Optimal mixed-level supersaturated design

Kai-Tai Fang[1]*, Dennis K. J. Lin[2] and Min-Qian Liu[3]

[1] Department of Mathematics, Hong Kong Baptist University, Hong Kong, China
(E-mail: ktfang@math.hkbu.edu.hk)
[2] Department of Supply Chain and Information Systems, The Pennsylvania State University,
University Park, PA 16802, U.S.A. (E-mail: DKL5@psu.edu)
[3] Department of Statistics, Nankai University, Tianjin 300071, China (E-mail: mqliu@263.net)

Abstract. A supersaturated design is essentially a fractional factorial in which the number of potential effects is greater than the number of runs. In this paper, $E(f_{NOD})$ criterion is employed for comparing supersaturated designs from the viewpoint of orthogonality and uniformity, and a lower bound of $E(f_{NOD})$ which can serve as a benchmark of design optimality is obtained. It is shown that the existing $E(s^2)$ and ave χ^2 criteria (for two- and three-level supersaturated designs respectively) are in fact special cases of this criterion. Furthermore, a construction method for mixed-level supersaturated designs is proposed and some properties of the resulting designs are investigated.

Key words: Discrepancy; Hamming distance; Orthogonal array; Supersaturated design; Uniformity; U-type design.

2000 Mathematics Subject Classifications: 62K15, 62K05, 62K99.

1 Introduction

In industrial and scientific experimental settings, scientists are constantly faced with distinguishing between the effects that are caused by particular factors and those that are due to random error. Often, there are a large number of effects to be investigated while the total number of experiments is limited because of excessive costs (e.g., with respect to money or time). With powerful statistical software readily available for data analysis (screening and predicting), there is no doubt that data collection (or design) is the most important part of such problems.

---

*Corresponding author.

As for the design of experiments, there has been increasing interest in the study of *supersaturated designs*. A supersaturated design is essentially a fractional factorial in which the number of potential effects is greater than the number of runs. Satterthwaite (1959) stands as a pioneer and proposed the idea of supersaturated design in random balanced designs. Booth and Cox (1962) first examined this problem systematically. After then, there had been little study on the subject of supersaturated designs until recently (e.g., Lin, 1993), except perhaps the work on the search design (see, Srivastava, 1975). Most studies have focused on two-level supersaturated designs. These two-level designs can be used for screening the factors in linear models. In some situations, however, certain factors have more than two levels. It may be undesirable to reduce the factor levels to two if it would result in severe loss in information. Examples include (a) a categorical factor with three machine types and (b) a continuous factor with three temperature settings. For case (a), the three machine types should all be included in the study for the purpose of screening and comparison. For case (b), if the response depends on the temperature in a non-monotone fashion, choice of two temperature settings may result that the temperature factor could not be screened out, and thus the curvilinear relation would not be explored. In these and other scenarios, multi-level designs may be adopted.

The main purpose of this article is to provide a class of universally optimal mixed-level supersaturated designs. In Section 2, design criteria for comparing supersaturated designs are discussed. Properties of the $E(f_{NOD})$ criterion from the viewpoint of orthogonality and uniformity are presented. Especially, a lower bound of $E(f_{NOD})$ is obtained as a benchmark of design optimality. A construction method for supersaturated design is proposed in Section 3, along with the discussion of properties of the resulting designs. Some designs are tabulated for practical use. Finally, conclusions are provided in Section 4. For the brevity of the main presentation, all proofs are deferred to an Appendix.

2 Design criteria

Some knowledge and related notations are as follows. Throughout this paper, let $X = (x_{ij})$ be an $n \times m$ matrix of a factorial design, x_i be the ith row of X and x^j be the jth column. Rows and columns are identified with the runs and factors respectively. X is called a *U-type design* in the class $\mathscr{U}(n; q_1, \ldots, q_m)$, if it has elements $1, \ldots, q_j$ at x^j such that these q_j elements appear in this column equally often. Here $q_1, \ldots, q_m$ are positive divisors of n. When some q_j's are equal, we denote it by $\mathscr{U}(n; q_1^{k_1} \cdots q_r^{k_r})$ with $\sum_{j=1}^{r} k_j = m$. U-type designs play the key role in the construction of uniform designs (Fang and Hickernell, 1995; Fang et al., 2000). A U-type design is called an *orthogonal array* of strength 2, denoted by $L_n(q_1, \ldots, q_m)$, if any two columns have all of their factor level-combinations appear equally often. In this case, $\sum_{j=1}^{m}(q_j - 1) \leq n - 1$. When $\sum_{j=1}^{m}(q_j - 1) = n - 1$, the design is called *saturated*. When $\sum_{j=1}^{m}(q_j - 1) > n - 1$, orthogonality is not obtainable and the design is called *supersaturated*, denoted by $S(n; q_1, \ldots, q_m)$. It is necessary that no two columns of a supersaturated design are fully aliased, i.e., no column of the design can be obtained from another by permuting levels. The following are some criteria for comparing fractional factorial designs.

