\sum_{x\in G} \chi(ux)\right|^2 = \sum_{x\in G} \chi(ux) \sum_{y\in G} \chi(-uy) = \sum_{x\in G}\sum_{y\in G} \chi(u(x-y)).$$

$$\sum_{u\in F_s} \left|\sum_{x\in G} \chi(ux)\right|^2 = \sum_{u\in F_s}\sum_{x\in G}\sum_{y\in G} \chi(u(x-y)) = \sum_{x\in G}\sum_{y\in G}\left(\sum_{u\in F_s} \chi(u(x-y))\right) = sk.$$

The last equation is due to the fact that $\sum_{u\in F_s} \chi(u(x-y))$ is equal to s if $x = y$ and 0 otherwise. Then $\sum_{u\in F_s^*} \left|\sum_{x\in G} \chi(ux)\right|^2 = \sum_{u\in F_s} \left|\sum_{x\in G} \chi(ux)\right|^2 - k^2 = sk - k^2$. □

Proof of Lemma 6. Consider a pair of columns: $X_1^2 + a_1X_1 + h_1$ and $X_1^2 + a_2X_1 + h_2$, where $h_1, h_2 \in H(X_2, \ldots, X_n)$ and $a_1, a_2 \in F_s$. With $z_1, z_2 \in F_s$, the number of times that (z_1, z_2) appears as a row in this subarray is equal to the number of solutions of $(X_1, \ldots, X_n)$ such that

$$X_1^2 + a_1X_1 + h_1 = z_1 \text{ and } X_1^2 + a_2X_1 + h_2 = z_2. \tag{4}$$

If $h_1 \neq h_2$, then for each value of X_1 we have two independent linear equations in $X_2, \ldots, X_n$, which leads to s^{n-3} solutions. Since there are s choices for X_1, there are s^{n-2} solutions to (4). Therefore, the two columns are orthogonal. If $h_1 = h_2$ and $a_1 \neq a_2$, then $(a_1 - a_2)X_1 = z_1 - z_2$. There is a unique solution for X_1. Given X_1, there are s^{n-2} solutions in $X_2, \ldots, X_n$. The total number of solutions to (4) is still s^{n-2}. Therefore, the two columns are orthogonal. Similarly, X_1 is orthogonal to $X_1^2 + aX_1 + h$ for any $a \in F_s$ and $h \in H(X_2, \ldots, X_n)$. Therefore, $Q_1(X_1, \ldots, X_n)$ is an OA. □

Lemma 11. *Consider columns $X_1^2 + a_1X_1 + h_1$ and $a_2X_1 + h_2$, where $h_1, h_2 \in L(X_2, \ldots, X_n)$ and $a_1, a_2 \in F_s$.*

(i) If h_1 and h_2 are independent, they are orthogonal.

(ii) For s odd, if h_1 and h_2 are dependent, they are semi-orthogonal.

(iii) For s even, if h_1 and h_2 are dependent and $a_1h_2 = a_2h_1$, they are orthogonal.

(iv) For s even, if h_1 and h_2 are dependent and $a_1h_2 \neq a_2h_1$, they are semi-orthogonal.

Proof. It follows from Lemmas 1–4 and 5a of Addelman and Kempthorne (1961). □

Proof of Theorem 4. The columns of $Q_1(X_1, \ldots, X_n)$ are X_1 and $X_1^2 + a_1X_1 + h_1$, and the columns of $H(X_1, \ldots, X_n)$ are X_1 and $a_2X_1 + h_2$, where $a_i \in F_s$ and $h_i \in H(X_2, \ldots, X_n)$. Since both $H(X_1, \ldots, X_n)$ and $Q_1(X_1, \ldots, X_n)$ are saturated OAs and they share column X_1, the optimality of the column juxtaposition of $H(X_1, \ldots, X_n)$ and $Q_1^*(X_1, \ldots, X_n)$ follows from Lemmas 3 and 4. By Lemma 5, the overall $A_2(H \cup Q_1^*) = A_2(Q_1^*) + [(s^n - s)/(s-1)](s-1) = (s^n - s)$ since Q_1^* is an OA.

