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SUPERSATURATED DESIGNS (UPDATE)

Many preliminary studies in industrial experimentation contain a large number of potentially relevant factors where only a few are believed to have actual effects. This is sometimes called *effect sparsity*. The basic problem is how to identify these few active factors in an efficient way. One approach is to use a so-called *supersaturated design* (also known as *oversaturated design*), namely, a factorial design with n observations and k factors, $k > n - 1$. If the first-order model is assumed (as in all main-effect* models) and if the number of significant factors is expected to be small, a supersaturated design can be very cost-effective.

Satterthwaite [15] suggested constructing such a design at random. Although the idea of *random balance designs* is interesting, these designs are not of maximum efficiency; see ref. [20], where also Youden et al. introduced the concept of *near-orthogonality* in a casual way. For example, in a three-dimensional space, one can accommodate at most three orthogonal vectors. However, if one replaces the property of perfect orthogonality with near-orthogonality, one can accommodate more than three vectors. Near-orthogonality is defined as the minimization of the maximum pairwise correlations among all design columns (for a perfect orthogonal design, all pairwise correlations are zero). When two designs have the same value for the maximum pairwise correlation, the authors suggest using the design with the fewest pairs of columns achieving this maximum. Following this comment, Booth and Cox [1] were the first to examine this problem via computer search. The optimality criterion

used there is the minimization of

$$E(s^2) = \binom{k}{2}^{-1} \sum s_{ij}^2,$$

where $s_{ij} = \boldsymbol{c}_i'\boldsymbol{c}_j$ and the summation is over all possible pairs of design columns $\boldsymbol{c}_i$ and $\boldsymbol{c}_j$. They provided seven supersaturated designs for $(n, k) = (12, 16)$, $(12, 20)$, $(12, 24)$, $(18, 24)$, $(18, 30)$, $(18, 36)$, and $(24, 30)$. Apart from these computer-generated designs, the construction problem was not addressed in the literature until Lin [8, 9].

USE OF HADAMARD MATRICES

Lin [9] proposed a class of special supersaturated designs that can be constructed easily via *half fractions of Hadamard matrices**. These designs examine $k = N - 2$ factors with $n = N/2$ runs, where N is the order of the Hadamard matrix used. Table 1 shows the original 12-run Plackett and Burman design*. If we take column 11 as the *branching column*, then the total 12 runs (rows) can be split into two groups: group I with the sign of $+1$ in column 11 (rows 2, 3, 5, 6, 7, and 11) and group II with the sign of -1 in column 11 (rows 1, 4, 8, 9, 10, and 12). Deleting column 11 from group I causes columns 1–10 to form a supersaturated design to examine $N - 2 = 10$ factors in $N/2 = 6$ runs (runs 1–6, as indicated in the table). If group II is used, the resulting supersaturated design is an equivalent one.

In general, a Plackett and Burman design matrix [14] can be split into two half fractions according to a specific branching column whose signs equal $+1$ or -1. Specifically, take only the rows which have $+1$ in the branching column. Then, the $N - 2$ columns other than the branching column will form a supersaturated design for $N - 2$ factors in $N/2$ runs. Of course, the underlying model is the first-order (main-effect) model. Comparisons with designs given by Satterthwaite [15] and Booth and Cox [1] are made in Table 2. Judged by $E(s^2)$, the designs given here are clearly superior to the others.

When the Hadamard matrix of order $N = 4t$ is of normalized form, that is, its first row and column are all $+1$'s, this half fraction relates to a balanced incomplete block design* (BIBD) with the parameters $(v, b, r, k) = (2t - 1, 4t - 2, 2t - 2, t - 1)$. Consequently, the $E(s^2)$ value for a supersaturated design from a half-fraction Hadamard matrix is $n^2(n - 3)/[(2n - 3)(n - 1)]$, which is the minimum within the class of designs of the same size. Promising theoretical results are being obtained for the construction of a half-fraction Hadamard matrix. Nguyen [13] points out such a connection and shows that supersaturated designs of this form are always $E(s^2)$-optimal. Some missing entries in Table 2 are related to BIBDs with repeated blocks. Since the BIBD is not unique, designs that are not given in Table 2 can be easily constructed

Table 1 Supersaturated Design Derived from the Hadamard Matrix of Order 12[a]