2.1 Existing criteria for two- and three-level factorials

For a two-level design X, the two levels are commonly denoted by -1 and 1. Let s_{ij} be the (i,j)-element of $X'X$. The popular $E(s^2)$ criterion, proposed by Booth and Cox (1962), is to minimize $E(s^2) = \sum_{1 \leq i < j \leq m} s_{ij}^2 / \binom{m}{2}$. Its lower bound was obtained by Nguyen (1996). Namely,

$$E(s^2) \geq \frac{n^2(m - n + 1)}{(m - 1)(n - 1)}. \tag{1}$$

For three-level supersaturated designs, Yamada and Lin (1999) defined a measure for dependency between two columns x^i and x^j by

$$\chi^2(x^i, x^j) = \sum_{u,v=1}^{3} \frac{\left(n_{uv}^{(ij)} - n/9\right)^2}{n/9}, \tag{2}$$

where $n_{uv}^{(ij)}$ is the number of (u, v)-pairs in (x^i, x^j), and $n/9$ is just the average frequency of all the nine (u, v)-pairs in (x^i, x^j). Then they defined a criterion for the whole design X by minimizing ave $\chi^2 = \sum_{1 \leq i < j \leq m} \chi^2(x^i, x^j) / \binom{m}{2}$ and also showed a lower bound of

$$\text{ave } \chi^2 \geq \frac{2n(2m - n + 1)}{(m - 1)(n - 1)}. \tag{3}$$

2.2 Discrepancy

The uniformity criterion has gained more popularity in recent years. It has played a crucial role in the construction of space-filling designs for computer experiments (Bates et al., 1996; Fang and Wang, 1994). It has also been shown to be intimately connected to many other design criteria. For example, Fang and Mukerjee (2000) provided an analytic connection between uniformity and aberration in two-level factorial designs. Recently, Liu and Hickernell (2002) and Liu (2002) proposed a kind of discrepancy, called the *discrete discrepancy*, to evaluate the uniformity of factorial designs with equal-level factors. Their results show that orthogonality and uniformity are strongly related to each other and the discrete discrepancy plays an important role in evaluating such equal-level experimental designs. Now we modify the discrete discrepancy to be used as a measure of uniformity of mixed-level designs.

A discrepancy measure of uniformity can be defined by a kernel function. Let $\mathcal{X}$ be a measurable subset of R^m. A kernel function $K(x, w)$ is any real-valued function defined on $\mathcal{X} \times \mathcal{X}$ and is symmetric in its arguments and non-negative definite, i.e.,

$$K(x, w) = K(w, x), \text{ for any } x, w \in \mathcal{X} \quad \text{and} \tag{4}$$

$$\sum_{i,j=1}^{n} a_i a_j K(x_i, x_j) \geq 0, \text{ for any } a_i, a_j \in R, \ x_i, x_j \in \mathcal{X}. \tag{5}$$

Let F_* denote the uniform distribution function over $\mathcal{X}$. For example, if $\mathcal{X} = \{1, \ldots, q\}^s$, then F_* just assigns probability q^{-s} to each member of this

set. Let $P = \{z_1, \ldots, z_n\} \subseteq \mathcal{X}$ be a set of design points and F_n denote the associated empirical distribution, where

$$F_n(x) = \frac{1}{n} \sum_{z \in P} 1_{\{z \leq x\}}.$$

Here $z = (z_1, \ldots, z_m) \leq x = (x_1, \ldots, x_m)$ means that $z_j \leq x_j$ for all j. Then given a kernel function $K(x, w)$, the discrepancy of P (Hickernell, 1999) is defined by

$$D(P; K) = \left\{ \int_{\mathcal{X}^2} K(x, w) d[F_*(x) - F_n(x)] d[F_*(w) - F_n(w)] \right\}^{\frac{1}{2}}$$

$$= \left\{ \int_{\mathcal{X}^2} K(x, w) dF_*(x) dF_*(w) - \frac{2}{n} \sum_{z \in P} \int_{\mathcal{X}} K(x, z) dF_*(x) \right.$$

$$\left. + \frac{1}{n^2} \sum_{z, z' \in P} K(z, z') \right\}^{\frac{1}{2}}. \tag{6}$$

Note that if the kernel $K(\cdot, \cdot)$ and the design region $\mathcal{X}$ are given, $D(P; K)$ depends only on the empirical distribution F_n of P, and measures how far apart F_n is from F_*. It tends to zero when F_n tends to F_*, and equals zero in the extreme case when $F_n = F_*$, such as when P is the full factorial design over $\mathcal{X} = \{1, \ldots, q\}^s$, i.e. each member of $\mathcal{X}$ appears once in P. So for a fixed number of points, n, a design with low-discrepancy is preferred (Fang and Wang, 1994).