(i) When s is odd, by Lemma 11, $X_1^2 + a_1X_1 + h_1$ and $a_2X_1 + h_2$ are semi-orthogonal if $h_1 = h_2$. Therefore, each column of $Q_1^*(X_1, \ldots, X_n)$ is semi-orthogonal to s columns of $H(X_1, \ldots, X_n)$. Since there are $(s^n - 1)/(s-1) - 1$ columns in $Q_1^*(X_1, \ldots, X_n)$, there are in total $s(s^n - s)/(s-1)$ semi-orthogonal pairs of columns with projected $A_2 = (s-1)/s$.

(ii) When s is even, by Lemma 11, $X_1^2 + a_1X_1 + h_1$ and $a_2X_1 + h_2$ are semi-orthogonal if $h_1 = h_2$ and $a_1 \neq a_2$. Therefore, each column of $Q_1^*(X_1, \ldots, X_n)$ is semi-orthogonal to $s-1$ columns of $H(X_1, \ldots, X_n)$. Since there are $(s^n - 1)/(s-1) - 1$ columns in $Q_1^*(X_1, \ldots, X_n)$, there are in total $s^n - s$ semi-orthogonal pairs of columns with projected $A_2 = 1$. □

Proof of Corollary 1. (i) Let $Y_1 = X_1$ and $Y_2 = X_1^2 + X_2$. It is a one-to-one mapping from (Y_1, Y_2) to (X_1, X_2). The columns of $Q_1(X_1, X_2)$ are $X_1 = Y_1$ and $X_1^2 + aX_1 + X_2 = aY_1 + Y_2$, where $a \in F_s$. Therefore, $Q_1(X_1, X_2) = H(Y_1, Y_2)$ is isomorphic to $H(X_1, X_2)$.

(ii) It follows from Theorems 8 and 9 to be proven later. □

Lemma 12. *Suppose $h_i \in L(X_3, \ldots, X_n)$ and $a_i, b_i \in F_s$ for $i = 1, 2$.*

(i) If h_1 and h_2 are independent, $X_1^2 + a_1X_1 + b_1X_2 + h_1$ and $X_2^2 + a_2X_2 + b_2X_1 + h_2$ are orthogonal.

(ii) If $b_2 \neq 0$, $X_1^2 + a_1X_1 + b_1X_2 + h_1$ and $X_2^2 + a_2X_2 + b_2X_1$ are orthogonal.

(iii) If h_1 and h_2 are dependent, the pair of columns $X_1^2 + a_1X_1 + b_1X_2 + h_1$ and $X_2^2 + a_2X_2 + b_2X_1 + h_2$ has projected $A_2 = (s-1)/s^2$ for s odd and $A_2 = 0$ or 1 for s even.

(iv) For s odd, the pair of columns $X_1^2 + a_1X_1 + X_2$ and $X_2^2 + a_2X_2 + X_1$ has projected $A_2 = (s-1)^2/s^2$.

(v) For s even, the pair of columns $X_1^2 + a_1X_1 + X_2$ and $X_2^2 + a_2X_2 + X_1$ has projected $A_2 = 0$, 1, 2 or 3.

(vi) For $s=4$, the pair of columns $X_1^2+a_1X_1+X_2$ and $X_2^2+a_2X_2+X_1$ has projected $A_2=3$ if $a_1=a_2=0$, $A_2=1$ if both $a_1\neq 0$ and $a_2\neq 0$, and $A_2=0$ otherwise.

Proof. (i) and (ii) The proofs are similar to that of Lemma 6.

(iii) Let $h_1=ch_2$, where $c\in F_s^*$. Let $z_1=x_1^2+a_1x_1+b_1x_2$ and $z_2=x_2^2+a_2x_2+b_2x_1$. Let χ be the canonical additive character defined in (3). By (2), the projected A_2 value of the pair is

$$\begin{aligned} A_2 &= s^{-2n}\sum_{u_1\in F_s^*}\sum_{u_2\in F_s^*}\left|\sum_{(x_1,\ldots,x_n)\in F_s^n}\chi(u_1(z_1+h_1)+u_2(z_2+h_2))\right|^2 \\ &= s^{-2n}\sum_{u_1\in F_s^*}\sum_{u_2\in F_s^*}\left|\sum_{(x_1,x_2)\in F_s^2}\chi(u_1z_1+u_2z_2)\sum_{(x_3,\ldots,x_n)\in F_s^{n-2}}\chi(u_1h_1+u_2h_2)\right|^2. \end{aligned}$$

