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A Note on Saturated First-Order Design with Foldover Structure

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A first-order saturated design is the smallest design resulting in unbiased estimates for all main effects. It could be misleading in the presence of interaction effects. This article provides a simple class of first-order saturated designs in which specific two-factor interactions are orthogonal to many of the main effects, while keeping rather high design efficiencies.

Keywords: D-optimal design; Foldover; Interaction effects; Main effect; Saturated design.

1. Introduction

Consider the first-order model of k variables in n runs,

$$\mathbf{y} = \beta_0\mathbf{1} + \beta_1\mathbf{x_1} + \ldots + \beta_k\mathbf{x_k} + \epsilon = X\beta + \epsilon,$$

where $\mathbf{y}$ is an $n \times 1$ vector of observations, $\mathbf{1}$ is an $n \times 1$ vector whose entries are all ones, $\mathbf{x_i}$ is an $n \times 1$ vector for the ith factor, β is the $(k+1) \times 1$ vector of coefficients to be estimated, and ϵ is the noise vector. When $n = k + 1$, the design matrix X is a $(k+1) \times (k+1)$ square matrix. This is the smallest design possible to estimate all β_i's; such a design is called a saturated (first-order) design. This is especially popular when the experimental costs are high. Construction of saturated design has received a great deal of attention in the literature. One main concern for a saturated design is that its estimates for the β_i's may be misleading in the presence of two-factor interactions.

This article proposes a new class of saturated (first-order) design in which specific two-factor interactions are orthogonal to as many main effects. It can be shown that the proposed designs are as near efficient as the optimal (D-optimal, say) design, but main effects are orthogonal to some two-factor interactions. For simplicity of presentation, all proofs are given in Appendix A.

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2. Proposed Design

Consider a two-level design matrix X of the form

$$X = \begin{pmatrix} X_1 & X_2 \\ X_1 & -X_2 \end{pmatrix}$$

where X_1 is an $(n/2) \times k_1$ matrix whose entries in the first column are all ones, X_2 is $(n/2) \times k_2$ matrix, and $k_1 + k_2 = n$, n is even. Divide the factors into two groups A and B. Factors in Group A follow the design of $\begin{pmatrix} X_1 \\ X_1 \end{pmatrix}$, while factors in Group B follow the design of $\begin{pmatrix} X_2 \\ -X_2 \end{pmatrix}$. It is obvious that all factors in Group B keep the foldover property, namely, all main effects are orthogonal to their two-factor interactions (see, e.g., Li and Lin 2003). Furthermore, we have the following property.

Property 1:

1. All main effects of x_i and x_j are orthogonal, for all x_i in Group A and x_j in Group B.
2. All two-factor interactions $x_i x_j$ are orthogonal to main effect x_k, for
   (a) all x_i and x_j in Group A, and x_k in Group B;
   (b) all x_i and x_j in Group B, and x_k in Group B;
   (c) all x_i in Group B, and x_j and x_k in Group A.

In short, all main effects in Group A are orthogonal to all main effects in Group B. If X_1 and X_2 are both orthogonal designs, X will be an orthogonal design. All main effects in Group B are orthogonal to two-factor interactions within Group B and within Group A, while all main effects in Group A are orthogonal to all two factor interactions with one factor in Group A and the other in Group B. Such a design will be rather robust against potential interaction effects (a nice property by foldover), but with only half the run size required of a full foldover. It is thus desirable to have as many design columns in Group B as possible. Property 2 given next, however, indicates that the maximal number of columns possible in Group B is $k_2 = n/2$ for the design matrix to be nonsingular.

Property 2: If X is full rank, then $k_1 = k_2 = n/2$.

Without loss of generality, each design column is coded ± 1 for high and low levels. Take D-optimality as an example, which maximizes the determinant of the $X'X$ matrix, $\| X'X \|$. Other optimalities can be used as well. It can be shown that:

Property 3: $\| X'X \| = 2^n \times \| X_1' X_1 \| \times \| X_2' X_2 \|$.

With Property 3 in mind, it is natural to employ D-optimal design of size $(n/2)$ for both X_1 and X_2 matrices. These D-optimal saturated designs are available in the literature, especially for small n (see, e.g., http://www.indiana edu/maxdet).

