# CRITERIA FOR SUPERSATURATED DESIGNS

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## 1. INTRODUCTION

Screening experiments typically contain a large number of potential factors. Practitioners are constantly faced with distinguishing between the factors that have an actual effect and those factors whose apparent effects are due to random error. The "null" factors are then adjusted to lower the cost, and the "non-null" (active) factors are used to yield better quality results. To distinguish the difference, a large number of factors can often be listed as possible sources of effect. It is not unusual, however, that among those factors only a small portion are, in fact, active. This is sometimes called "effect sparsity." Usually, further investigation on the nonsignificant effects is not of interest. Estimating all effects may be wasteful if the goal is simply to detect those few active factors.

When there are many factors, the usual advice given to them is to run so-called main-effect designs (Resolution III designs in the orthogonal case) which require at least $k$+1 runs for investigating $k$ factors. However, estimating all main effects may be wasteful if the goal is only to *detect* those active factors. This is particularly true when the number of factors is large and a small number of runs is required. In such situations, a supersaturated design can save considerable costs.

A supersaturated design is a fraction of a factorial design with $n$ observations in which the number of factors, $k$ is more than $n$-1. When such a design is used, the abandonment of orthogonality is inevitable, because otherwise, these columns would form a set of more than $n$ orthogonal vectors in $n$ dimensional space. The usefulness of such a supersaturated design relies upon the realism of effect sparsity; namely, the number of the dominant active factors is small. As previously mentioned, the goal here is to identify these active factors. For a brief review of early work in supersaturated design, see Lin (1991).

Apart from some ad hoc procedures and computer-generated designs, the construction problem has not been addressed until very recently. See, Lin (1991, 1993a, 1995), Wu (1993). Most of these supersaturated designs, though constructed based upon different viewpoints, show that a Hadamard matrix is indeed a useful tool for constructing a supersaturated design. Indeed, Deng, Lin and Wang (1994) provide a universal form of a supersaturated design using a Hadamard matrix, which will cover all of the above construction methods as special cases. Moreover, they show that a supersaturated design constructed with such a universal form is superior to others, in terms of various criteria.

In this paper, we discuss several existing criteria for evaluating the goodness of a supersaturated design. Two specific criteria for orthogonality and estimability respectively are proposed.

## 2. CLASSICAL CRITERIA FOR SUPERSATURATED DESIGNS

To screen a large number of factors in a small number of runs, the abandonment of orthogonality in a supersaturated design is inevitable. Since lack of orthogonality results in lower efficiency, it is always desirable to make the design as nearly orthogonal as possible when the perfect orthogonality is unattainable. This clearly suggests several criteria to be suitable for supersaturated designs.

(C1) $s = \max(s_{ij})$, where $s_{ij} = x_i'x_j$ for all $1 \le i < j \le k$.

Here we denote the ith column of the design matrix X by $x_i$. The value of s is the maximum correlation among any pair of design columns. Certainly, the smaller, the better.

(C2) $E(s^2) = \sum s_{ij}^2 / \binom{k}{2}$, where $s_{ij} = x_i'x_j$ for all $1 \le i < j \le k$.

Booth and Cox (1962) first proposed the $E(s^2)$ criterion to evaluate the goodness of a supersaturated design, and it has been intensively used by others.

Note that once the few dominant active factors are identified, the initial design is then projected into a much smaller dimension. The implicit assumption under $E(s^2)$ criterion is that there are, at most, two active factors. If the number of active factors, $c$, is larger than 2, there is no guarantee that the projective (reduced) design will be of full rank, i.e., a main effect model consists only of those active factors that may not be estimable.

(C3) $\rho = \sum r_{ij}^2 / \binom{k}{2}$, where $r_{ij} = \mathrm{Corr}(x_i, x_j)$ for all $1 \le i < j \le k$.

Lin (1994) modifies the $E(s^2)$, by taking into the run size $n$ into account and proposes an equivalent criterion, mean square correlation $\rho$ as shown above. The disadvantage of $E(s^2)$ is also shared by the criterion $\rho$.

## 3. EXTENSION OF SOME OPTIMAL DESIGN CRITERIA

Let $X_{n \times k}$ be the design matrix with entries $\pm 1$, and let $c$ be the number of active factors, i.e., the number of design columns of the projected design matrix. For a given $s = (l_1, \ldots, l_c)$, s set of size $c$ from $(1, \ldots, k)$, we can construct a $n$ x $c$ sub-matrix $X_s$ from X. Following the idea of $E(s^2)$ which gives an efficiency measurement in an average sense, we can measure the "orthogonality" of X as follows:

$$V_c(X) = \frac{1}{\binom{k}{c}} \cdot \sum \nu(X_s), \qquad (1)$$

where $\nu(X_s)$ is a function to measure the "orthogonality" of $X_s$ and the summation is taken over all possible choice of $s$.