Since $h_1=ch_2$, the last summation is equal to s^{n-2} if $cu_1+u_2=0$ and 0 otherwise. Therefore,

$$\begin{aligned} A_2 &= s^{-4}\sum_{u_1\in F_s^*}\left|\sum_{(x_1,x_2)\in F_s^2}\chi(u_1(z_1-cz_2))\right|^2 \\ &= s^{-4}\sum_{u_1\in F_s^*}\left|\sum_{x_1\in F_s}\chi(u_1x_1^2+(u_1a_1-cu_1b_2)x_1)\sum_{x_2\in F_s}\chi(-cu_1x_2^2+(-cu_1a_2+u_1b_1)x_2)\right|^2. \end{aligned}$$

For s odd, $A_2=s^{-4}(s-1)s^2=(s-1)/s^2$ follows from Lemma 8. For s even, from Lemma 9, A_2 is equal to the number of $u_1\in F_s^*$ such that $u_1=(u_1a_1-cu_1b_2)^2$ and $-cu_1=(-cu_1a_2+u_1b_1)^2$. Clearly, the two equations have at most one solution in F_s^*. Therefore, A_2 is equal to 0 or 1.

(iv) Similar to (iii), we have

$$A_2=s^{-4}\sum_{u_1\in F_s^*}\sum_{u_2\in F_s^*}\left|\sum_{x_1\in F_s}\chi(u_1x_1^2+(u_1a_1+u_2)x_1)\sum_{x_2\in F_s}\chi(u_2x_2^2+(u_2a_2+u_1)x_2)\right|^2. \tag{5}$$

Since s is odd, $A_2=s^{-4}(s-1)^2s^2=(s-1)^2/s^2$ follows from Lemma 8.

(v) As in (iv), we have (5). Since s is even, by Lemma 9, A_2 is equal to the number of $u_1\in F_s^*$ and $u_2\in F_s^*$ such that

$$u_1=(u_1a_1+u_2)^2 \text{ and } u_2=(u_2a_2+u_1)^2. \tag{6}$$

We show that the number of solutions to (6) is at most 3; therefore, $A_2=0,1,2$ or 3. From (6), $u_1(u_2a_2+u_1)^2=u_2(u_1a_1+u_2)^2$. Let $c=u_1^{-1}u_2$. The last equation simplifies to $(ca_2+1)^2=c(a_1+c)^2$. There are at most three solutions for $c\in F_s^*$ as long as it is a cubic polynomial in c. For each $c\in F_s^*$, there is a unique solution to (6): $u_1=(a_1+c)^{-2}$ and $u_2=(a_2+c^{-1})^{-2}$, provided the inverses exist.

(vi) When $s=4$, the equation $(ca_2+1)^2 = c(a_1+c)^2$ is the same as $c^3+a_2^2c^2+a_1^2c+1=0$. It is easy to verify that it has three solutions if $a_1=a_2=0$, one solution if $a_1 \neq 0$ and $a_2 \neq 0$, and no solution otherwise. For each c, there is a unique solution to (6): $u_1=(a_1+c)^{-2}$ and $u_2=(a_2+c^{-1})^{-2}$. □

Remark 1. For s odd, if Lemma 7 is used instead of Lemma 8, the statement in (iii) can be strengthened as follows. The pair has all s^2 level combinations. Suppose $h_1=ch_2$. If c is a quadratic residue, s combinations occurring $(2s-1)s^{n-3}$ times and $s(s-1)$ combinations occurring $(s-1)s^{n-3}$ times; otherwise, s combinations occurring s^{n-3} times and $s(s-1)$ combinations occurring $(s+1)s^{n-3}$ times.

Proof of Theorem 5. Without loss of generality, we assume $h_1=X_1$ and $h_2=X_2$. Since both $Q_{X_1}(X_1,\ldots,X_n)$ and $Q_{X_2}(X_1,\ldots,X_n)$ are saturated OAs, the GMA optimality and the overall $A_2=s^n-1$ follow from Lemmas 3, 4 and 5.

