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Recent Developments in Supersaturated Designs

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1. AGRICULTURAL AND INDUSTRIAL EXPERIMENTS

Industrial management is becoming increasingly aware of the benefits of running statistically designed experiments. Statistical experimental designs, developed by Sir R. A. Fisher in the 1920s, largely originated from agricultural problems. Designing experiments for industrial problems and designing experiments for agricultural problems are similar in their basic concerns. There are, however, many differences. The differences listed in Table 1 are based on the overall characteristics of all problems. Exceptions can be found in some particular cases, of course.

Industrial problems tend to contain a much larger number of factors under investigation and usually involve a much smaller total number of runs.

Industrial results are more reproducible; that is, industrial problems contain a much smaller replicated variation (pure error) than that of agricultural problems.

Industrial experimenters are obliged to run their experimental points in sequence and naturally plan their follow-up experiments guided by previous results; in contrast, agricultural problems harvest all results at one time. Doubts and complications can be resolved in industry by immediate follow-up experiments. Confirmatory experimentation is readily available for industrial problems and becomes a routine procedure to resolve assumptions.
Table 1 Differences Between Agricultural and Industrial Experiments

<table>
<thead>
<tr>
<th>Subject</th>
<th>Agriculture</th>
<th>Industry</th>
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</thead>
<tbody>
<tr>
<td>Number of factors</td>
<td>Small</td>
<td>Large</td>
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<tr>
<td>Number of runs</td>
<td>Large</td>
<td>Small</td>
</tr>
<tr>
<td>Reproducibility</td>
<td>Less likely</td>
<td>More likely</td>
</tr>
<tr>
<td>Time taken</td>
<td>Long</td>
<td>Short</td>
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<tr>
<td>Blocking</td>
<td>Nature</td>
<td>Not obvious</td>
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<tr>
<td>Missing values</td>
<td>Often</td>
<td>Seldom</td>
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The concept of blocking arose naturally in agriculture but often is not obvious for industrial problems. Usually, industrial practitioners need certain specialized training to recognize and handle blocking variables. Missing values seem to occur more often in agriculture (mainly due to natural losses) than in industry. Usually, such problems can be avoided for industrial problems by carrying out well-designed experiments.

The supersaturated design method considered in this chapter suggests one kind of screening method for industrial problems involving a large number of potential relevant factors. It may not be an appropriate proposal for some agricultural problems.

2. INTRODUCTION

Consider the simple fact that where there is an effect, there is a cause. Quality engineers are constantly faced with distinguishing between the effects that are caused by particular factors and those that are due to random error. The “null” factors are then adjusted to lower the cost: the “non-null” (effective) factors are used to yield better quality. To distinguish between them, a large number of factors can often be listed as possible sources of effects. Preliminary investigations (e.g., using professional knowledge) may quickly remove some of these “candidate factors.” It is not unusual, however, to find that more than 20 sources of effects exist and that among those factors only a small portion are actually active. This is sometimes called “effect sparsity.” A problem frequently encountered in this area is that of how to reduce the total number of experiments. This is particularly important in situations where an individual run is expensive (e.g., with respect to money or time). With powerful statistical software readily available for data analysis, there is no doubt that data collection is the most important part of such problems.

To obtain an unbiased estimate of the main effect of each factor, the number of experiments must exceed (or at least be equal to) the number of factors plus one (for estimating the overall grand average). When the two numbers are equal, the design is called a saturated design; it is the minimum effort required to estimate all main effects. The standard advice given to users in such a screening process is to use the saturated design, which is “optimal” based on certain theoretical optimality criteria. However, the nonsignificant effects are not of interest. Estimating all main effects may be wasteful if the goal is simply to detect the few active factors. If the number of active factors is indeed small, then the use of a slightly biased estimate will still allow one to accomplish the identification of the active factors but significantly reduce the amount of experimental work. Developing such screening designs has long been a well-recognized problem, certainly since Satterthwaite (1959).