For any factorial design $X \in \mathcal{U}(n; q_1, \ldots, q_m)$, $\mathcal{X} = \{1, \ldots, q_1\} \times \cdots \times \{1, \ldots, q_m\}$ comprising all possible level combinations of the m factors, F_* assigns probability $(q_1 \times \cdots \times q_m)^{-1}$ to each member of $\mathcal{X}$. Let

$$K_j(x, w) = \begin{cases} a & \text{if } x = w, \\ b & \text{if } x \neq w, \end{cases} \quad \text{for } x, w \in \{1, \ldots, q_j\}, \quad a > b > 0,$$

and

$$K_d(x, w) = \prod_{j=1}^{m} K_j(x_j, w_j), \quad \text{for any } x, w \in \mathcal{X}. \tag{7}$$

And then $K_d(x, w)$ is a kernel function and satisfies conditions (4) and (5). The corresponding discrete discrepancy can be used for measuring the uniformity of mixed-level design points.

2.3 $E(f_{NOD})$ criterion

For any two design columns x^i and x^j, define

$$f_{NOD}^{ij} = \sum_{u=1}^{q_i} \sum_{v=1}^{q_j} \left(n_{uv}^{(ij)} - \frac{n}{q_i q_j} \right)^2, \tag{8}$$

where $n_{uv}^{(ij)}$ is the number of (u, v)-pairs in (x^i, x^j), and $n/(q_i q_j)$ stands for the average frequency of level-combinations in each pair of columns x^i and x^j. Here, the subscript NOD stands for *non-orthogonality of the design*. A criterion $E(f_{NOD})$ is defined as minimizing

$$E(f_{NOD}) = \sum_{1 \le i < j \le m} f_{NOD}^{ij} \Big/ \binom{m}{2}. \tag{9}$$

It is obvious that $E(f_{NOD}) = 0$ for an orthogonal array. Let $\lambda_{kl} = \sum_{j=1}^{m} 1_{\{x_{kj} = x_{lj}\}}$, where 1_A is the indicator function of A, i.e. λ_{kl} is the number of coincidences between the two rows x_k and x_l. It is obvious that $\lambda_{kk} = m$. Note that the measure $E(f_{NOD})$ is motivated by taking $\theta(x) = x$ and $\phi(x) = x^2$ from the work of Ma, Fang and Liski (2000).

For the $E(f_{NOD})$ criterion, the following theorem gives its expression and lower bound (in terms of λ_{kl}'s).

Theorem 1. *For any design* $X \in \mathcal{U}(n; q_1, \ldots, q_m)$,

$$E(f_{NOD}) = \frac{\sum_{k,l=1, k \ne l}^{n} \lambda_{kl}^2}{m(m-1)} + C(n, q_1, \ldots, q_m) \tag{10}$$

$$\ge \frac{n(\sum_{j=1}^{m} n/q_j - m)^2}{m(m-1)(n-1)} + C(n, q_1, \ldots, q_m), \tag{11}$$

where $C(n, q_1, \ldots, q_m) = \frac{nm}{m-1} - \frac{1}{m(m-1)} \left(\sum_{i=1}^{m} \frac{n^2}{q_i} + \sum_{i,j=1, j \ne i}^{m} \frac{n^2}{q_i q_j} \right)$ *depends on* X *only through* $n, q_1, \ldots, q_m$, *and the lower bound of* $E(f_{NOD})$ *on the right-hand side of (11) can be achieved if and only if* $\lambda = (\sum_{j=1}^{m} n/q_j - m)/(n-1)$ *is a positive integer and all the* $\lambda_{kl}'s$ *for* $k \ne l$ *are equal to* λ.

When all the q_j's are equal to q, the theorem reduces to the following.

Corollary 1. *For any design* $X \in \mathcal{U}(n; q^m)$,

$$E(f_{NOD}) \ge \frac{mn}{(m-1)(n-1)} \left(\frac{n}{q} - 1 \right)^2 + \frac{n}{m-1} \left(m - \frac{n}{q} \right) - \left(\frac{n}{q} \right)^2, \tag{12}$$

and the lower bound of $E(f_{NOD})$ *on the right-hand side of (12) can be achieved if and only if* $\lambda = m(n/q - 1)/(n - 1)$ *is a positive integer and all the* $\lambda_{kl}'s$ *for* $k \ne l$ *are equal to* λ.

Based on Theorem 1 and its corollary, the $E(f_{NOD})$ criterion can be used as a measure of non-orthogonality for constructing supersaturated designs and the lower bound can be used as a benchmark of design optimality. ·

2.4 The connections between $E(f_{NOD})$ *criterion and other criteria*

It is easy to see the $E(s^2)$ and ave χ^2 criteria are in fact special cases of the $E(f_{NOD})$ criterion. Thus we have the following lemma.