(i) The columns of $Q_{X_1}(X_1,\ldots,X_n)$ fall into three types: (a) X_1, (b) $X_1^2+a_1X_1+X_2$, and (c) $X_1^2+a_1X_1+b_1X_2+g_1$, where $a_1,b_1 \in F_s$ and $g_1 \in H(X_3,\ldots,X_n)$. Similarly, the columns of $Q_{X_2}(X_1,\ldots,X_n)$ fall into three types: (a) X_2, (b) $X_2^2+a_2X_2+X_1$, and (c) $X_2^2+a_2X_2+b_2X_1+g_2$, where $a_2,b_2 \in F_s$ and $g_2 \in H(X_3,\ldots,X_n)$. The projected A_2 values of all possible pairs can be found in Lemmas 11(ii), 11(i), 12(iv), 12(ii), and 12(i)(iii), respectively. In summary, we have the following aliasing patterns:

	X_2	$X_2^2+a_2X_2+X_1$	$X_2^2+a_2X_2+b_2X_1+g_2$
X_1	0	$(s-1)/s$	0
$X_1^2+a_1X_1+X_2$	$(s-1)/s$	$(s-1)^2/s^2$	0
$X_1^2+a_1X_1+b_1X_2+g_1$	0	0	$\delta_{g_1,g_2}(s-1)/s^2$

where δ_{g_1,g_2} is equal to 1 if g_1 and g_2 are dependent and 0 otherwise. Each type (c) column in $Q_{X_1}(X_1,\ldots,X_n)$ is partially aliased with s^2 type (c) columns in $Q_{X_2}(X_1,\ldots,X_n)$. The result follows from the fact that the numbers of columns for each type are (a) 1, (b) s, and (c) $(s^n-s^2)/(s-1)$, respectively.

(ii) From Lemmas 11 and 12, the possible projected A_2 values are 0, 1, 2 or 3.

(iii) From Lemmas 11 and 12, the possible projected A_2 values are 0, 1 or 3. Lemma 12(vi) shows that there is one fully aliased pair: $X_1^2+X_2$ and $X_2^2+X_1$, which has projected $A_2=3$. Since the overall $A_2=4^n-1$, there must be 4^n-4 pairs with projected $A_2=1$. □

Proof of Theorem 6. It follows from Theorem 5. □

Proof of Theorem 7. We only need prove the GMA optimality. Since all linear functions form a saturated OA, the number of coincidences between any pair of rows of the resulting SSD is a constant when $k = (s^n - 1)/(s - 1)$ and differs by at most one when $k = (s^n - 1)/(s - 1) - 1$. Therefore, the GMA optimality follows from Lemma 3. □

Lemma 13. *Let $G \subset F_s$ and $|G| = k$. Suppose X_1 takes on values from G only and all other X_i take on values from F_s. Suppose $h_1, h_2 \in L(X_2, \ldots, X_n)$ and $a_1, a_2 \in F_s$.*

(i) If h_1 and h_2 are independent, $a_1X_1 + h_1$ and $a_2X_1 + h_2$ are orthogonal .

(ii) If $h_1 = h_2$ and $a_1 \neq a_2$, the pair of columns $a_1X_1 + h_1$ and $a_2X_1 + h_2$ has projected $A_2 = (s - k)/k$.

Proof. (i) It is obvious.

(ii) Let χ be a nontrivial additive character of F_s. By (2), the projected A_2 value of the pair is

$$\begin{aligned} A_2 &= (ks^{n-1})^{-2} \sum_{u_1 \in F_s^*} \sum_{u_2 \in F_s^*} \left| \sum_{x_1 \in G} \sum_{(x_2,\ldots x_n) \in F_s^{n-1}} \chi(u_1(a_1x_1 + h_1) + u_2(a_2x_1 + h_2)) \right|^2 \\ &= (ks^{n-1})^{-2} \sum_{u_1 \in F_s^*} \sum_{u_2 \in F_s^*} \left| \sum_{x_1 \in G} \chi((u_1a_1 + u_2a_2)x_1) \sum_{(x_2,\ldots x_n) \in F_s^{n-1}} \chi(u_1h_1 + u_2h_2) \right|^2 . \end{aligned}$$

The last summation is equal to s^{n-1} if $u_1h_1 + u_2h_2 = 0$ and 0 otherwise. Since $h_1 = h_2$, $A_2 = k^{-2} \sum_{u_1 \in F_s^*} \left|\sum_{x_1 \in G} \chi(u_1(a_1 - a_2)x_1)\right|^2 = (s - k)/k$ follows from Lemma 10. □

