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SUPERSATURATED DESIGN: THEORY AND APPLICATION

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1 Agriculture and Industrial Experiments

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

- In contrast to agriculture problems, industrial problems tend to contain a much larger number of factors under investigation and usually involve a much smaller number of runs in total.

- Industrial results are more reproducible, i.e., industrial problems contain a much smaller replicated variation (pure error) than that of agriculture problems.

- Industrial experimenters are obliged to run their experimental points in sequence and naturally plan their follow-up experiments guided by previous results; unlike agriculture, which harvests 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 become a routine procedure to resolve assumptions.

- The concept of blocking arises 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 industry. Usually, such problems can be avoided for industrial problems by well-designed experiments.

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

Table 1: Differences Between Agriculture 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>
</tr>
<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>
</tr>
<tr>
<td>Blocking</td>
<td>Nature</td>
<td>Not Obvious</td>
</tr>
<tr>
<td>Missing Values</td>
<td>Often</td>
<td>Seldom</td>
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</tbody>
</table>

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 factors which have an effect and those that are due to random error. Those "null" factors are then adjusted to lower the cost; those "non-null" (effective) factors are used to yield better quality. To distinguish the difference, a large number of factors can often be listed as possible sources of effect. 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 twenty sources of an effects exist, and among those factors only a small portion are actually active. This is sometimes called "effect sparsity". A problem frequently encountered in this area is how to reduce the total number of experiments. This is particularly important in situations where the cost of an individual run is expensive (e.g., regarding 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.

For 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 these two numbers are equal, the design is called a saturated design, which is the minimum effort possible to estimate all main effects. Standard advice given to users in such a screening process is to use the saturated design, which is "optimal" based upon 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 those few active factors. If the number of active factors is indeed small, 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 grouped into several groups, the so-called group screening designs can be used (see, for example, Watson, 1961). Only those factors in groups that are found to have large effects are studied further. The grouping scheme seems to be crucial but has seldom been discussed. The basic assumptions here (such as the directions of possible effects are known, etc), in fact, heavily depend upon the grouping scheme. While such methods may be appropriate in certain situation (e.g., blood tests), we are interested in systematic supersaturated designs for two-level factorial designs that can be examine k factors in N < k + 1 experiments where no grouping scheme needs to be made. Recently work in this area includes, for example, Lin (1991, 1993a, 1993b, 1994, 1995); Tang and Wu (1993); Wu (1993); Deng and Lin (1994, 1996); Chen and Lin (1995); Cheng (1995, 1997); Deng, Lin and Wang (1996, 1997); and Nguyen (1996).

3 Supersaturated Designs Using Hadamard Matrices

Recently, Lin (1993) proposed a class of special supersaturated designs which can be easily constructed via half-fractions of Hadamard matrices. These designs can examine k = N - 2 factors with n = N/2 runs, where N is the order of 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 the 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 1 2). Deleting column 11 from Group I causes the columns 1-10 then 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 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. Judged by a criterion proposed by Booth and Cox (1962), these designs have been shown to be superior to other existing supersaturated designs.

Table 2: A Supersaturated Design Derived From the Hadamard Matrix of Order 12

<table>
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The construction methods here are simple. However, knowing in advance that Hadamard matrices entail 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 λ=t-1. Consequently, the E(s²) value (see next section) for a supersaturated design from a half-
fraction Hadamard matrix is \( n^2(n-3)/[(2n-3)(n-1)] \) which can be shown to be the minimum within the class of the design with same size. Potentially promising theoretical results seem possible for the construction of a half-fraction Hadamard matrix. Theoretical implications deserve detailed scrutiny as will be discussed below. More details in this issue, please consult with Cheng (1997) and Nguyen (1996).

Note that the interaction columns of Hadamard matrices are only partially confounded with any 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 thus 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 there.

4 Optimality Criteria

When a supersaturated design is needed, 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 "near orthogonal" as possible. One way to measure the degree of non-orthogonality 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 interested to find what value can be achieved for the third quantity. Some computational results have been reported in Lin (1995). No theoretical results are currently available, however. It is believed that some results from the coding theory can be very helpful in this direction. Further refinement is currently under investigation.

If two designs have the same \( s \), we prefer the one in which the number 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), which is computed by \( \sum s_i f_i \left( \begin{array}{c} k \\ 2 \end{array} \right) \), where \( f_i \) is the frequency of \( s_i \) of all \( \left( \begin{array}{c} k \\ 2 \end{array} \right) \) pairs of columns.