Lemma 1. *For any design* $X \in \mathcal{U}(n; q_1, \ldots, q_m)$, *the three design criteria* $E(f_{NOD})$, $E(s^2)$ *and* aveχ^2 *satisfy the following relations:*

$$E(f_{NOD}) = \frac{n}{9} \text{ave } \chi^2, \text{ when } q_i = 3, i = 1, \ldots, m, \text{ and} \tag{13}$$

$$E(f_{NOD}) = \frac{1}{4} E(s^2), \text{ when } q_i = 2, i = 1, \ldots, m, \text{ with two levels } -1 \text{ and } 1. \tag{14}$$

Furthermore, the lower bound of $E(f_{NOD})$ in (11) includes those lower bounds of $E(s^2)$ in (1) and of ave χ^2 in (3) as special cases, and these three forms of lower bounds also satisfy similar relations in (13) and (14).

This lemma indicates a strong justification for using minimizing $E(f_{NOD})$ as a criterion for supersaturated designs. Unlike the $E(s^2)$ and ave χ^2, the $E(f_{NOD})$ can be used for mixed-level designs. However, the lower bound of $E(f_{NOD})$ in (11) may not be obtainable. This happens when $\lambda = (\sum_{j=1}^{m} n/q_j - m)/(n - 1)$ is not a positive integer or when it is a positive integer but some λ_{kl}'s for $k \neq l$ are not equal to this positive integer. In this paper, we only discuss supersaturated designs with $E(f_{NOD})$ achieving its lower bound and call these designs $E(f_{NOD})$-*optimal supersaturated designs* (for two- or three-level supersaturated designs, they are also $E(s^2)$-*optimal* or ave χ^2-*optimal*). The following analytical expression and lower bound of the corresponding discrete discrepancy can be easily derived.

Theorem 2. *For any set of design $X \in \mathcal{U}(n; q_1, \ldots, q_m)$,*

$$D^2(X; K_d) = -\prod_{j=1}^{m}\left[\frac{a + (q_j - 1)b}{q_j}\right] + \frac{a^m}{n} + \frac{b^m}{n^2}\sum_{k,l=1, l\neq k}^{n}\left(\frac{a}{b}\right)^{\lambda_{kl}}, \tag{15}$$

$$\geq -\prod_{j=1}^{m}\left[\frac{a + (q_j - 1)b}{q_j}\right] + \frac{a^m}{n} + \frac{n-1}{n}b^m\left(\frac{a}{b}\right)^{\lambda}, \tag{16}$$

and the lower bound on the right-hand side of (16) can be achieved if and only if $\lambda = (\sum_{j=1}^{m} n/q_j - m)/(n - 1)$ is a positive integer and all the $\lambda_{kl}'s$ for $k \neq l$ are equal to λ. In this case, the design is an $E(f_{NOD})$-optimal design.

We call a design $X \in \mathcal{U}(n; q_1, \ldots, q_m)$ a *uniform design* under $D(X; K_d)$ if its square discrepancy $D^2(X; K_d)$ achieves the lower bound in (16). Theorem 2 leads to the equivalence between $E(f_{NOD})$ optimality and uniformity of any supersaturated design X. If X is $E(f_{NOD})$-optimal, then it is also a uniform design in the sense of $D(X; K_d)$, and vice versa.

Remark 1 Let $H_{kl} = m - \lambda_{kl}$. This is known as the *Hamming distance* between rows x_k and x_l, which is the number of positions where they differ. From Theorems 1 and 2, we know that the non-orthogonality and uniformity of a U-type design is determined by its Hamming distances. If a U-type supersaturated design has equal Hamming distances between its rows, it is both an $E(f_{NOD})$-optimal design and a uniform design in the sense of $D(X; K_d)$ over $\mathcal{U}(n; q_1, \ldots, q_m)$, and this is also true on the contrary. However, when the lower bound of $E(f_{NOD})$ in (11), and thus the lower bound of $D^2(X; K_d)$ in (16), is not obtainable, the Hamming distances can not be all equal. In this case, we seek a design whose Hamming distances distribute as evenly as possible over $\mathcal{U}(n; q_1, \ldots, q_m)$.

Remark 2. The uniformity of $E(s^2)$- and ave χ^2-optimal supersaturated designs can be obtained directly based on Theorems 1 and 2, as special cases of supersaturated designs with equal-level factors.

3 Design construction

In this section we will present a method of constructing $E(f_{NOD})$-optimal mixed-level supersaturated designs and study the properties of the resulting designs.