When all factors can be reasonably arranged into several groups, the so-called group screening designs can be used (see, e.g., Watson, 1961). Only those factors in groups that are found to have large effects are studied further here. The grouping scheme seems to be crucial but has seldom been discussed. The basic assumptions (such as assuming that the directions of possible effects are known) in fact, depend heavily on the grouping scheme. While such methods may be appropriate in certain situations (e.g., blood tests), we are interested in systematic supersaturated designs for two-level factorial designs that can examine \( k \) factors in \( N < k + 1 \) experiments in which no grouping scheme is needed. Recent work in this area includes, for example, that of Lin (1991, 1993a, 1993b, 1995, 1998), Tang and Wu (1997), Wu (1993), Deng and Lin (1994), Chen and Lin (1998), Cheng (1997), Deng et al. (1994, 1996a, 1996b), Yamada and Lin (1997) and Nguyen (1996).

3. SUPERSATURATED DESIGNS USING HADAMARD MATRICES

Lin (1993a) proposed a class of special supersaturated designs that can be easily constructed via half-fractions of the Hadamard matrices. These designs can examine \( k = N - 2 \) factors with \( n = N/2 \) runs, where \( N \) is the order of the Hadamard matrix used. The Plackett and Burman (1946) designs, which can be viewed as a special class of Hadamard matrices, are used to illustrate the basic construction method.

Table 2 shows the original 12-run Plackett and Burman design. If we take column 11 as the branching column, then the runs (rows) can be split into two groups: group I with the sign of +1 in column 11 (rows 2, 3, 5, 6, 7, 10, 12, 13) and group II with the sign of -1 in column 11 (rows 1, 4, 7, 8, 9, 11, 14, 15).
Table 2  A Supersaturated Design Derived from the Hadamard Matrix of Order 12

<table>
<thead>
<tr>
<th>Run</th>
<th>Row</th>
<th>1</th>
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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 Table 2). It can be shown that if group II is used, the resulting supersaturated design is an equivalent one. In general, a Plackett and Burman (1946) design matrix can be split into two half-fractions according to a specific branching column whose signs equal +1 or -1. Specifically, take only the rows that 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. Judged by a criterion proposed by Booth and Cox (1962), these designs have been shown to be superior to other existing supersaturated designs.

The construction methods here are simple. However, knowing in advance that Hadamard matrices entertain many “good” mathematical properties, the optimality properties of these supersaturated designs deserve further investigation. For example, the half-fraction Hadamard matrix of order \( n = N/2 = 4t \) is closely related to a balanced incomplete block design with \((v, b, r, k) = (2t - 1, 4t - 2, 2t - 2, t - 1)\) and \( \lambda = t - 1 \). Consequently, the \( E(s^2) \) value (see Section 4) for a supersaturated design from a half-fraction Hadamard matrix is \( n^2(3n - 3)/[(2n - 3)(n - 1)] \), which can be shown to be the minimum within the class of designs with the same size. Potentially promising theoretical results seem possible for the construction of a half-fraction Hadamard matrix. Theoretical implications deserve detailed scrutiny and are discussed below. For more details regarding this issue, please consult Cheng (1977) and Nguyen (1996).

Note that the interaction columns of Hadamard matrices are only partially confounded with other main-effect columns. Wu (1993) 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 has \( N \) runs and can accommodate up to \( N(N - 1)/2 \) factors. When there are \( k = N(N - 1)/2 \) factors to be studied, choosing columns becomes an important issue to be addressed.

4. CAPACITY CONSIDERATIONS

As mentioned, when a supersaturated design is used, the abandonment of perfect orthogonality is inevitable. The designs given in Lin (1993a) based on half-fractions of Hadamard matrices have a very nice mathematical structure but can be used only to examine \( N - 2 \) factors in \( N/2 \) runs, where \( N \) is the order of the Hadamard matrix used. Moreover, these designs do not control the value of the maximal pairwise correlation \( r \). and, in fact, large values of \( r \) occur in some cases.

Consider a two-level \( k \)-factor design in \( n \) observations with maximal pairwise correlation \( r \). Given any two of the quantities \((n, k, r)\), Lin (1995) presents the possible values that can be achieved for the third quantity. Moreover, designs given in Lin (1995) may be adequate to allow examination of many prespecified two-factor interactions. Some of the results are summarized in Table 3.