Run	Row	I	1	2	3	4	5	6	7	8	9	10	(11)
	1	+	+	+	−	+	+	+	−	−	−	+	−
1	2	+	+	−	+	+	+	−	−	−	+	−	+
2	3	+	−	+	+	+	−	−	−	+	−	+	+
	4	+	+	+	+	−	−	−	+	−	+	+	−
3	5	+	+	+	−	−	−	+	−	+	+	−	+
4	6	+	+	−	−	−	+	−	+	+	−	+	+
5	7	+	−	−	−	+	−	+	+	−	+	+	+
	8	+	−	−	+	−	+	+	−	+	+	+	−
	9	+	−	+	−	+	+	−	+	+	+	−	−
	10	+	+	−	+	+	−	+	+	+	−	−	−
6	11	+	−	+	+	−	+	+	+	−	−	−	+
	12	+	−	−	−	−	−	−	−	−	−	−	−

[a]Using column 11 as the branching column.

Table 2 Comparison of the Expectations of s^2 for Selected Designs

		$E(s^2)$			HFHM[a]
n	k	Random Balance	Booth and Cox	HFHM[a]	largest r
12	22	13.09	—	6.85	0.333
	16	13.09	7.06	6.27	
	18	13.09	9.68	6.59	
	24	13.09	10.26	—	
18	34	19.06	—	9.82	0.333
	24	19.06	13.04	9.22	
	30	19.06	15.34	9.74	
	36	19.06	16.44	—	
24	46	25.04	—	12.80	0.333
	30	25.04	12.06	11.59	
6	10	7.20	—	4.00	0.333
10	18	11.11	—	5.88	0.600
14	26	15.07	—	7.84	0.429
22	42	23.05	—	11.80	0.273
26	49	27.04	—	13.80	0.385
30	58	31.03	—	15.79	0.200

[a]Half-fraction Hadamard matrices.

from the corresponding BIBDs without repeated blocks [13, 3].

The interaction columns of Hadamard matrices* are only partially confounded with main-effect columns. Wu [18] makes use of such a property and proposes a supersaturated design that consists of all main-effect and two-factor interaction columns from any given Hadamard matrix of order N. The resulting design thus has N runs and can accommodate up to $N(N-1)/2$ factors. When $k < N(N-1)/2$ factors are to be studied, choosing columns becomes an important issue. In fact, when the number of factors is slightly larger than the number of runs, the results given in Deng et al. [5] can be useful; see also refs. [7, 16, 19].

CAPACITY CONSIDERATIONS

As mentioned, when such a supersaturated design is used, the abandonment of perfect orthogonality is inevitable. The designs given in Lin [9] based on half fractions of Hadamard matrices have a very nice mathematical structure but can only be used to examine $N-2$ factors in $N/2$ runs, where N is the order of Hadamard matrix used. Moreover, these designs do not control the value of the maximum pairwise correlation r, and large values of r occur in some cases (see Table 2).

Consider a two-level k-factor design in n observations with maximum pairwise correlation r. Given any two of the quantities (n, k, r), Lin [8, 11] presents the possible values that can be achieved for the third quantity. Moreover, designs given in ref. [11] may be adequate to allow examination of many prespecified two-factor interactions.

Table 3 shows the maximum number of factors, $k_{\max}$, that can be accommodated when both n (even) and r are specified for $3 \leq n \leq 25$ and $0 \leq r \leq \frac{1}{3}$. For a complete list, see Lin [11]. For $r \leq \frac{1}{3}$, many factors can be accommodated. For fixed n, as the value of r increases, $k_{\max}$ also increases; that is, the larger the nonorthogonality, the more factors can be accommodated. In fact, $k_{\max}$ increases rapidly. Certainly, the more factors accommodated, the more complicated are the biased estimation relationships that occur, leading to more diffi-

Table 3 Maximal Number of Factors Found

Number of Runs, n	Maximal Number, k_{max}				
	$nr = 0$[a]	2	4	6	8
4	3				
6	—	10			
8	7	—			
10	—	12			
12	11	—	66		
14	—	13	—	113	
16	15	—	42	—	
18	—	17	—	111	
20	19	—	34		
22	—	20	—	92	—
24	23	—	33	—	276