3.1 Construction method

Many $E(s^2)$-optimal designs have been constructed (for example, Lin, 1993 and 1995; Tang and Wu, 1997; Liu and Zhang, 2000). Yamada and Lin (1999) and Yamada et al. (1999) presented two construction methods for three-level supersaturated designs based on ave χ^2 criterion. It can be verified that only the two designs with 9 runs of Yamada et al. (1999) achieve the lower bound of ave χ^2 (also $E(f_{NOD})$). Recently Fang, Lin and Ma (2000) obtained a new class of multi-level supersaturated designs by collapsing a U-type uniform design to an orthogonal array. Many of their designs are $E(f_{NOD})$-optimal also. The following theorem plays an important role in our construction method of mixed-level supersaturated designs.

Theorem 3. *Suppose X is a saturated orthogonal array $L_n(q^m)$, where*

Case (i) q is a prime power, $n = q^t$, $m = (n-1)/(q-1)$ and $t \geq 2$, or
Case (ii) $q = 2$, $n = 4t$, $m = 4t - 1$ and $t \geq 1$, then the Hamming distances between different rows are equal to q^{t-1} in Case (i) or $2t$ in Case (ii). That is, the design is $E(f_{NOD})$-optimal and the most uniform.

Recall that Lin (1993) provided a method of constructing two-level supersaturated designs of size $(n, m) = (2t, 4t - 2)$ using a half fraction of a Hadamard matrix (HFHM). The Hadamard matrices are saturated orthogonal arrays with parameters satisfying Case (ii) of Theorem 3. Thus the $E(f_{NOD})$ (as well as $E(s^2)$) optimality of the resulted supersaturated designs easily follows from Corollary 1 as the resulting designs have equal Hamming distances from Theorem 3.

We next present a method of constructing $E(f_{NOD})$-optimal mixed-level supersaturated designs from saturated orthogonal arrays with parameters satisfying Case (i) of Theorem 3. Let X be such an orthogonal array $L_n(q^m)$, the construction method can be carried out as follows:

Step 1. Choose a column from X, say the kth column (k), split the total n rows of X into q groups, such that Group i has all the $n/q = q^{t-1}$ level i's in column (k). We call this column (k) the *branching column*.

Step 2. Given p $(2 \leq p < q)$, delete any $q - p$ group (if $q - p = 1$) or groups (if $q - p > 1$) of X, the remaining p groups form a mixed-level supersaturated design $S(pq^{t-1}; p^1 q^{m-1})$ to examine one p-level factor on the branching column and $m - 1$ q-level factors on other columns.

This method can be regarded as an extension of Lin's (1993) HFHM, and we call it *fractions of saturated orthogonal arrays* (FSOA for simplicity). These supersaturated designs are $E(f_{NOD})$-optimal, as will be shown in Theorem 4. Now let us take the $L_{16}(4^5)$ saturated orthogonal array as an illustrative example. Table 1 shows the $L_{16}(4^5)$ design. If we take column (1) as the *branching column*, then the total $n = 16$ rows can be split into $q = 4$ groups,

Table 1. Supersaturated designs derived from $L_{16}(4^5)$ (using 1 as the branching column)

$S(12;3^14^4)$	$S(8;2^14^4)$	Row	1	2	3	4	5
1		1	1	1	1	1	1
2		2	1	2	2	2	2
3		3	1	3	3	3	3
4		4	1	4	4	4	4
5	1	5	2	1	2	3	4
6	2	6	2	2	1	4	3
7	3	7	2	3	4	1	2
8	4	8	2	4	3	2	1
	5	9	3	1	3	4	2
	6	10	3	2	4	3	1
	7	11	3	3	1	2	4
	8	12	3	4	2	1	3
9		13	4	1	4	2	3
10		14	4	2	3	1	4
11		15	4	3	2	4	1
12		16	4	4	1	3	2

i.e., rows 1–4, 5–8, 9–12, and 13–16. Deleting any group causes the remaining rows to form a mixed-level supersaturated design $S(12;3^14^4)$ to examine one 3-level factor and four 4-level factors, i.e., rows 1–8 and 13–16. Deleting any two groups causes the remaining rows to form a mixed-level supersaturated design $S(8;2^14^4)$, to examine one 2-level factor and four 4-level factors (rows 5–12). In Table 1 we give two such designs whose designs are entitled $S(12;3^14^4)$ and $S(8;2^14^4)$ respectively.

3.2 Properties

Section 3.1 presented the construction procedure for mixed-level supersaturated designs. As for which column will be selected as the branching column and which group or groups will be deleted from an $L_n(q^m)$, we have the following theorem which is proved in the Appendix.