Take $n = 6$ as an example; $n/2$ is 3 and a D-optimal 3×3 saturated design is known to be

$$X_1 = X_2 = \begin{pmatrix} 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}.$$

Therefore, the proposed saturated design for five factors is

$$X = \begin{pmatrix} X_1 & X_2 \\ X_1 & -X_2 \end{pmatrix} = \begin{array}{c} \begin{array}{cccccc} I & x_1 & x_2 & x_3 & x_4 & x_5 \end{array} \\ \begin{pmatrix} 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & 1 \end{pmatrix} \end{array}.$$

The design matrix has the following properties:

1. Main effects of factors x_1, x_2 are orthogonal to main effects of factors x_3, x_4, x_5.
2. Main effects of factors x_1, x_2 are orthogonal to two-factor interactions of $x_1x_3, x_1x_4, x_1x_5, x_2x_3, x_2x_4, x_2x_5$.
3. Main effects of factors x_3, x_4, x_5 are orthogonal to two-factor interactions of $x_1x_2, x_3x_4, x_3x_5, x_4x_5$.
4. $\| X'X \| = 2^{14}$.

If a 6×6 D-optimal design is used, its determinant is $\| X'X \| = 5^2 \times 2^{10}$. In terms of d-efficiency (as explained later) the proposed design has 92.8% d-efficiency. However, none of main effects for the D-optimal design are orthogonal to any two-factor interactions (except the trivial cases that interaction x_ix_j is always orthogonal to main effects x_i and x_j).

Table 1 displays the comparisons of d-efficiencies between the $n \times n$ D-optimal designs and the proposed saturated designs, for $2 \le n \le 60$. Define (see, e.g., Lin 1993) d-efficiency $= \| X'X \|^{1/n} /n$, and the relative ratio RR is defined as

$$RR = \frac{\text{d-eff}_P}{\text{d-eff}_D},$$

where d-eff$_P$ and d-eff$_D$ are the d-efficiencies for the proposed design and the D-optimal design, respectively.

From Table 1, it is obvious that the loss of d-efficiency is rather limited—the relative ratio is between 90.5% and 100%. However, the proposed design is robust to many (although not all) interaction effects. The same observation can be made for larger designs. Comparisons for $62 \le n \le 120$ are given in Appendix B. It is interesting to note that the proposed design for $n = 94$ results in a higher d-efficiency than the published D-optimal design (see, e.g., Koukouvinos et al. 2000).

To use these newly proposed designs in practice, the experimenter should group all factors into two groups, such that potential two-factor interactions only occur within each group, but not between groups. Then assign sensitive factors to Group B.

3. Final Remarks

As pointed out by one referee, "Clearly for any saturated first-order design every 2-factor interaction must be confounded (partially or completely) with at least one main effect." With foldover structure, the proposed designs allows some specific two-factor interactions to be orthogonal to as many main effects as possible. The general property is described in Property 1 for practical uses.

Table 1
Comparisons of d-efficiencies between D-optimal design and the proposed design

n	d-eff$_D$(%)	d-eff$_P$(%)	RR(%)*	n	d-eff$_D$(%)	d-eff$_P$(%)	RR(%)*
2	100	100	100	32	100	100	100
4	100	100	100	34	98.0†	96.6	98.6
6	90.5	84.0	92.8	36	100	96.7	96.7
8	100	100	100	38	98.4	95.4	97.0
10	94.1	94.1	100	40	100	100	100
12	100	90.5	90.5	42	98.6	97.6	99.0
14	95.7	87.8	91.7	44	100	96.8	96.8
16	100	100	100	46	98.7	95.8	97.1
18	96.7	93.2	96.4	48	100	100	100
20	100	94.1	94.1	50	98.8	98.8	100
22	96.8†	91.5	94.5	52	100	97.7	97.7
24	100	100	100	54	98.9	96.7	97.8
26	97.7	97.7	100	56	100	100	100
28	100	95.7	95.7	58	98.7†	98.0	99.3
30	98.0	94.1	96.0	60	100	98.0	98.0

*$RR =$ d-eff$_P$/d-eff$_D$, where d-eff$_P$ and d-eff$_D$ are the d-efficiencies for the proposed design and the D-optimal design, respectively.

†These designs are believed to be D-optimal, but have not been proved to be so.

If A-optimality is preferable (rather than the D-optimality), it can be shown that Property 4 holds:

Property 4: $tr(X'X) = 2tr(X_1'X_1) + 2tr(X_2'X_2)$.

Thus, to obtain the largest $tr(X'X)$, an A-optimal design should be employed for X_1 and X_2. Other optimalities can be investigated in a similar manner. Other criteria can be evaluated as well. For example, if average squared correlation (Miller and Sitter 2005) is considered, it can be shown that the proposed designs perform well in general.