As an extension of the classical design optimality, some natural choices of $\nu(X_s)$ are:

(C4) $\nu(X_s) = \det(X_s'X_s)^{-1}$.

(C5) $\nu(X_s) = \mathrm{trace}\,(X_s'X_s)^{-1}$.

(C6) $\nu(X_s) = \lambda_{(c)}(X_s'X_s)^{-1}$, where $\lambda_{(c)}$ denotes the largest eigenvalue of the matrix $(X_s'X_s)^{-1}$.

Notes:

1. When $c = k \le n$, these criteria are corresponding to: (i) D optimal, (ii)

A optimal, and (iii) E optimal criteria, respectively. When $k > n$ (see Section 5), the value of $c$ can not be larger than $k$, and in fact, is normally much smaller than $k$.

2. When $c = 2$, all criteria are reduced to the criterion similar to the one proposed by Booth and Cox (1962) and Lin (1993a). One should note that the first two criteria will optimize a design by minimizing

$$E\left(\frac{1}{n^2 - s^2}\right),$$

where as the criterion considered by Booth and Cox (1962) and Lin (1993a) is

$$E(s^2).$$

Note also that

$$\frac{1}{n^2-s^2} = \frac{1}{n^2}\,\frac{1}{1-s^2/n^2} = \frac{1}{n^2}\left(1+\frac{s^2}{n^2}+\ldots\right).$$

Therefore, criteria (C4) - (C6) and (C2) should be approximately equivalent to each other because $s^2$ is normally much smaller than $n^2$.

## 4. A NEW CLASS OF B-OPTIMAL CRITERIA

Clearly, if a vector y is orthogonal to a group of vectors $Z = (z_1, z_2, \ldots, z_p)$, then the regression sum squares must be null, when regress y on $(z_1, z_2, \ldots, z_p)$. Namely, $y'Z(Z'Z)^{-1}Z'y=0$. Thus, the value of $y'Z(Z'Z)^{-1}Z'y$, or equivalently $b'(Z'Z)b$, where $b = (Z'Z)^{-1}Z'y$ is the regression coefficient, provides a good measurement on how orthogonal the vector y to Z. Motivated by this, the proposed criterion, called "B optimality," reflects the dependence of a column to all other $c - 1$ columns by computing the regression coefficients of one column in $X_s$, $X_i$, over the remaining columns $X_{s-i}$. For any specific projection design $X_s$ with size $n \times c$, we average $x_i'X_{s-i}(X_{s-i}'X_{s-i})^{-1}X_{s-i}'x_i$ over all possible $i (i = 1,2,\ldots,c)$ as a measurement of the design orthogonality. Of course, the value of $c$ is typically small (See, for example, Lin, 1993b).

In general, consider a class of new functions $v_g(X_s)$ to measure the "orthogonality" of $X_s$ for $V_c(X)$ in (1):

$$v_g(X_s) = \sum_{i \in s} \beta_{s-i}(X_{s-i}'X_{s-i})^g \beta_{s-i}, \qquad (2)$$

namely,

(C7)

$$V_c(X) = \frac{1}{\binom{k}{c}} \cdot \sum_{|s|=c} \sum_{i \in s} \beta_{s-i}'(X_{s-i}'X_{s-i})^g \beta_{s-i},$$

where

(i) $\beta_{s-i} = (X_{s-i}'X_{s-i})^{-1}X_{s-1}'x_i$,

(ii) $x_i$ is the $n \times 1$ column corresponding to the $i$-th unit in $s$,

(iii) $X_{s-i}$ is the $n \times (c\text{-}1)$ matrix corresponding to units in $s-\{i\}$,

and $g$ can be any scalar value to present the degree of penalty to the non-singularity of the $X_{s-i}'X_{s-i}$ matrix. Note that for g=1, the B-criterion is equivalent to the well known VIF criterion (Variance Inflation Factor). In principle, the B-criterion can apply to any design when the projection property is under concern, regardless the number of levels, the number of factors and the number of runs.

To compute the value of $v_g(X_s)$ given in (2), we need the value of $(X'_{s-i}X_{s-i})^{-1}$ for each $i \in s$. Now, $(X'_{s-i}X_{s-i})^{-1}$ easily can be computed from $(X'_sX_s)^{-1}$. Theorem 1 below gives the formula for $v_1(X_s)$ and $v_0(X_s)$ in terms of the elements in $(X'_sX_s)^{-1}$. Throughout this section, we will consider, without loss of generality, the sample s = $(l_1,...l_c)$ as s=(1,...,c).