Theorem 4. *Let X be a saturated orthogonal array $L_n(q^m)$, where $q > 2$ is a prime power, $n = q^t$, $m = (n - 1)/(q - 1)$ and $t \geq 2$. The mixed-level supersaturated designs $S(pq^{t-1};p^1q^{m-1})$ obtained by the FSOA method are $E(f_{NOD})$-optimal and the $p(2 \leq p < q)$-level factor is orthogonal to those q-level factors, no matter which column is selected as the branching column and which group is (or groups are) deleted. Furthermore, if $t = 2$, the q-level factors of $S(pq;p^1q^q)$ are equally correlated in the meaning of f_{NOD}^{ij}, i.e. all the f_{NOD}^{ij}'s for $j \neq i$ are equal to $pq - p^2$, and $E(f_{NOD}) = p(q - p)(q - 1)/(q + 1)$.*

Based on this theorem, we can construct $E(f_{NOD})$-optimal mixed-level supersaturated designs by the FSOA method from any given saturated orthogonal array $L_n(q^m)$, where q is a prime power, $n = q^t$, $m = (n - 1)/(q - 1)$ and $t \geq 2$ (choosing any branching column and any groups). Especially when $t = 2$, the resulting design $S(pq;p^1q^q)$ has two kinds of f_{NOD}^{ij}'s for $j \neq i$. It is zero when one factor is the $p(2 \leq p < q)$-level, and $pq - p^2$ when

both factors are q-level. Note that the p-level factor is an important one as it is orthogonal to others. When $t > 2$, the values of f_{NOD}^{ij} are somewhat complicated. This case needs further study. We are, however, able to offer the following theorem.

Theorem 5. *Let X be a saturated orthogonal array $L_n(q^m)$, where $q > 2$ is a prime power, $n = q^t$, $m = (n-1)/(q-1)$ and $t \geq 2$. For any mixed-level supersaturated design $S(pq^{t-1}; p^1 q^{m-1})$ obtained by the FSOA method, there are no fully aliased factors.*

Saturated orthogonal arrays are available in many design books. Hedayat, Sloane and Stufken (1999), for example, provided a systematic account of the theory and applications of orthogonal arrays. (A large number of the saturated orthogonal arrays constructed in the book can be found at http://www.research.att.com/~njas/oadir/.) Using saturated orthogonal arrays with parameters satisfying Case (i) of Theorem 3, mixed-level supersaturated designs can be constructed by the FSOA method described earlier. Table 2 gives a list of such designs for $q < 10$ and $t = 2$, with their $E(f_{NOD})$ and f_{NOD}^{ij} values. Also listed are the ratios of f_{NOD}^{ij} to f_{NOD}^{ii}, where $f_{NOD}^{ii} = qp^2 - p^2$ is the maximum of f_{NOD}^{ij}'s only when two q-level factors are fully aliased. The ratio $f_{NOD}^{ij}/f_{NOD}^{ii}$ also measures the non-orthogonality among the q-level factors. Note that this ratio equals 1

Table 2. Mixed-level supersaturated designs $S(pq; p^1 q^q)$ obtained by FSOA for prime power $q < 10$

$n = pq$	q	p	$E(f_{NOD})$	f_{NOD}^{ij}	ratio*
6	3	2	1.00	2	0.2500
8	4	2	2.40	4	0.3333
12	4	3	1.80	3	0.1111
10	5	2	4.00	6	0.3750
15	5	3	4.00	6	0.1667
20	5	4	2.67	4	0.0625
14	7	2	7.50	10	0.4167
21	7	3	9.00	12	0.2222
28	7	4	9.00	12	0.1250
35	7	5	7.50	10	0.0667
42	7	6	4.50	6	0.0278
16	8	2	9.33	12	0.4286
24	8	3	11.67	15	0.2381
32	8	4	12.44	16	0.1429
40	8	5	11.67	15	0.0857
48	8	6	9.33	12	0.0476
56	8	7	5.44	7	0.0204
18	9	2	11.20	14	0.4375
27	9	3	14.40	18	0.2500
36	9	4	16.00	20	0.1562
45	9	5	16.00	20	0.1000
54	9	6	14.40	18	0.0625
63	9	7	11.20	14	0.0357
72	9	8	6.40	8	0.0156

* ratio $= f_{NOD}^{ij}/f_{NOD}^{ii}$

when the two q-level factors are fully aliased and 0 when they are orthogonal to each other. So from the viewpoint of orthogonality, designs with small ratios are preferred. And most designs listed in Table 2 have ratios less than or equal to 0.25, some ratios are even less than 0.1, which means that there are strong nearly-orthogonality among the q-level factors of the corresponding designs. Also note that the $p(2 \leq p < q)$-level factor is orthogonal to those q-level factors. Designs for $q \geq 10$ were not listed because they are of less practical value, although they can be easily constructed by the FSOA method and their corresponding non-orthogonality values can be computed straightforwardly.

4 Conclusions

We have proposed a criterion (the $E(f_{NOD})$ criterion) and a construction method (the FSOA method) for mixed-level supersaturated designs. The mixed-level supersaturated designs constructed here are optimal in terms of the $E(f_{NOD})$ criterion, i.e., they are optimal not only from the viewpoint of minimizing non-orthogonality but also from the viewpoint of space-filling uniformity. In a factorial design, it is necessary that no two columns are fully aliased, as we cannot use two fully aliased columns to accommodate two different factors. In any of the newly constructed supersaturated designs, there are no fully aliased factors and all the factors have desirable nearly-orthogonality among them.

