

An Algorithmic Approach to Constructing Supersaturated Designs

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Supersaturated designs are very cost-effective to scientists and engineers at the primary stage of scientific investigation. This article describes a method of constructing supersaturated designs from balanced incomplete block designs that is a generalization of the method of Lin for constructing these designs and a more general approach to constructing these designs.

KEY WORDS: Computer-aided designs; Cyclic incomplete block designs; Interchange algorithm; Near-orthogonal array; Saturated designs; Screening designs.

Because the main objective of a screening experiment is to identify a few significant factors for further studies, scientists and engineers require designs with the minimum number of runs. Many *saturated* designs (designs with the number of factors m equal to $n - 1$, where n is the number of runs) have proved useful for this purpose. There are situations, however, in which scientists and engineers cannot even afford the number of runs required for these designs.

Consider an example in which a car manufacturer is conducting a passenger-impact crash test on a planned new four-wheel-drive (4WD) range. The objective is to find a subset of 54 safety features such as modified airbags, bull-bar, bonded windscreen, (twin front) crush cans, and so forth to be included in the new car's total safety system. A suitable design for this test is a Hadamard matrix of order 56 that requires 56 runs (car prototypes). The question is what type of design is to be used when the research and development of the car manufacturer allows at most half of the number of required cars for this test.

Designs suitable for this example are called supersaturated designs. These designs were introduced by Booth and Cox (1962) and were recently studied further by Lin (1993a) and Wu (1993) (see also Satterthwaite 1959). These designs are very cost-effective with respect to the number of runs and as such are highly desirable in the context of industrial experimentation. This article describes a method of constructing supersaturated designs from balanced incomplete block designs (BIBD's), and a more general approach to constructing these designs.

1. CRITERIA FOR COMPARING SUPERSATURATED DESIGNS

Let X be an $n \times m$ design matrix of a design with n runs (rows) and m two-level factors (columns) each with $\frac{1}{2}n$ of +1's or high-level values and $\frac{1}{2}n$ of -1's or low-level values ($m \geq n - 1$). Let s_{ij} be the element in the i th row and j th column of $X'X$. Booth and Cox (1962) proposed as a criterion for comparing designs the minimization of $\text{ave}(s^2)$,

where $\text{ave}(s^2) = \sum_{i < j} s_{ij}^2 / \binom{m}{2}$. Clearly for orthogonal designs $\text{ave}(s^2) = 0$.

The rationale of the Booth-Cox criterion can be explained by using the singular value decomposition to decompose X as $U\Lambda^{1/2}V'$, where matrices U and V are orthogonal and Λ is diagonal. It can then be shown that $X'X$ and XX' share the same set of nonzero eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_r$, where $r = \text{rank}(X'X) = \text{rank}(XX')$. Moreover, $\text{tr}(X'X) = \text{tr}(XX') = \sum \lambda_i = mn = \text{const.}$ and $\text{tr}((X'X)^2) = \text{tr}((XX')^2) = \sum \lambda_i^2$. Thus minimizing $\sum_{i < j} s_{ij}^2$, which is equivalent to minimizing $\text{tr}((X'X)^2)$, is the same as making the λ_i 's as equal as possible with $\sum \lambda_i = \text{const.}$ This in a sense is an approximation of the A -optimality criterion, which requires the minimization of $\sum \lambda_i^{-1}$, or the D -optimality criterion, which requires the maximization of $\prod \lambda_i$ (see Kiefer 1959).

Because the sum of each column of X is 0, the sum of the elements of XX' is 0—that is, the sum of the off-diagonal elements of XX' equal to $-nm$ (nm is the sum of the diagonal elements of XX'). Thus, the sum of squares of the elements of XX' (and $X'X$) will reach the minimum if XX' is of the form $(m - x)I_n + xJ_n$, where $x = -m/(n - 1)$ [assuming that m is divisible by $(n - 1)$], I_n is the identity matrix, and J_n is the $n \times n$ matrix of 1's. In this case $\text{ave}(s^2) = n(m^2 + (n - 1)x^2 - mn)/(m(m - 1)) = n^2(m - n + 1)/((n - 1)(m - 1))$. This quantity can be used as a *lower bound* for $\text{ave}(s^2)$ when m is divisible by $n - 1$. Note that for $m = n - 1$ this quantity becomes 0, and for $m = 2(n - 1)$ this quantity becomes $n^2/(2n - 3)$.