Proof of Theorem 8. Without loss of generality, take X_1 as the branching column. The columns are $aX_1 + h$, where $a \in F_s$ and $h \in H(X_3, \ldots, X_n)$. By Lemma 13, each column is partially aliased with $s-1$ columns with projected $A_2 = (s-k)/k$ and orthogonal to all other columns. Since there are $(s^n - s)/(s - 1)$ columns, there are $(s^n - s)/2$ pairs of nonorthogonal columns with projected $A_2 = (s - k)/k$. Therefore, the overall $A_2 = (s^n - s)(s - k)/(2k)$. Finally, the GMA optimality follows from Lemmas 3 and 4. □

Lemma 14. *Let $G \subset F_s$ and $|G| = k$. Take $X_1^2 + X_2$ as the branching column of $Q_1(X_1, \ldots, X_n)$, that is, suppose all X_i, $i \neq 2$ take on values from F_s and $X_1^2 + X_2$ takes on values from G only. Suppose $h \in H(X_2, \ldots, X_n)$ and $a_1, a_2, b_1, b_2 \in F_s$.*

(i) The pair of columns X_1 and $X_1^2 + a_1X_1 + X_2$ has projected $A_2 = (s - k)/k$.

(ii) If $a_1 \neq a_2$, the pair of columns $X_1^2 + a_1X_1 + X_2$ and $X_1^2 + a_2X_1 + X_2$ has projected $A_2 = (s-k)/k$.

(iii) For s odd, if $b_1 \neq b_2$, the pair of columns $X_1^2 + a_1X_1 + b_1X_2 + h$ and $X_1^2 + a_2X_1 + b_2X_2 + h$ has projected $A_2 = (s-k)/(ks)$.

(iv) For s even, if $b_1 \neq b_2$ and $a_1 \neq a_2$, the pair of columns $X_1^2 + a_1X_1 + b_1X_2 + h$ and $X_1^2 + a_2X_1 + b_2X_2 + h$ has projected $A_2 \leq 1$.

(v) For $s = 4$, if $b_1 \neq b_2$ and $a_1 \neq a_2$, the pair of columns $X_1^2 + a_1X_1 + b_1X_2 + h$ and $X_1^2 + a_2X_1 + b_2X_2 + h$ has projected $A_2 = 0$ or 1 for $k = 2$, and projected $A_2 = 1/9$ for $k = 3$.

Proof. Let $Y = X_1^2 + X_2$. Then Y are independent of X_i for $i \neq 2$.

(i) and (ii) The proofs are similar to Lemma 13(ii).

(iii) Let χ be a nontrivial additive character of F_s. Let $z_i = x_1^2 + a_ix_1 + b_ix_2 = (1-b_i)x_1^2 + a_ix_1 + b_iy$ for $i = 1, 2$. By (2), the projected A_2 value of the pair is

$$\begin{aligned} A_2 &= (ks^{n-1})^{-2} \sum_{u_1 \in F_s^*} \sum_{u_2 \in F_s^*} \left| \sum_{x_1 \in F_s} \sum_{y \in G} \sum_{(x_3,\ldots,x_n) \in F_s^{n-2}} \chi(u_1(z_1+h) + u_2(z_2+h)) \right|^2 \\ &= (ks^{n-1})^{-2} \sum_{u_1 \in F_s^*} \sum_{u_2 \in F_s^*} \left| \sum_{x_1 \in F_s} \sum_{y \in G} \chi(u_1z_1 + u_2z_2) \sum_{(x_3,\ldots,x_n) \in F_s^{n-2}} \chi((u_1+u_2)h) \right|^2. \end{aligned}$$

The last summation is equal to s^{n-2} if $u_1 + u_2 = 0$ and 0 otherwise. Then,

$$\begin{aligned} A_2 &= (ks)^{-2} \sum_{u_1 \in F_s^*} \left| \sum_{x_1 \in F_s} \sum_{y \in G} \chi(u_1(z_1 - z_2)) \right|^2 \\ &= (ks)^{-2} \sum_{u_1 \in F_s^*} \left| \sum_{x_1 \in F_s} \chi(u_1(b_2-b_1)x_1^2 + u_1(a_1-a_2)x_1) \sum_{y \in G} \chi(u_1(b_1-b_2)y) \right|^2. \end{aligned} \quad (7)$$