Appendix

Proof of Theorem 1. Let $N_{ij} = (n_{uv}^{(ij)})$. For each column x^j of X, let $Z^j = (z_{ku}^j)$ be an $n \times q_j$ matrix, where

$$z_{ku}^j = \begin{cases} 1, & \text{if } x_{kj} = u, \\ 0, & \text{otherwise,} \end{cases} \quad k = 1,\ldots,n, \quad u = 1,\ldots,q_j, \tag{17}$$

and let $Z = (Z^1,\ldots,Z^m)$. From (17), it can be easily verified that Z satisfies $ZZ' = (\lambda_{kl})$, and

$$Z'Z = \begin{pmatrix} \frac{n}{q_1}I_{q_1} & N_{12} & \cdots & N_{1m} \\ N_{21} & \frac{n}{q_2}I_{q_2} & \cdots & N_{2m} \\ \cdots & \cdots & \cdots & \cdots \\ N_{m1} & N_{m2} & \cdots & \frac{n}{q_m}I_{q_m} \end{pmatrix}.$$

And from the definition of f_{NOD}^{ij},

$$f_{NOD}^{ij} = \sum_{u=1}^{q_i} \sum_{v=1}^{q_j} \left(\left(n_{uv}^{(ij)} \right)^2 - 2n_{uv}^{(ij)} \frac{n}{q_i q_j} + \frac{n^2}{(q_i q_j)^2} \right)$$

$$= \sum_{u=1}^{q_i} \sum_{v=1}^{q_j} \left(n_{uv}^{(ij)} \right)^2 - \frac{n^2}{q_i q_j}$$

$$= \mathrm{tr}(N_{ij} N_{ji}) - \frac{n^2}{q_i q_j}.$$

So

$$E(f_{NOD}) = \sum_{1 \le i < j \le m} \left(\mathrm{tr}(N_{ij} N_{ji}) - \frac{n^2}{q_i q_j} \right) \Big/ \binom{m}{2}$$

$$= \frac{\sum_{i,j=1, j \ne i}^m \mathrm{tr}(N_{ij} N_{ji})}{m(m-1)} - \frac{\sum_{i,j=1, j \ne i}^m n^2/(q_i q_j)}{m(m-1)}$$

$$= \frac{\mathrm{tr}(Z'Z)^2 - \sum_{i=1}^m n^2/q_i}{m(m-1)} - \frac{\sum_{i,j=1, j \ne i}^m n^2/(q_i q_j)}{m(m-1)},$$

as $\mathrm{tr}(Z'Z)^2 = \mathrm{tr}(ZZ')^2 = \sum_{k,l=1}^n \lambda_{kl}^2$ and $\lambda_{kk} = m$, we obtain (10).

For a U-type design, it is obvious that

$$\sum_{l=1, l \ne k}^n \lambda_{kl} = \sum_{j=1}^m n/q_j - m, \quad k = 1, \ldots, n. \tag{18}$$

Then from (10) and the well known arithmetic-geometric means inequality, (11) holds under constraint (18), and because λ_{kl}'s are integers, the lowerbound of $E(f_{NOD})$ on the right hand side of (11) can be achieved ifand only if λ is a positive integer and all the λ_{kl}'s for $k \ne l$ are equal to λ. ∎

Proof of Theorem 2 (15) just from the definition of discrepancy $D(X; K)$ (6) and

$$K_d(x_k, x_l) = \prod_{x_{ki} = x_{li}} K_i(x_{ki}, x_{li}) \prod_{x_{ki} \ne x_{li}} K_i(x_{ki}, x_{li})$$

$$= a^{\lambda_{kl}} b^{m - \lambda_{kl}} = b^m \left(\frac{a}{b} \right)^{\lambda_{kl}},$$

where x_k and x_l are two rows and $\lambda_{kk} = m$. The proof of (16) is similar to that of (11) and the last conclusion just follows from Theorem 1. ∎

Proof of Theorem 3 As for the existence of such orthogonal arrays, please see Hedayat, Sloane and Stufken (1999, Theorems 3.20 and 7.5).

Case (i) From the definition of orthogonal array, $E(f_{NOD}) = 0$. On the other hand, if we substitute the parameters in this theorem into the lower bound of $E(f_{NOD})$ in (12), note that all the q_j's, $j = 1, \ldots, m$, are equal to q here, the lower bound is just equal to zero, that means X is $E(f_{NOD})$-optimal. So from Corollary 3, all the λ_{kl}'s for $k \ne l$ are equal to $m(n/q - 1)/(n - 1) =$

$(q^{t-1} - 1)/(q - 1)$. As $H_{kl} = m - \lambda_{kl}$, then we know all the Hamming distances between different rows are equal to q^{t-1}.