Furthermore, a more general class is design of the form

$$X = \begin{pmatrix} X_1 & X_2 \\ X_3 & -X_2 \end{pmatrix},$$

where $X_1 \neq X_3$. Since

$$X'X = \begin{pmatrix} X_1' & X_3' \\ X_2' & -X_2' \end{pmatrix} \times \begin{pmatrix} X_1 & X_2 \\ X_3 & -X_2 \end{pmatrix} = \begin{pmatrix} X_1'X_1 + X_3'X_3 & X_1'X_2 - X_3'X_2 \\ X_2'X_1 - X_2'X_3 & 2X_2'X_2 \end{pmatrix},$$

thus, if $X_1'X_2 - X_3'X_2 = 0$, then main effects of factors in Group A will be orthogonal to main effects of factors in Group B. This deserves further investigation.

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Appendix A: Proofs for All Properties

Proof of Property 1

1. Since factor x_i is from Group A and factor x_j from Group B, the corresponding columns are $(x_{1i}, x_{2i}, \ldots, x_{n/2i}, x_{1i}, x_{2i}, \ldots, x_{n/2i})'$ and $(x_{1j}, x_{2j}, \ldots, x_{n/2j}, -x_{1j}, -x_{2j}, \ldots, -x_{n/2j})'$, respectively. The inner product of the two vectors is $\sum_{m=1}^{n/2} x_{mi} \times x_{mj} + \sum_{m=1}^{n/2} x_{mi} \times (-x_{mj}) = 0$.
2. (a) The interaction of two factors is $(x_{1i} \times x_{1j}, x_{2i} \times x_{2j}, \ldots, x_{n/2i} \times x_{n/2j}, x_{1i} \times x_{1j}, x_{2i} \times x_{2j}, \ldots, x_{n/2i} \times x_{n/2j})'$; then the inner product of the main effect of factor x_k and this interaction is $\sum_{m=1}^{n/2} x_{mi} \times x_{mj} \times x_{mk} + \sum_{m=1}^{n/2} x_{mi} \times x_{mj} \times (-x_{mk}) = 0$.

(b) The interaction of two factors is $(x_{1i} \times x_{1j}, x_{2i} \times x_{2j}, \ldots, x_{n/2i} \times x_{n/2j}, (-x_{1i}) \times (-x_{1j}), (-x_{2i}) \times (-x_{2j}), \ldots, (-x_{n/2i}) \times (-x_{n/2j}))'$; then the inner product of the main effect of factor x_k and this interaction is $\sum_{m=1}^{n/2} x_{mi} \times x_{mj} \times x_{mk} + \sum_{m=1}^{n/2} (-x_{mi}) \times (-x_{mj}) \times (-x_{mk}) = 0$.

(c) The two-factor interaction is $(x_{1i} \times x_{1j}, x_{2i} \times x_{2j}, \ldots, x_{n/2i} \times x_{n/2j}, (-x_{1i}) \times x_{1j}, (-x_{2i}) \times x_{2j}, \ldots, (-x_{n/2i}) \times x_{n/2j})'$. Then the inner product of the main effect of factor x_k and this interaction is $\sum_{m=1}^{n/2} x_{mi} \times x_{mj} \times x_{mk} + \sum_{m=1}^{n/2} (-x_{mi}) \times x_{mj} \times x_{mk} = 0$.

Proof of Property 2

For any square matrix, if X is full rank, then X must be full rank of its columns. Thus

$$rank \begin{pmatrix} X_2 \\ -X_2 \end{pmatrix} = k_2,$$

where X_2 is an $(n/2) \times k_2$ matrix. For an $(n/2) \times 1$ vector with elements $\pm$, the largest number of linear independent vectors is $n/2$.

If $k_2 > n/2$, there exists a set of k_2 scalars, $\alpha_1, \alpha_2, \ldots, \alpha_{k_2}$, not all zeros, such that

$$\alpha_1 \mathbf{x_{21}} + \alpha_2 \mathbf{x_{22}} + \ldots + \alpha_{k_2} \mathbf{x_{2k_2}} = 0$$

where $\mathbf{x_{2i}}$ denotes the ith column vector of X_2, $i = 1, 2, \ldots, k_2$. Then we have

$$\alpha_1 \begin{pmatrix} \mathbf{x_{21}} \\ -\mathbf{x_{21}} \end{pmatrix} + \alpha_2 \begin{pmatrix} \mathbf{x_{22}} \\ -\mathbf{x_{22}} \end{pmatrix} + \ldots + \alpha_{k_2} \begin{pmatrix} \mathbf{x_{2k_2}} \\ -\mathbf{x_{2k_2}} \end{pmatrix} = 0.$$

This implies that

$$rank \begin{pmatrix} X_2 \\ -X_2 \end{pmatrix} < k_2,$$

which conflicts the proposition that

$$rank \begin{pmatrix} X_2 \\ -X_2 \end{pmatrix} = k_2.$$

Thus, k_2 must be $\leq n/2$. Applying the same argument to X_1, we have $k_1 \leq n/2$. Since $k_1 + k_2 = n$, thus the claim of $k_1 = k_2 = n/2$.