Another reasonable criterion for comparing supersaturated designs is to minimize the frequency of $s_{ij} = \pm s_{\max}$, where $s_{\max} = \max |s_{ij}|$. This criterion and the $\text{ave}(s^2)$ criterion typically agree on which of the two designs is better. There are, however, examples that show that these two cri-

Table 1. Generating Vectors of BIBD-Based Supersaturated Designs of Size $(n, m) = (2t, 4t - 2)$, $3 \leq t \leq 15$

t	n	m	Generating vectors
3	6	10	(+ - - - +) (- + - + -)
4*	8	14	(- + + - - - +) (- + + - + - -)
5	10	18	(+ + - + - - - + -) (- + + + - - - - -)
6	12	22	(- + + + - - + - - +) (+ - - - - + + - + - +)
7	14	26	(- + + + - + + - - - -) (+ + - + - - + - + - - +)
8*	16	30	(+ - + + + + - - + - - - + -) (- + - - + + - + - - - + + -)
9	18	34	(- - - + - + + - + - + + - -) (+ + - - + + - - - + - - + +)
10*	20	38	(- + + - + + + - - - - + - - - +) (- + - + + - - - - + + + - - - +)
11	22	42	(+ + + + - + - - - - + + - - - +) (- + + - - + + - - - + + + - - - +)
12	24	46	(+ + - - + + - + - - - - + + + - - -) (- + - + - - - - + - - - + + + - - + +)
13*	26	50	(- + + + + - - + - + + + - - + + - - -) (- + - - - + + + + - - + + - - - + + - -)
14*	28	54	(- - + + + - - + - - + - + + - - + - - - +) (+ - - - + + - - - - - + + - + + - - - + +)
15	30	58	(+ + - - - + - - - - + - + + + + - - + + - - - +) (+ - - - + - - + - + + - - + + - + - - - + + -)

* t value associated with new design.

4. Different generating arrays (obtained from different cyclic BIBD's) might result in designs with the same $\text{ave}(s^2)$ but different s_{\max} . For example, for $(n, m) = (26, 50)$, the s_{\max} of BIBD-based designs can be 6, 8, 10, and so forth.

3. A GENERAL ALGORITHM

A supersaturated design can be considered as a near-orthogonal array (NOA) with columns at two levels (Nguyen in press). Before describing the NOA algorithm, I will present some matrix results. Without loss of generality, let the i th and u th rows of X be two row vectors of the form $(+1 \mathbf{i}')$ and $(-1 \mathbf{u}')$, where \mathbf{i}' and \mathbf{u}' are two $1 \times (m - 1)$ row vectors. It is not difficult to show that the effect on $X'X$ obtained by swapping of the signs of the first elements of these two rows of X is the same as adding the following matrix to the $X'X$ matrix:

$$\left(\begin{array}{c|c} 0 & 2(\mathbf{u}' - \mathbf{i}') \\ \hline 2(\mathbf{u} - \mathbf{i}) & \mathbf{0}_{m-1} \end{array} \right), \quad (1)$$

where $\mathbf{0}_{m-1}$ is the $(m - 1) \times (m - 1)$ matrix of 0's.

The NOA algorithm based on the preceding matrix results has two steps:

1. Construct a *starting* design by allocating randomly half of the entries of each column of X to +1 and half to -1. Form $X'X$ and calculate $f = \sum_{i < j} s_{ij}^2$.
2. For column j of X ($j = 1, 2, \dots, m$) repeat searching a pair of i th and u th elements having different signs in this column such that the swap of these two elements will result in the biggest reduction in f . If the search is successful, update f , X , and $X'X$ using (1). If f cannot be reduced further, go to the next column.

Step 2 is repeated until $f = 0$ or f reaches its lower bound (when m is divisible by $n - 1$) or f cannot be reduced by any further sign-swaps.

The NOA algorithm is a typical example of an *inter-change* algorithm. Other examples of this type of algorithm in different design settings were discussed by Nguyen and Williams (1993) and Nguyen (1994). The algorithms of Booth and Cox (1962) and Lin (1995) for constructing supersaturated designs and of Lin (1993b) for constructing saturated designs are examples of *exchange* algorithms (see Nguyen and Miller 1992). In this class of algorithms, a column of X is replaced by an entirely new column from the candidate list.

Remarks

1. Because $X'X$ is symmetric, the NOA algorithm only needs to work with the upper diagonal elements.
2. To calculate the change in f and update f in Step 2, note that only the nonzero elements of the vector $2(u' - i')$ will affect the increase (or decrease) of a corresponding element of $X'X$.
3. Among several designs generated by the NOA algorithm with same f [or $\text{ave}(s^2)$] but with different s_{\max} 's, the one with the smallest s_{\max} is chosen.
4. To replace the $\text{ave}(s^2)$ criterion by the s_{\max} criterion, f in the preceding algorithm is replaced by $f_{s_{\max}}$, the frequency of $s_{ij} = \pm s_{\max}$.