Table 3 shows the maximum number of factors, \( k_{\text{max}} \), that can be accommodated when both \( n \) and \( r \) are specified for \( 3 \leq n \leq 25 \) and \( 0 \leq r \leq 1/3 \) (Table 3a for even \( n \) and Table 3b for odd \( n \)). We see that for \( r \leq 1/3 \), many factors can be accommodated. For fixed \( n \), as the value of \( r \) increases, \( k_{\text{max}} \) also increases. That is, the larger the nonorthogonality, the more factors can be accommodated. In fact, \( k_{\text{max}} \) increases rapidly in this setting. Certainly the more factors accommodated, the more complicated are the biased estimation relationships that occur, leading to more difficulty in data analysis. On the other hand, for fixed \( r \), the value of \( k_{\text{max}} \) increases rapidly as \( n \) increases. For \( r \leq 1/3 \), one can accommodate at most 111 factors in 18 runs or 66 factors in 12 runs; for \( r \leq 1/4 \), one can accommodate 42 factors in 16 runs; for \( r \leq 1/5 \), one can accommodate 34 factors in 20 runs. Provided that these maximal correlations are acceptable, this can be an efficient design strategy.
5. OPTIMALITY CRITERIA

When a supersaturated design is employed, as previously mentioned, the abandonment of orthogonality is inevitable. It is well known that lack of orthogonality results in lower efficiency; therefore, we seek a design that is as "nearly orthogonal" as possible. One way to measure the degree of nonorthogonality between two columns, \( c_i \) and \( c_j \), is to consider their cross-product, \( s_{ij} = c_i' c_j \); a larger \( |s_{ij}| \) implies less orthogonality. Denote the largest \( |s_{ij}| \) among all pairs of columns for a given design by \( s \), and we desire a minimum value for \( s \) (\( s = 0 \) implies orthogonality). The quantity \( s \) can be viewed as the degree of orthogonality that the experimenter is willing to give up—the smaller, the better. This is by nature an important criterion. Given any two of the quantities \((n, k, s)\), it is of interest to determine what value can be achieved for the third quantity. Some computational results were reported by Lin (1995). No theoretical results are currently available, however. It is believed that some results from coding theory can be very helpful in this direction. Further refinement is currently under investigation.

If two designs have the same value of \( s \), we prefer the one in which the value of \( |s_{ij}| = s \) is a minimum. This is intimately connected with the expectation of \( s^2 \). \( E(s^2) \) first proposed by Booth and Cox (1962) and computed as \( \sum s_{ij}^2 f_i \binom{k}{2} \), where \( f_i \) is the frequency of \( s_i \) among all \( \binom{k}{2} \) pairs of columns.

Intuitively, \( E(s^2) \) gives the increment in the variance of estimation arising from nonorthogonality. It is, however, a measurement for pairwise relationships only. More general criteria were obtained by Wu (1993) and Deng et al. (1994, 1996b). Deng and Lin (1994) outlined eight criteria useful for supersaturated designs: \( s = \max |c_i'c_j| \); \( E(s^2) \); \( \rho \) (Lin, 1995); \( D_r, A_r, E_r \) (Wu, 1993); \( B \) criterion (Deng et al., 1996a, 1996b); and \( r \)-rank (see Section 8). Further theoretical justification is currently under study. Optimal designs in light of these approaches deserve further investigations. In addition, the notion of multifactor (non)orthogonality is closely related to the multicollinearity in linear model theory.

6. DATA ANALYSIS METHODS

Several methods have been proposed to analyze the \( k \) effects, given only the \( n < k \) observations from the random balance design concepts (see, e.g., Satterthwaite, 1959). These methods can also be applied here. Quick methods such as these provide an appealing, straightforward comparison among
With simulated \( p \) values, but the errors can be made very small, particularly with control variates. The analysis of data from supersaturated designs along this direction can be found in Westfall et al. (1998).

7. EXAMPLES

Examples of supersaturated designs as real data sets can be found in Lin (1993, 1995). Here we apply the concept of supersaturated design to identify interaction effects from a main-effect orthogonal design. This example is adapted from Lin (1998). Consider the experiment in Hunter et al. (1982). A 12-run Plackett and Burman design was used to study the effects of seven factors (designated here as \( A, B, \ldots, G \)) on the fatigue life of weld-repaired castings. The design and responses are given in Table 4 (temporarily ignore columns 8–28). For the details of factors and level values, see Hunter et al. (1982).