Proof of Property 3

$$X'X = \begin{pmatrix} X_1' & X_1' \\ X_2' & -X_2' \end{pmatrix} \times \begin{pmatrix} X_1 & X_2 \\ X_1 & -X_2 \end{pmatrix} = \begin{pmatrix} 2X_1'X_1 & 0 \\ 0 & 2X_2'X_2 \end{pmatrix}$$

Therefore,

$$\| X'X \| = \left\| \begin{matrix} 2X_1'X_1 & 0 \\ 0 & 2X_2'X_2 \end{matrix} \right\| = 2^n \times \| X_1'X_1 \| \times \| X_2'X_2 \| .$$

Proof of Property 4

Assume λ is an eigenvalue of $X'X$, we have $\| \lambda I_{n\times n} - X'X \| = 0$. Now,

$$\begin{aligned} \| \lambda I_{n\times n} - X'X \| &= \left\| \begin{pmatrix} \lambda I_{n/2\times n/2} & 0 \\ 0 & \lambda I_{n/2\times n/2} \end{pmatrix} - \begin{pmatrix} 2X_1'X_1 & 0 \\ 0 & 2X_2'X_2 \end{pmatrix} \right\| \\ &= \left\| \begin{matrix} \lambda I_{n/2\times n/2} - 2X_1'X_1 & 0 \\ 0 & \lambda I_{n/2\times n/2} - 2X_2'X_2 \end{matrix} \right\| \\ &= \left\| \lambda I_{n/2\times n/2} - 2X_1'X_1 \right\| \times \left\| \lambda I_{n/2\times n/2} - 2X_2'X_2 \right\| . \end{aligned}$$

Thus, $\| \lambda I_{n/2\times n/2} - 2X_1'X_1 \| \times \| \lambda I_{n/2\times n/2} - 2X_2'X_2 \| = 0$. This implies that (a) $\lambda/2$ is an eigenvalue of either $X_1'X_1$ or $X_2'X_2$ and (b) if $\lambda/2$ is an eigenvalue of $X_1'X_1$ or $X_2'X_2$, then λ is an eigenvalue of $X'X$. So we have

$$tr(X'X) = 2tr(X_1'X_1) + 2tr(X_2'X_2).$$

Appendix B: Comparisons of d-efficiencies between D-optimal design and the proposed design (for $62 \le n \le 120$, as a supplement to Table 2.1)

Table 2

Comparisons of d-efficiencies between D-optimal design and the proposed design (for $62 \le n \le 120$)

n	d-eff$_D$(%)	d-eff$_P$(%)	RR(%)*	n	d-eff$_D$(%)	d-eff$_P$(%)	RR(%)*
62	99.1	97.0	97.9	92	100	98.7	98.7
64	100	100	100	94	94.1†	97.9	104‡
66	99.1	98.1	99.0	96	100	100	100
68	100	98.0	98.0	98	99.4	98.5	99.1
70	98.0†	96.8	98.8	100	100	98.8	98.8
72	100	100	100	102	99.4	97.7	98.3
74	99.2	98.8	99.6	104	100	100	100
76	100	98.4	98.4	106	99.4†	98.5	99.1
78	99.1†	97.4	98.3	108	100	98.9	98.9
80	100	100	100	110	99.4	97.9	98.5
82	99.3	99.3	100	112	100	100	100
84	100	98.6	98.6	114	99.5	99.1	99.6
86	99.3	97.4	98.1	116	100	98.7	98.7
88	100	100	100	118	99.5	98.5	99.0
90	99.3	98.3	99.0	120	100	100	100

* $RR = \text{d-eff}_P/\text{d-eff}_D$, where d-eff$_P$ and d-eff$_D$ are the d-efficiencies for the proposed design and the D-optimal design, respectively.

†These designs are believed to be D-optimal, but have not been proved to be so.

‡The proposed design for $n = 94$ is shown to have a higher d-efficiency than the published D-optimal design (see, for example, Koukouvinos, Mitrouli and Seberry (2000)).