4. COMPARISON WITH OTHER DESIGNS

For designs with $(n, m) = (2t, 4t - 2)$ and $t = 3, 5, 6, 7, 9, 11, 12$, and 15 , the HFHM-based supersaturated designs of Lin (1993a) and my BIBD-based designs have the same value of $\text{ave}(s^2)$ and r_{\max} (the maximum correlation in terms of the absolute value between two columns of X calculated as s_{\max}/n). For $t = 4, 8, 10, 13$, and 14 , my BIBD-based designs are new. These designs were obtained from the generating vectors in Table 1. They are $\text{ave}(s^2)$ optimal (Table 2). As mentioned in Section 2, deleting a column of these designs does not change $\text{ave}(s^2)$. The design for $(n, m) = (26, 49)$ in Table 2 was obtained by deleting a column of a design for $(n, m) = (26, 50)$ (see Remark 3 of Sec. 2). This design has the same $\text{ave}(s^2)$ as the corresponding design of Lin (1993a) but has a smaller r_{\max} than Lin's.

Designs for $(n, m) = (12, 16)$, $(12, 18)$, $(12, 24)$, $(18, 24)$, $(18, 30)$, $(18, 36)$, and $(24, 30)$ in Table 2 were constructed by the NOA algorithm. The design for $(n, m) = (24, 30)$ is design (A) in Section 1. An alternative design [design (B) in Sec. 1], obtained by the s_{\max} criterion, has $\text{ave}(s^2) = 8.72$

Table 2. Comparison of Selected Designs in Terms of $\text{ave}(s^2)$
(the smaller the better)

n	m	Booth & Cox	Lin	Wu	Nguyen	r_{\max}^b
12	22	—	6.86	7.40	6.86 ^a	.333
	16	7.06	6.27	6.00	5.20	.333
	18	9.68	6.59	6.59	5.96	.333
	24	10.26	—	8.17	7.83	.333
18	34	—	9.82	—	9.82 ^a	.333
	24	13.04	9.22	—	7.13	.333
	30	15.34	9.74	—	9.37	.333
	36	16.44	—	—	10.96	.333
24	46	—	12.80	13.29	12.80 ^a	.333
	30	12.06	11.59	9.27	7.91	.333
6	10	—	4.00	—	4.00 ^a	.333
8	14	—	—	—	4.92 ^a	.500
10	18	—	5.88	—	5.88 ^a	.600
14	26	—	7.84	—	7.84 ^a	.429
16	30	—	—	—	8.83 ^a	.250
20	38	—	—	11.36	10.81 ^a	.400
22	42	—	11.80	—	11.80 ^a	.273
26	50	—	—	—	13.80 ^a	.230
26	49	—	13.80	—	13.80 ^a	.230
28	54	—	—	15.33	14.79 ^a	.285
30	58	—	15.79	—	15.79 ^a	.200

^a $\text{ave}(s^2)$ optimal design.

^b r_{\max} of Nguyen's design.

and $r_{\max} = .166$. My designs improve those of Booth and Cox (1962), Lin (1993a), and Wu (1993) not only with respect to $\text{ave}(s^2)$ but also with respect to r_{\max} . For example, for $(n, m) = (12, 16)$ and $(12, 24)$, although the designs of Wu (1993) have 45 and 141 $s_{ij} = \pm 4$'s, respectively, my designs have only 34 $s_{ij} = \pm 4$'s for the former and 135 $s_{ij} = \pm 4$'s for the latter, where 4 is s_{\max} of these designs. For $(n, m) = (24, 30)$, although the design of Wu (1993) has 63 $s_{ij} = \pm 8$'s, my corresponding design [design (B) in Sec. 1] has $s_{\max} = 4$.

Note that, in the passenger-impact crash test in the Introduction, the airbag (first factor) explodes and starts to deflate within the spell of an eyeblink. If the car-manufacturer engineers suspect that the bull-bar (second factor) distorts this tuning (because a 4WD has an inherently rigid chassis structure), using my design for $(n, m) = (28, 54)$, the interaction between these two factors can be tested. In Wu's design, this interaction is fully *aliased* with the 28th factor.