Intuitively, \( E(s^2) \) gives the increment in variance of estimation arising from non-orthogonality. It is, however, a measurement for pairwise relationships only. More general criteria have been obtained in Deng, Wang and Lin (1997) and Wu (1993). Deng and Lin (1994) outline eight various criteria useful for supersaturated designs. Further theoretical justification is currently under study. Optimal design in light of these approaches deserves further investigations. In addition, the notion of multi-factor orthogonality is closely related to the multicollinearity in linear model content. It is anticipated that results from the current project can be very useful in both areas.

5 Data Analysis Methods

Several methods have been proposed to analyze the \( k \) effects, given only the \( n (< k) \) observations from the random balance design contents (see, for example, Satterthwaite, 1959). 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 available information can be extracted using them; combining several of these methods provides a more satisfying effect. In addition, three data analysis methods for data resulting from a supersaturated design are discussed as follows in Lin (1995): (1) normal plotting, (2) stepwise selection procedure, and (3) ridge regression.

To study so many columns in only a few runs, the probability of a false positive reading (Type-I error) is a major risk here. The principal investigator plans to study an alternative to forward selection procedure to control these false positive rates. Let \( X = \{i_1, i_2, \cdots, i_p\} \) and \( A = \{i_p + 1, \cdots, i_k\} \) denote indexes of inert and active factors, so that \( N \cup A = \{1, \cdots, k\} = S \). If \( X \) denotes the \( n \times p \) design matrix, our model is \( Y = \mu + X\beta + \epsilon \) where \( Y \) is the \( n \times 1 \) observable data vector, \( \mu \) is the intercept term and \( 1 \) is an \( n \)-vector of \( 1 \)'s; \( \beta \) is a \( k \times 1 \) fixed and unknown vector of factor effects, and \( \epsilon \) is the noise vector. In the multiple hypothesis-testing framework, we have null and alternative pairs \( H_j : \beta_j = 0 \) and \( H_j^c : \beta_j \neq 0 \), with \( H_j \) true for \( j \in N \), and \( H_j^c \) true for \( j \in A \).

Forward selection proceeds by identifying the maximum F-statistics at successive stages. Let \( F_j^{(s)} \) denotes the F-statistics for testing \( H_j \).
at stage $s$. Consequently, define $j_s = \arg \max_{j \in S \setminus \{j_1, \ldots, j_{s-1}\}} F_j^{(s)}$ where $F_j^{(s)} = \frac{\text{RSS}(j, j_1, \ldots, j_{s-1})}{\text{MSE}(j_1, j_2, \ldots, j_{s-1})}$. Letting $\max_{j \in S \setminus \{j_1, \ldots, j_{s-1}\}} F_j^{(s)} = F^{(s)}$, the forward selection procedure is defined by selecting variables $j_1, \ldots, j_s$, where $F^{(s)} \leq \alpha$ and $F^{(s+1)} > \alpha$. If $F^{(s)} > \alpha$, then no variables are selected.

The Type-I (false positive) error may be controlled using the adjusted $p$-values method (Westfall and Young, 1993). Algorithmically, at stage $s$, if $F^{(s)} > \alpha$, then stop; otherwise, enter $X_j$ and continue. This procedure controls the Type-I error rate exactly at level $\alpha$ under the complete null hypothesis, since $P(\text{Rejects at least one } H_i \mid \text{all } H_i \text{ true}) = P(F^{(s)} \leq F_i^{(s)}) = \alpha$.

In addition, if the first $s$ variables are forced, and the test is used to evaluate the significance of the next entering variable (of the remaining $k - s$), the procedure is again exact under the complete null hypothesis of no effects among the $k - s$ remaining variables. The exactness disappears 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, Young and Lin (1997).

6 Theoretical Construction Methods

Recently, Deng, Lin and Wang (1997) proposed a supersaturated design of the form $X = [H, RH, C]$ 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 in this way, the $X$ matrix covers many existing supersaturated designs as special cases. This includes the supersaturated designs proposed by Lin (1993), Wu (1993) and Tang and Wu (1993). Some justifications of its optimal properties have been obtained.