Since s is odd, by Lemma 8 and then Lemma 10,

$$A_2 = (ks)^{-2} \sum_{u_1 \in F_s^*} s \left| \sum_{y \in G} \chi(u_1(b_1-b_2)y) \right|^2 = (s-k)/(ks).$$

(iv) Let χ be the canonical additive character defined in (3). As in (iii), we have (7). Since s is even, by Lemma 9, (7) is simplified to

$$A_2 = (ks)^{-2}s^2 \left| \sum_{y \in G} \chi(-(b_1-b_2)^2/(a_1-a_2)^2 y) \right|^2 \leq k^{-2} \left| \sum_{y \in G} 1 \right|^2 = 1.$$

(v) As in (iv), $A_2 = k^{-2} \left| \sum_{y \in G} \chi(uy) \right|^2$, where $u = -(b_1 - b_2)^2/(a_1 - a_2)^2 \neq 0$. Since χ is the canonical additive character and $s = 4$, $\chi(\cdot) = \pm 1$. Therefore, for $k = 2$, $A_2 = 0$ or 1; for $k = 3$, $A_2 = 1/9$. □

Proof of Theorem 9. The GMA optimality follows from Lemmas 3 and 4. Since both designs in Theorems 8 and 9 have GMA, they must have the same overall $A_2 = (s^n - s)(s - k)/(2k)$.

(i) The columns of $Q_1(X_1, \ldots, X_n)$ are X_1, $X_1^2 + aX_1 + X_2$ and $X_1^2 + aX_1 + bX_2 + h$, where $a, b \in F_s$ and $h \in H(X_3, \ldots, X_n)$. By Lemma 14(i), the pair of columns X_1 and $X_1^2 + aX_1 + X_2$ has projected $A_2 = (s - k)/k$ when $a \neq 0$, and there are $s - 1$ such pairs; by Lemma 14(ii), the pair of columns $X_1^2 + a_1X_1 + X_2$ and $X_1^2 + a_2X_1 + X_2$ has projected $A_2 = (s - k)/k$ when $a_1 \neq a_2$, and there are $\binom{s-1}{2}$ such pairs since column $X_1^2 + X_2$ is removed; and by Lemma 14(iii), the pair of columns $X_1^2 + a_1X_1 + b_1X_2 + h$ and $X_1^2 + a_2X_1 + b_2X_2 + h$ has projected $A_2 = (s - k)/(ks)$ when $b_1 \neq b_2$, and there are $s^2\binom{s}{2}(s^{n-2} - 1)/(s - 1) = s(s^n - s^2)/2$ such pairs. It is easy to verify that all other pairs of columns are orthogonal.

(ii) and (iii) The proofs are similar to (i) and are omitted. □

6 Some small designs and comparison

Applying the construction methods, we can get many optimal multi-level SSDs. Tables 1–3 list the frequencies of projected nonzero A_2 values for some optimal 3-, 4-, and 5-level SSDs. All SSDs have the property that the number of coincidences between any pair of rows differs from each other by at most one; therefore, their overall A_2 values achieve the lower bound in Theorem 1 and they are optimal under GMA.

When $s = 4$ and $n = 2$, according to Theorem 6, the column juxtaposition of all five saturated OAs has 10 pairs of fully aliased columns. After removing one column from each pair, we obtain 15 columns with projected $A_2 = 0$ or 1. It can be verified that the overall A_2 value is 45 and achieves the lower bound in Theorem 1; therefore, this SSD is optimal under GMA. Similarly, when $s = 4$ and $n = 3$, the column juxtaposition of all 21 saturated OAs has 210 pairs of fully aliased columns. After removing one column from each pair, we obtain 231 columns with projected $A_2 = 0$ or 1. It can be verified that the overall A_2 value is 3465 and achieves the lower bound in Theorem 1; therefore, this SSD is also optimal under GMA.

Yamada et al. (1999) constructed some 3-level SSDs with $N = 9, 18$ and 27 runs. Fang et al.