5. CONCLUDING REMARKS

Although it is beyond the scope of this article to compare the NOA algorithm with the one of Lin (1993b) for constructing saturated designs, it is worth mentioning some saturated designs constructed by NOA that improve on Lin's designs. For $n = 17$, my saturated design has $\text{ave}(s^2) = 1.94$ as compared to 2.06 of Lin's corresponding design. Although Lin's design has 6 $s_{ij} = \pm 5$, mine has $s_{\max} = 3$. The following is my saturated design for $n = 22$ with $\text{ave}(s^2) = 3.64$ as compared to 4.33 of Lin's corresponding design. Although Lin's design has 6 $s_{ij} = \pm 6$, mine has $s_{\max} = 2$.

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Note that if the condition of equal occurrence of +1's and -1's for the entries in each column is re-

laxed, the Kronecker product of a Hadamard of order 2 and a saturated design for $n = 11$ and $\text{ave}(s^2) = 1$ will produce a design saturated for $n = 22$ with $\text{ave}(s^2) = 1.90$. However, 10 columns of this design has 12 entries that equal -1 but only 10 entries that equal $+1$.

An additional application of the NOA algorithm is to augment an existing supersaturated design with additional two-level columns. In the passenger-impact crash test in the Introduction, if the engineers decide to include the 55th safety feature, say computerized seat belt, in the test, they can augment the design for $(n, m) = (28, 54)$ in Table 2 with an additional two-level column to obtain a design for $(n, m) = (28, 55)$ with $\text{ave}(s^2) = 15.31$ and $s_{\max} = .285$. The extension of this idea to construct orthogonal and near-orthogonal arrays with mixed levels was discussed by Nguyen (in press).

The running time of the NOA algorithm varies with m and n . For design of size $(n, m) = (12, 66)$, a solution with $\text{ave}(s^2) = 11.08$ (optimal) and $s_{\max} = 4$ is obtained in 25 out of 100 tries. The average time per try for this combination is about four seconds on a 66 MHz 486DX2 PC. Naturally, NOA cannot improve $\text{ave}(s^2)$ of the BIBD-type designs. The biggest Hadamard matrix NOA can construct is of order 20.

Data from an experiment using supersaturated designs can be analyzed by stepwise selection or subset selection procedure (e.g., see Miller 1990). Examples of this type of analysis were given by Lin (1993a, 1995).

The NOA algorithm is implemented in a PASCAL program with the same name. Please contact me at namky@forprod.csiro.au regarding the availability of this program and the CIB program that I used to obtain cyclic BIBD solutions in Section 2.

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REFERENCES

- Booth, K. H. V., and Cox, D. R. (1962), "Some Systematic Supersaturated Designs," *Technometrics*, 4, 489–495.
- Hedayat, A., and Wallis, W. D. (1978), "Hadamard Matrix and Their Applications," *The Annals of Statistics*, 6, 1184–1238.
- John, J. A., and Williams, E. R. (1995), *Cyclic and Computer Generated Design* (2nd ed.), New York: Chapman & Hall.
- Kiefer, J. (1959), "Optimum Experimental Design," *Journal of the Royal Statistical Society, Ser. B*, 21, 272–319.
- Lin, D. K. J. (1993a), "A New Class of Supersaturated Designs," *Technometrics*, 35, 28–31.
- (1993b), "Another Look at First-Order Saturated Designs: The p -Efficient Designs," *Technometrics*, 35, 284–292.
- (1995), "Generating Systematic Supersaturated Designs," *Technometrics*, 37, 213–225.
- Miller, A. J. (1990), *Subset Selection in Regression*, New York: Chapman & Hall.
- Nguyen, N.-K. (1994), "Construction of Optimal Incomplete Block Designs by Computer," *Technometrics*, 36, 300–307.
- (in press), "A Note on the Construction of Near-Orthogonal Arrays With Mixed Levels and Economic Run Size," *Technometrics*, 38.
- Nguyen, N.-K., and Miller, A. J. (1992), "A Review of Some Exchange Algorithms for Constructing Discrete D -Optimal Designs," *Computational Statistics & Data Analysis*, 14, 489–498.
- Nguyen, N.-K., and Williams, E. R. (1993), "An Algorithm for Constructing Optimal Resolvable Row-Column Designs," *Australian Journal of Statistics*, 35, 363–370.
- Satterthwaite, F. (1959), "Random Balance Experimentation" (with discussion), *Technometrics*, 1, 111–137.
- Wu, C. F. J. (1993), "Construction of Supersaturated Designs Through Partially Aliased Interactions," *Biometrika*, 80, 661–669.