Plackett and Burman designs are traditionally known as main-effect designs, because if all interactions can temporarily be ignored, they can be used to estimate all main effects. There are many ways to analyze such a main-effect design. One popular way is the normal plot [see Hamada and Wu (1992), Figure 1]. Using this method, it appears that factor \( F \) is the only significant main effect. Consequently a main-effect model is fitted as follows:

\[
\hat{y} = 5.73 + 0.458F \quad \text{with} \quad R^2 = 44.5\%.
\]

Note that the low \( R^2 \) is not very impressive. Is it safe to ignore the interaction effects? Hunter et al. claim that the design did not generate enough information to identify specific conjectured interaction effects. If this is not the case here, is it possible to detect significant interaction effects? Hamada and Wu (1992) introduced the concept of effect heredity. After main effects were identified, they used forward selection regression to identify significant effects among a group consisting of (1) the effects already identified and (2) the two-factor interactions having at least one component factor appearing among the main effects of those already identified. In this particular example, a model for factor \( F \) and interaction \( FG \) was chosen:

\[
\hat{y} = 5.7 + 0.458F - 0.459FG. \quad R^2 = 89\%
\]

Now, if we generate all interaction columns, \( AB, AC, \ldots, FG \), together with all main-effect columns, \( A, B, \ldots, G \), we have \( 7 + 21 = 28 \) columns. Treat all of these 28 columns in 12 runs as a supersaturated design (Lin, 1993) as shown in Table 4. The largest correlation between any pair of the design columns is \( \pm 1/3 \). The results from a regular stepwise regression analysis (with \( \alpha = 5\% \) for entering variables) yields the model.
\[ \hat{y} = 5.73 + 0.394F - 0.395FG - 0.191AE. \quad R^2 = 95\% \]  

(2)

a significantly better fit to the data than Eq. (1). An application of the
adjusted p-value method (Westfall, et al. 1998) reaches the same conclusion
in this example.

Note that the AE interaction, in general, would never be chosen under
the effect heredity assumption. Of course, most practitioners may consider
adding main effects A, E, and G to the final model because of the signific-
ce of interactions FG and AF. The goal here is only to identify potential
interaction effects. In general, for most main-effect designs, such as Plackett
and Burman type designs (except for $2^{k-p}$ fractional factorials), one can
apply the following procedure [see Lin (1998) for the limitations]:

**Step 1.** Generate all interaction columns and combine them with the
main-effect columns. We now have \( k(k+1)/2 \) design columns.

**Step 2.** Analyze these \( k(k+1)/2 \) columns with \( n \) experimental runs as a
supersaturated design. Data analysis methods for such a supersatura-
ted design are available.

Note that if the interactions are indeed inert, the procedure will work well,
and if the effect heredity assumption is indeed true, the procedure will end
up with the same conclusion as that of Hamada and Wu (1992). The
proposed procedure will always result in better (or equal) performance than
that of Hamada and Wu’s procedure.

### 8. THEORETICAL CONSTRUCTION METHODS

Deng et al. (1994) proposed a supersaturated design of the form
\( X_s = [H, RHC] \), where \( H \) is a normalized Hadamard matrix, \( R \) is an orthogonal
matrix, and \( C \) is an \( n \times (n - c) \) matrix representing the operation of
column selection. Besides the fact that some new designs with nice properties
can be obtained this way, the \( X_s \) matrix covers many existing supersaturated
designs. This includes the supersaturated designs proposed by Lin (1993a),
Wu (1993), and Tang and Wu (1993). Some justifications of its optimal
properties have been obtained as follows.

It can be shown that

\[
X_s'X_s = \begin{pmatrix}
I_n & H'RHC \\
C'H'R'H & I_{n-c}
\end{pmatrix} = \begin{pmatrix}
I_n & WC \\
C'W'C & I_{n-c}
\end{pmatrix}
\]

where \( W = H'R'H = (w_{ij}) = (h_j'Rh_i) \) and \( h_j \) is the \( j \)th column of \( H \). Further,
the following theorem can be demonstrated.
Theorem

Let \( H \) be a Hadamard matrix of order \( n \) and \( B = (b_1, \ldots, b_r) \) be an \( n \times r \) matrix with all entries \( \pm 1 \) and \( V = H' B = (v_{ij}) = h_i/b_j \). Then

1. For any fixed \( 1 \leq j \leq r \), \( n^2 = \sum_{i=1}^{n} v_{ij}^2 \).
2. In particular, let \( B = RH \) and \( W = H' RH = (w_{ij}) \). We have
   a. \( (1/n)W \) is an \( n \times n \) orthogonal matrix.
   b. \( n^2 = \sum_{j=1}^{n} w_{ij}^2 = \sum_{j=1}^{n} w_{ij}^2 \).
   c. \( w_{ij} \) is always a multiple of 4.
   d. If \( H' \) is column-balanced, then \( \pm n = \sum_{i=1}^{n} w_{ij} = \sum_{j=1}^{n} w_{ij} \).

