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Review of Classical Methods in Supersaturated Designs (SSD) for factor Screening

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Abstract
Supersaturated designs are fractional factorial designs that have too few runs to allow the estimation of the main effects of all the factors in the experiment. There has been a great deal of interest in the development of these designs for factor screening in recent years. A review of supersaturated design is presented, including criteria for design selection, with reference to the popular E(s^2) criterion and classical methods for constructing supersaturated designs. Classical methods have been suggested for the analysis of data from supersaturated designs and these are critically reviewed and illustrated.
Keywords: Supersaturated, Classical method, Screening, fractional factorial and E(S^2)

1.0 Introduction

All factor screening designs are intended for situations in which there are too many factors to study in detail. If the number of factors is very large and/or each experimental run is very expensive, then it may be impractical to use even the Resolution III two-level designs, which allow all main effects to be estimated. In such cases, it might be useful to run experiments with fewer runs than there are factors to try to identify a small number of factors that appear to have dominant effects.
A supersaturated design is a design for which there are fewer runs than effects to be estimated in a proposed model. Usually the term "supersaturated" is used more specifically for a design for which there are insufficient degrees of freedom for estimating the main effects only, that is, for designs with n runs where estimating the main effects would require more than n −1 degrees of freedom.
The use of screening designs of the restricted type are investigated. In the early literature on the subject, and often today, the term was used still more specifically for a design with n runs in which there are more than n −1 two-level factors. The discussion here concentrates on these two-level designs and their use in factor screening. For recent work on factors with more than two levels, see Lu et al. (2003).

Supersaturated designs have their roots in random balance experimentation, which was briefly popular in industry in the 1950s,until the discussion of the papers by Satterthwaite (1959) and Budne (1959). In these experiments, the combinations of the factor levels are chosen at random, subject to having equal numbers of runs at each level of each factor, and they can include more factors than there are runs. Box (1959) suggested that the latter idea was worth pursuing in the context of designed experiments. However, the idea of random balance itself was totally refuted as a useful way of running experiments and has rarely been seen since. Booth and Cox (1962) presented the first supersaturated designs, but no more work on the subject was published for more than 30 years. The papers by Lin (1993) and Wu (1993) sparked a renewed interest in the subject. Since then there has been a large and increasing number of papers published in the statistical literature, mostly on methods of constructing supersaturated designs. It is less clear how much they are being used in practice. There appear to be no published case studies featuring the use of supersaturated designs, although the most likely area for their application is in early discovery experiments which are unlikely to be sent for publication. In my own view, industrial statisticians are reluctant to recommend supersaturated designs because there are no successful case studies in the literature, but the difficulties in interpreting the data might also be a deterrent. This paper reviews the recent work on supersaturated designs in factor screening, concentrating on methods of obtaining designs and analytical methods that are most likely use in practice.

2.0 E(s^2)-Optimal Designs

We assume that each factor has two levels, coded +1 and −1, often written as "+" and " - ". As in almost all of the literature, we assume that each factor is observed at each level an equal number of times, although Allen and Bernshteyn (2003) recently relaxed this assumption.

2.1 Criteria of Optimality

Consider the "main effects only" model,

$$Y = \beta_0 + \sum_{j=1}^{f} \beta_j X_j + \varepsilon, \quad \text{.....(1)}$$

where Y is a response variable, $\beta_0,\beta_1,...,\beta_f$ are unknown parameters, $x_1,...,x_f$ are the coded levels of the *f* factors, ε is an error term with $E(\varepsilon) = 0$ and $V(\varepsilon) = \sigma^2$, and error terms are independent. The model in matrix notation is

$$Y = X\beta + \varepsilon \quad \text{.....(2)}$$

TABLE 1. Designs for 14 factors in 8 runs.