Theorem 1. Let $X_s=(x_1,...,x_c)$ be a matrix with full-rank of dimension nxc and let

$$W=(X'_sX_s)^{-1} = (w_{ij}).$$

then,

(i) $$v_1(X_s) = nc - \sum_{i=1}^{c} \frac{1}{w_{ii}}$$

and

(ii) $$v_0(X_s) = \sum_{i \neq j}^{c} \frac{w_{ij}^2}{w_{ii}^2} \qquad \blacksquare$$

## 5. RESOLUTION-RANK CRITERION

Note that once these active factors are identified, the initial design is then projected into a much smaller dimension (see Lin, 1993b). A criterion based upon such an important projection property, called resolution rank, is defined as follows.

(C8) DEFINITION. Let X be a column-balanced design matrix. We define the resolution-rank (r-rank, for short) of X as $f = d - 1$, where $d$ is the minimum number subset columns (excluding ±1) that will be linearly dependent.

Clearly, if a supersaturated design, X, has an r-rank of $f$, then when X is projected to any submatrix of $f$ (or less) factors, the main effects of the projected design are all estimable. Moreover, in many situations where the r-ranks are very different for two supersaturated designs, their $D_f$ and $A_f$ values are nearly identical (The maximum difference is around 1%.).

Theorem 2. If no columns in any supersaturated design, X, are fully aliased, then its r-rank at least 3. $\blacksquare$

Table below shows the comparisons on a specific 16-run supersaturated design generated by the method of Wu (1993) and Deng, Lin and Wang (1994) respectively. Clearly, a r-rank of 4 and 7 can easily distinguish the superiority of the later design, while the $A_f$ and $D_f$ values are too close to tell.

| | Wu (1993) | | DLW (1994) | |
|---|---|---|---|---|
| $f$ | $A_f$ | $D_f$ | $A_f$ | $D_f$ |
| 2 | 0.130 | 11.340 | 0.130 | 11.339 |
| 3 | 0.205 | 9.583 | 0.204 | 9.581 |
| 4 | 0.290 | 8.123 | 0.287 | 8.118 |
| 5 | | | 0.380 | 6.903 |
| 6 | | | 0.489 | 5.886 |
| 7 | | | 0.619 | 5.024 |

## 6. DISCUSSION

Supersaturated designs can save considerable costs in screening experimentation. Many experimenters are trying such a design on real examples. To evaluate the goodness of supersaturated design, we reviewed certain classical criteria (C1) - (C3) and extended some optimal design criteria suitable for supersaturated design (C4) - (C6).

Moreover, two important criteria based on projection are proposed: (i) B-optimal criterion (C7), and (ii) resolution-rank (C8) criterion. The former directly associates with multi-factor orthogonality, while the latter associates with the estimability of the projective design.

In summary, eight criteria have been discussed in this paper. They are

(C1) $s = \max s_{ij}$

(C2) $E(s^2) = \Sigma s_{ij}^2 / \binom{k}{2}$

(C3) $\rho = \Sigma r_{ij}^2 / \binom{k}{2}$

(C4) $$\text{D-criterion} = \frac{1}{\binom{k}{c}} \Sigma \det (X_s'X_s)^{-1}$$

(C5) $$\text{A-criterion} = \frac{1}{\binom{k}{c}} \Sigma \operatorname{trace} (X_s'X_s)^{-1}$$

(C6) $$\text{E-criterion} = \frac{1}{\binom{k}{c}} \Sigma \lambda_{(c)}(X_s'X_s)^{-1}$$

(C7) $$\text{B-criterion} = \frac{1}{\binom{k}{c}} \Sigma \beta_{s-i}'(X_{s-i}'X_{s-i})^{g}\beta_{s-i}$$

(C8) resolution rank.

## REFERENCES


Booth, K.H.V. and Cox, D.R. (1962), "Some Systematic Supersaturated Designs," *Technometrics*, **4** 489-495.

Deng, L.Y., Lin, D.K.J. and Wang, J. (1993), "A Measurement of Multi-factor Orthogonality," Working Paper, No. 273, College of Business Administration, The University of Tennessee.

Deng, L.Y., Lin, D.K.J. and Wang, J. (1994), "Supersaturated Design Using Hadamard Matrix," IBM Research Report, No. RC19470, IBM Watson Research Center.

Lin, D.K.J. (1991), "Systematic Supersaturated Designs," Working Paper, No. 264, College of Business Administration, The University of Tennessee.

Lin, D.K.J. (1993a), "A New Class of Supersaturated Designs," *Technometrics*, **35**, 28-31.

Lin, D.K.J. (1993b), "Another Look at First-Order Saturated Designs: The p-efficient Designs." *Technometrics*, **35**, 284-292.

Lin, D.K.J. (1995), "Generating Systematic Supersaturated Designs," *Technometrics*, to appear.

Wu, C.F.J. (1993), "Construction of Supersaturated Designs Through Partially Aliased Interactions," *Biometrika*, **80**, 661-669.