[a]Maximum absolute cross product, $nr = |\mathbf{c}_i'\mathbf{c}_j|$, $r \leq \frac{1}{3}$.

culty in data analysis. On the other hand, for fixed r, the value of k_{max} increases rapidly as n increases. For $r \leq \frac{1}{3}$, one can accommodate at most 111 factors in 18 runs or 66 factors in 12 runs; for $r \leq \frac{1}{4}$, one can accommodate 42 factors in 16 runs; for $r \leq \frac{1}{5}$, one can accommodate 34 factors in 20 runs. Provided that these maximum correlations are acceptable, this can be an efficient design. The identifiability* problem for a supersaturated design has been addressed [2].

OPTIMALITY CRITERIA AND DATA ANALYSIS METHODS

Besides the pairwise correlation type criteria, such as $E(s^2)$ or r mentioned above, Wu [18] proposes other criteria that can be obtained by straightforward extension of classical optimal-design theory (*see* OPTIMUM DESIGN OF EXPERIMENTS). For example, if we consider the average of the determinants of all the possible submatrices consisting of f columns, we can define *D-optimality* (in an average sense) for a given supersaturated design. Specifically, define

$$D_f = \binom{k}{f}^{-1} \sum \det(\mathbf{X}_f'\mathbf{X}_f)^{-1},$$

where $\mathbf{X}_f$ is the design matrix consisting only of the f selected columns and the summation is taken over all possible combinations of f columns. One can define *A-optimality*, *E-optimality*, and so on, in a similar manner.

Once the active effects are identified, the initial design is then projected into a much smaller dimension. Such a projection property is very important in designing supersaturated experiments [12, 10, 6]. If we know the number of active factors in advance, the criteria proposed by Wu [18] can be useful. Unfortunately, this is not the case in most screening experiments. Deng et al. [7] thus propose the criterion of *resolution rank*, defined as r-rank $= d - 1$, where d is the minimum number of subset columns that will be linearly dependent. Clearly, if a supersaturated design has an r-rank f, then when the original design is projected into any submatrix of size f (or less), the main effects of the projective design are all estimable. Properties of r-rank criteria are further discussed in ref. [7]. Deng and Lin [4] review and discuss eight useful criteria for evaluating supersaturated designs.

Several methods have been proposed to analyze the k effects, given only the n ($< k$) observations from the contents of the random balance design [15]. These methods can also be applied here. Quick methods such as these provide an appealing straightforward comparison among factors, but it is questionable how much useful information can be extracted with them—combining several of these methods provides a more satisfactory result. In addition, there are three methods for analyzing data resulting from a supersaturated design [11]: (1) normal plotting, (2) stepwise selection, and (3) ridge regression*. In studying so many columns in only a few runs, the probability of a false positive reading (Type I error) is a major risk. Recently, Westfall et al. [17] proposed a relatively conservative approach based on the adjusted P-value* method to control the Type I error. For real data examples see refs. [9, 11, 17].

CONCLUDING REMARKS

1. Using supersaturated designs involves more risks than using designs with more

runs. However, their use is far superior to experimentation approaches such as subjective selection of factors or changing factors one at a time. The one-at-a-time procedure can be shown to have unresolvable confounding patterns, and such confounding patterns are important for data analysis and follow-up experiments.

2. Supersaturated designs are very useful in the early stages of an experimental investigation of complicated systems and processes involving many factors. They are not useful for a terminal experiment. Knowledge of the confounding patterns makes possible the interpretation of the results and provides understanding of how to plan follow-up experiments.
3. The success of a supersaturated design depends heavily on the effect-sparsity assumption. Consequently, the projection properties play an important role in designing a supersaturated experiment.
4. Combining several analysis methods for the data resulting from a supersaturated design is always recommended. Besides the stepwise selection procedure (and other methods mentioned in Lin [9]), the PLS (partial least squares*), adjusted P-value [17], and Bayesian approaches are promising procedures used to identify active factors.
5. Another suitable use for these designs is in testing *robustness*, where the objective is not to identify important factors, but to vary all possible factors so that the response will remain within specifications.

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(HADAMARD MATRICES OPTIMUM DESIGN OF EXPERIMENTS PLACKETT AND BURMAN DESIGNS SUPERSATURATED DESIGNS)

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