Factors													
1	2	3	4	5	6	7	8	9	10	11	12	13	14
+	+	+	+	+	+	+	+	+	+	+	+	+	+
-	-	+	+	-	-	+	+	-	-	+	+	-	-
-	+	-	-	+	-	+	+	-	+	-	-	+	-
+	-	-	-	-	+	+	+	+	-	-	-	-	+
-	+	-	+	-	+	-	-	+	-	+	-	+	-
+	-	-	+	+	-	-	-	-	+	+	-	-	+
+	+	+	-	-	-	-	-	-	-	-	+	+	+
-	-	+	-	+	+	-	-	+	+	-	+	-	-

In a supersaturated design, even for this main effects only model, the matrix X'X is non singular, where ' denotes transpose, and so no unique least squares estimates of the parameters β can be obtained. Consider, for example, the small supersaturated design shown in Table 1. This has

$$X'X = \begin{bmatrix}
8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8
\end{bmatrix}$$

The diagonal elements of this matrix are fixed by the number of runs. Best of all is when the off-diagonal elements are all zero, in which case all main effects are estimated independently. It is, of course, impossible to get an X'X matrix for 14 factors in 8 runs with rank greater than 8. However, these considerations suggest that a good design will be one that makes the off-diagonal elements as small as possible (in absolute value). Letting the $(i, j)^{th}$ element of X'X be s_{ij}, Booth and Cox (1962) suggested two criteria based on the sizes of the s_{ij}. The first criterion they used was to choose a design with minimum $\max_{i \neq j} |S_{ij}|$, and among all such designs to choose one with the fewest s_{ij} that achieves this maximum.

The second suggestion of Booth and Cox was to choose a design that minimizes

$$E(S^2) = \frac{2}{f(f-1)} \sum_{i<j} S_{ij}^2 \quad \text{.....(3)}$$

This has become the most commonly used criterion in the literature on supersaturated designs. Sometimes these two criteria are combined, for example, by choosing a supersaturated design that minimizes $E(s^2)$ subject to some upper bound on $\max_{i \neq j} |S_{ij}|$. Cheng and Tang (2001) gave upper bounds on the number of factors that could be included in a supersaturated design subject to $\max_{i \neq j} |S_{ij}| \leq c$, where c is a constant.

Booth and Cox (1962) gave two other interpretations of $E(s^2)$. They showed that if there are only *p* important factors and their main effects are so large that they can be easily identified, then the average variance of their estimated main effects is approximately

$$\frac{\sigma^2}{n}\left\{1 + \frac{(p-1)E(S^2)}{n^2}\right\} \quad \text{.....(4)}$$

Thus, an $E(s^2)$-optimal design also minimizes this quantity. As *p* becomes larger, this approximation becomes poorer and the assumption that the large effects can be identified becomes less plausible, so it is most relevant for $p = 2$ and perhaps $p = 3$. Wu (1993) showed that $E(s^2)$-optimal designs also maximize the average D-efficiency over all models with just two main effects.

The second interpretation of $E(s^2)$ arises from considering the estimation of the main effect of a single factor X_j, for example if only one factor appears to have a very large effect. The simple linear regression estimate of β_j from the model

$$Y_i = \beta_0 + \beta_j x_{ji} + \varepsilon_i \quad \text{.....(5)}$$

$$\hat{\beta}_j = \sum_{i=1}^{n} x_{ji} y_i / n, \qquad \text{with } V(\hat{\beta}_j) = \frac{\sigma^2}{n}, \quad \text{.....(6)}$$

and is based on the assumption that all other factors will have zero effects. If, in fact, all other factors have effects of magnitude 2δ, with their directions being chosen at random, then the true variance of the single estimated main effect is not σ^2/n, but