Case (ii) The proof is similar to Case (i), we omit the details.   ■

Proof of Theorem 4. From Theorem 3, X has equal Hamming distances between different rows, so deleting rows doesn't change the Hamming distances between the remaining rows. After deleting any group or groups according to any branching column, the resulting mixed-level design is still a U-type design, so its $E(f_{NOD})$-optimality just follows from Theorem 1. The orthogonality between the p-level factor and other q-level factors can be easily obtained from that of the original array.

If $t = 2$, for any two factors there are q^2 level-combinations each occurring once in the original array. In the mixed-level supersaturated design $S(pq; p^1 q^q)$ derived from FSOA, for any two q-level factors, there are pq level-combinations each occurring once and other $q^2 - pq$ level-combinations don't occur. We can compute all the f_{NOD}^{ij}'s for $j \neq i$ from (8), which are equal to $pq - p^2$, the $E(f_{NOD})$ value can be calculated either from its definition (9) or from the lower bound in (11) which are the same one.   ■

Proof of Theorem 5. We only need to consider the q-level factors. Suppose there are two fully aliased factors, $\hat{x}^i$ and $\hat{x}^j$ (say), then there are only q level-combinations each occurring pq^{t-2} times, the other $q^2 - q$ level-combinations don't occur. As there are q^2 level-combinations in the original factors x^i and x^j which are orthogonal to each other, the other $q^2 - q$ level-combinations must appear pq^{t-2} times also in the deleted group or groups. Therefore, we know there are altogether $q^2 \times pq^{t-2} = pq^t$ rows in the original array, which contradicts the assumption that there are only q^t rows, as $p \geq 2$.   ■

References

1. Bates RA, Buck RJ, Riccomagno E, Wynn HP (1996) Experimental design and observation for large systems. J R Statist Soc B 58:77–94
2. Booth KHV, Cox DR (1962) Some systematic supersaturated designs. Technometrics 4:489–495
3. Fang KT, Hickernell FJ (1995) The uniform design and its applications. Bull Inst Internat Statist, 50th Session, Book 1, 333–349
4. Fang KT, Lin DKJ, Winker P, Zhang Y (2000) Uniform design: theory and applications. Technometrics 42:237–248
5. Fang KT, Lin DKJ, Ma CX (2000) On the construction of multi-level supersaturated designs. J Statist Plann Inference 86:239–252
6. Fang KT, Mukerjee R (2000) A connection between uniformity and aberration in regular fractions of two-level factorials. Biometrika 87:193–198
7. Fang KT, Wang Y (1994) Number-theoretic methods in statistics. Chapman and Hall, London
8. Hedayat AS, Sloane NJA, Stufken J (1999) Orthogonal arrays: theory and applications. Springer, New York
9. Hickernell FJ (1999) Goodness-of-fit statistics, discrepancies and robust designs. Statist Probab Lett 44:73–78
10. Lin DKJ (1993) A new class of supersaturated designs. Technometrics 35:28–31
11. Lin DKJ (1995) Generating systematic supersaturated designs. Technometrics 37:213–225

12. Liu MQ (2002) Using discrepancy to evaluate fractional factorial designs. In: eds, Fang KT, Hickernell FJ, Niederreiter H, Monte Carlo and Quasi-Monte Carlo Methods 2000, Springer-Verlag, 357–368

13. Liu MQ, Hickernell FJ (2002) $E(s^2)$-optimality and minimum discrepancy in 2-level supersaturated designs. Statist Sinica, 12(3), 931–939

14. Liu MQ, Zhang RC (2000) Construction of $E(s^2)$ optimal supersaturated designs using cyclic BIBDs. J Statist Plann Inference 91:139–150

15. Ma CX, Fang KT, Liski E (2000) A new approach in constructing orthogonal and nearly orthogonal arrays. Metrika 50:255–268

16. Nguyen NK (1996) An algorithmic approach to constructing supersaturated designs. Technometrics 38:69–73

17. Satterthwaite F (1959) Random balance experimentation (with discussion). Technometrics 1:111–137

18. Srivastava JN (1975) Design for searching non-negligible effects. In: Srivastava JN (ed), Survey of Statistical design and Linear Models, North-Holland, Amsterdam

19. Tang B, Wu CFJ (1997) A method for constructing supersaturated designs and its $E(s^2)$ optimality. Canad J Statist 25:191–201

20. Yamada S, Ikebe YT, Hashiguchi H, Niki N (1999) Construction of three-level supersaturated design. J Statist Plann Inference 81:183–193

21. Yamada S, Lin DKJ (1999) Three-level supersaturated designs. Statist Probab Lett 45:31–39