(2000) constructed some multi-level SSDs with $N = 9, 16, 18, 25$ and 27 runs. Here we compare their designs with ours. Since our designs are optimal under GMA, we compare the maximum aliasing among the columns. Table 4 compares their designs with ours in terms of the maximum projected A_2 values. For $N = 9, 25, 27$, we have two classes of SSDs from Theorems 6 and 7. The latter designs have smaller maximum projected A_2 values than the former designs (although the latter designs may have larger overall A_2 values than the former designs). In Table 4, our designs have the smallest maximum projected A_2 values except in one case. For $N = 18$, $s = 3$ and $m = 12$, the design by Fang et al. has the smallest maximum projected A_2 value. However, their design has an overall $A_2 = 7.72$ and is not optimal while the other two designs have an overall $A_2 = 6$ and is optimal.

The advantage of our construction methods over the algorithms of Yamada et al. and Fang et al. is evident from Table 4. Neither algorithm is efficient in controlling the maximum aliasing among columns when the number of runs, columns or levels is large. In contrast, our construction methods work efficiently for large and small SSDs. Moreover, since the columns are represented by linear and quadratic polynomials, we can study in depth the aliasing among columns, which is useful in factor assignment. For example, since one column is orthogonal to all other columns in the half Addelman-Kempthorne array, the experimenter should assign the most important factor to this column.

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Table 1: Some optimal three-level supersaturated designs

		Projected A_2 Values					
N	m	2/3	1/2	4/9	2/9	1/6	Source
6	3		3				Theorem 8, $n = 2, k = 2$
9	7	9					Theorem 4, $n = 2$
9	12			54			Theorem 7, $n = 2, k = 4$
9	16	36		54			Theorem 6, $n = 2, k = 4$
18	12		12				Theorem 8, $n = 3, k = 2$
18	12		3			27	Theorem 9, $n = 3, k = 2$
27	25	36					Theorem 4, $n = 3$
27	156			702	6318		Theorem 7, $n = 3, k = 13$
27	169	468		702	6318		Theorem 6, $n = 3, k = 13$
54	40		36				Theorem 8, $n = 4, k = 2$
54	40		3			108	Theorem 9, $n = 4, k = 2$

Table 2: Some optimal four-level supersaturated designs

		Projected A_2 Values			
N	m	1	1/3	1/9	Source
8	4	6			Theorem 8, $n = 2, k = 2$
12	4		6		Theorem 8, $n = 2, k = 3$
16	9	12			Theorem 4, $n = 2$
16	15	45			Theorem 6[a], $n = 2$
32	20	30			Theorem 8, $n = 3, k = 2$
48	20		30		Theorem 8, $n = 3, k = 3$
48	20		6	72	Theorem 9, $n = 3, k = 3$
64	41	60			Theorem 4, $n = 3$
64	231	3465			Theorem 6[a], $n = 3$

[a] The design is obtained by removing fully aliased columns.

Table 3: Some optimal five-level supersaturated designs

		Projected A_2 Values							
N	m	3/2	4/5	16/25	2/3	3/10	1/4	2/15	Source
10	5	10							Theorem 8, $n = 2, k = 2$
15	5				10				Theorem 8, $n = 2, k = 3$
20	5						10		Theorem 8, $n = 2, k = 4$
25	11		25						Theorem 4, $n = 2$
25	30			375					Theorem 7, $n = 2, k = 6$
25	36		150	375					Theorem 6, $n = 2, k = 6$
50	30	60							Theorem 8, $n = 3, k = 2$
50	30	10				250			Theorem 9, $n = 3, k = 2$
75	30				60				Theorem 8, $n = 3, k = 3$
75	30				10			250	Theorem 9, $n = 3, k = 3$

Table 4: Comparison of supersaturated designs in terms of maximum projected A_2 values

N	s	m	Authors	Fang et al.	Yamada et al.
9	3	12	.44 or .67	.67	.67
9	3	16	.67	.67	.67
16	4	15	1	1.12	
18	3	12	.5	.44	.5[b]
25	5	24	.64 or .8	2.48	
25	5	30	.64 or .8		
25	5	36	.8		
27	3	52	.44 or .67	.59	.67
27	3	156	.44 or .67		1.11
27	3	169	.67		1.11

[b] This design is constructed according to their Theorem 3.