Corollary

For any \( R \) and \( C \) such that (1) \( R' R = I \) and (2) rank \( (C) = n - c \), all \( X_e \) matrices have an identical \( E(s^2) \) value.

This implies that the popular \( E(s^2) \) criterion used in supersaturated designs is invariant for any choice of \( R \) and \( C \). Therefore, it is not effective for comparing supersaturated designs. In fact, following the argument in Tang and Wu (1993), the designs given here will always have the minimum \( E(s^2) \) values within the class of designs of the same size. One important feature of the goodness of a supersaturated screening design is its projection property (see Lin 1993b). We thus consider the \( r \)-rank property as defined below.

Definition

Let \( X \) be a column-balanced design matrix. The resolution \( r \)-rank (or \( r \) rank, for short) of \( X \) is defined as \( f = d - 1 \), where \( d \) is the minimum number of columns that are linearly dependent.

The following results are provided by Deng et al. (1994).

1. If no column in any supersaturated design \( X \) is fully aliased, then the \( r \) rank of \( X \) is at least 3.
2. \( n R h_i = \sum_{j=1}^{n} w_{ij} h_i \).
3. Let \( W = H' D(h_i) H \), where \( D(h_i) \) is the diagonal matrix associated with \( h_i \), namely, the \( i \)th column vector of \( H \); and \( n = 4r \). Then
   a. If \( r \) is odd, then there can be exactly three 0's in each row or each column of \( W \). The rest of \( w_{ij} \) can only be of the form \( \pm 8k + 4 \), for some nonnegative integer \( k \).
   b. If \( r \) is even, then every entry \( w_{ij} \) in \( W \) can be of the form \( \pm 8k \), for some nonnegative integer \( k \).

These results are only the first step. Extension of these results to a more general class of supersaturated designs in the form \( S_K = (R_1 H C_1, \ldots, R_K H C_K) \) is promising.

9. COMPUTER ALGORITHMIC CONSTRUCTION METHODS

More and more researchers are benefiting from using computer power to construct designs for specific needs. Unlike some cases from the optimal design perspective (such as \( D \)-optimal design), computer construction of supersaturated designs is not well developed yet. Lin (1991) introduced the first computer algorithm to construct supersaturated designs. Denote the largest correlation in absolute value among all design columns by \( r \), as a simple measure of the degree of nonorthogonality that can willingly be given up. Lin (1995) examines the maximal number of factors that can be accommodated in such a design when \( r \) and \( n \) are given.

At Church at GenCorp Company used the projection properties in Lin and Draper (1992, 1993) to develop a software package named DOE0 to generate designs for mixed-level discrete variables. Such a program has been used at several sites in GenCorp. A program named DOESS is one of the results and is currently in a test stage. Dr. Nam-Ky Nguyen (CSIRO, Australia) also independently works on this subject. He uses an exchange procedure to construct supersaturated designs and near-orthogonal arrays. A commercial product called Genex is available for sale to the public as a result. Algorithmic approaches to constructing supersaturated designs seem to have been a hot topic in recent years. For example, Li and Wu (1997) developed a so-called columnwise-pairwise exchange algorithm. Such an algorithm seems to perform well for constructing supersaturated designs by various criteria.

10. CONCLUSION

1. Using supersaturated designs involves more risk than using designs with more runs. However, it is far superior to other experimental approaches such as subjectively selecting factors or changing factors one at a time. The latter can be shown to have unresolvable confounding patterns, though such confounding patterns are important for data analysis and follow-up experiments.
2. Supersaturated designs are very useful in early stages of experimental investigation of complicated systems and processes involving many factors. They are not used for a terminal experiment.
Knowledge of the confounding patterns makes possible the interpretation of the results and provides the understanding of how to plan the 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 data analysis methods to analyze the data resulting from a supersaturated design is always recommended. Besides the stepwise selection procedure [and other methods mentioned in Lin (1993)], PLS (partial least squares), adjusted $p$ value (see Westfall et al. (1998)), and Bayesian approaches are promising procedures for use in identifying active factors.

5. Another particularly 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 the specifications.

REFERENCES