It can be shown that

$$X'X = \begin{pmatrix} nI_n & H'RH & C'H'R'H \\ C'W' & nI_{n-c} \end{pmatrix} = \begin{pmatrix} nI_n & WC \\ C'W' & nI_{n-c} \end{pmatrix}$$

where $W = H'RH = (w_{ij}) = (h_i'R_i)$ and $h_i$ is the $j$th column of $H$. It can be further shown that:

**THEOREM** Let $H$ be a Hadamard matrix of order $n$, and $B = (b_1, \ldots, b_r)$ be a $n \times r$ 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 $B = RH$, $W = H'R = (w_{ij})$, we have
   - $\frac{1}{n}W$ is an $n \times n$ orthogonal matrix,
   - $\sum_{i=1}^n w_{ij}^2 = \sum_{j=1}^n w_{ij}^2$,
   - $w_{ij}$ is always a multiple of 4, and
   - 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($C$) = $n - c$, then the $X$ matrix has the same E($s^2$) values.

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 in 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 a class of the same size. One important feature of the goodness of a supersaturated screening design is its projection property (see, Lin, 1993b; Cheng, 1995). We thus consider the r-rank property as defined below.

**Definition.** Let $X$ be a column-balanced design matrix. The resolution rank (or r-rank, for short) of $X$ is defined as $r = d + 1$, where $d$ is the minimum number subset columns that will be linearly dependent.

The following results have been obtained (see, Deng, Lin and Wang, 1997).

1. If no column in any supersaturated design, $X$, is fully aliased, then the r-rank of $X$ is at least 3.

2. $nRh_j = \sum_{i=1}^n w_{ij}h_i$.

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 $n = 4t$, then
   - If $t$ 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 $k$.
   - If $t$ 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. The principal investigator proposes to extend these results to a more general class of supersaturated design in the
following form: \( S_K = (R_1HC_1, \ldots, R_KHC_K) \). We anticipate obtaining a general theorem for supersaturated designs in the future study.

7 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 measurement of the degree of the non-orthogonality willing to 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.

Mr. Church, at GenCorp Company, utilized the projection properties in Draper and Lin (1992) to develop a software package named "DOE90" to generate designs for mixed-level discrete variables. Such a program has been used by several sites in GenCorp. A program named "DOESS" is one of the results, which 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. Algorithmic approach of constructing supersaturated design seems to be a hot topic in the recent year. Many nice work are anticipated in the near future.

8 Examples

Examples of supersaturated designs with 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 (1995). Consider the experiment in Hunter, Hodi and Eager (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 3 (tentatively ignore Columns 8-28). For the details of factors and level values, see Hunter, Hodi and Eager (1982).

Plackett and Burman designs are traditionally known as main-effect designs, because if all interactions can tentatively 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, Hadama and Wu, 1992, Figure 1). It appears that factor F is the only significant main effect. Consequently a main-effect model is fitted as follows: \( \hat{\gamma} = 5.73 + 0.458F \) with \( R^2 = 44.5\% \).

Note that the low \( R^2 \) is not so impressive. Can we safely 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, can we 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, which consists of: (i) the effects are already identified, and (ii) the two-factor interactions have at least one component factor appearing among the main effects in (i). In this particular example, a model for factor F and interaction FG was chosen, and given below:

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

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 those 28 columns in 12 runs as a supersaturated design (Lin, 1993) as shown in Table 3. The largest correlation between any pairs of the 28 design columns is \( \pm 1/3 \). The results from a regular stepwise regression analysis (with \( \alpha = 5\% \) for entering variables) yields the model

\[
\hat{\gamma} = 5.73 + 0.394F - 0.395FG - 0.191AE \quad (R^2 = 95\%)
\]

is a significantly better fit to the data than is (1). Note that the AE interaction, in general, would never be chosen under the effect heredity assumption. Of course, most practitioners may consider to add main effects A, E, and G to the final model, because of the significance of interactions FG and AE. 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, 1994, for the limitations):

Step 1. Generate all interaction columns, and combine them with the main-effect columns. We have now \( k(k+1)/2 \) 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 supersaturated 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 a better (or equal) performance to Hadama and Wu's procedure.

9 Conclusion

1. Using supersaturated designs involves more risky than using designs with more runs. However, their use is far superior to other experimentation approaches, such as subjective selection of factors or changing factors one-at-a-time. The latter can be shown to have unsolvable confounding patterns while such confounding patterns are important for data analysis and follow-up experiments.

2. Supersaturated designs are very useful in early stages of the 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, Young and Lin (1997)), and Bayesian approaches are promising procedures used to identify 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.

10 References