$$\frac{\sigma^2}{n} + \frac{(f-1)}{4n^2}\sigma^2 E(S^2) \quad \text{.....(7)}$$

Cheng et al. (2002) showed that supersaturated designs with a property called "minimum G_2-aberration" are $E(s^2)$-optimal and suggested that G_2-aberration might be a useful criterion for supersaturated designs. Liu and Hickernall (2002) showed that $E(s^2)$ is similar, but not identical, to a form of discrepancy, that is, a measure of how far the points of the design are from being uniformly distributed in the factor space. They also showed that, under certain conditions, the most uniform designs are $E(s^2)$-optimal. It is unknown how the concept of discrepancy is related to the statistical properties of the designs. A different criterion was used by Allen and Bernshteyn (2003) to construct supersaturated designs. A prior probabilities of factors being active (having non negligible effects) and inactive (having negligible effects) and then searched for designs that maximize the probability of correctly selecting the active factors. In all of the examples they studied, they found that designs which optimize this criterion are also $E(s^2)$-optimal, but that the converse is not true. This suggests that they could restrict their search for designs to the class of $E(s^2)$-optimal designs. Other criteria have been suggested, but rarely used, for constructing supersaturated designs, although they are sometimes used for comparing different $E(s^2)$- optimal designs. One of these is to minimize the average D- or A- efficiency over all submodels with *p* factors, $2 \leq p < f$ (Wu, 1993; Liu and Dean, 2004). Deng et al. (1996) suggested using the multiple regression of a column in the design on $p-1$ other columns. The regression sum of squares then gives a measure of the nonorthogonality of this column to the others. The average of this regression sum of squares over all sets of columns can be used as a criterion for comparing designs, although the computation of this criterion is a major task in itself. Deng et al. (1999) defined the resolution-rank of a supersaturated design as the maximum *p* such that any *p* columns of the design are linearly independent. They suggested maximizing the resolution-rank, although again the computation of this criterion is prohibitive for large *f*. Holcomb and Carlyle (2002) suggested

using the ratio of the largest eigenvalue of X'X and the smallest nonzero eigenvalue and stated that this was related to A-efficiency. None of these criteria have been studied further.

In order to know whether a given design is optimal, it is helpful to have lower bounds on $E(s^2)$. Increasingly tight, or more widely applicable, bounds have been given by Nguyen (1996), Tang and Wu (1997), Liu and Zhang (2000a,b), Butler et al. (2001), and Bulutoglu and Cheng (2004). The bounds of Bulutoglu and Cheng cover all cases with n even and with each factor having two levels with n/2 runs at each level, that is, all of the cases we are considering here. These results allow us to identify many $E(s^2)$-optimal supersaturated designs.

3.0 **Data Analysis**

Standard methods for analyzing data from fractional factorial designs cannot be used with data from supersaturated designs, because the least squares estimates are not unique and, given any reasonable assumptions, there is no way to estimate all the main effects simultaneously. Several methods of analysis have been suggested in the literature and are discussed in the context of data from half of an experiment reported by Williams (1968) and analyzed by several authors.
Twenty-three factors were varied in 28 runs and one continuous response was observed. The half-fraction analyzed by Lin (1993) is shown in Table 2, which incorporates the corrections noted by Box and Draper (1987) and Abraham et al. (1999). Most methods of analysis assume that the objective is to identify a few active factors, those with non-negligible main effects, to separate them from the inactive factors, those with negligible main effects.

Table 2: Design and data for half-replicate of Williams' experiment

									Factors													Response
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	Y
+	+	+	-	-	-	+	+	+	+	+	-	+	-	-	+	-	-	+	-	-	-	+	133
+	-	-	-	-	-	+	+	+	-	-	-	+	+	+	-	+	-	-	+	+	-	-	62
+	+	-	+	+	-	-	-	-	+	-	+	+	+	+	+	-	-	-	-	+	+	-	45
+	+	-	+	-	+	-	-	-	+	+	-	+	-	+	-	+	+	+	-	-	-	-	52
-	-	+	+	+	+	-	+	+	-	-	-	+	-	+	+	-	-	+	-	+	+	+	56
-	-	+	+	+	+	+	-	+	+	+	-	-	+	+	+	+	+	+	+	+	-	-	47
-	-	-	-	+	-	-	+	-	+	-	+	+	+	-	+	+	+	+	+	-	-	+	88
-	+	+	-	-	+	-	+	-	+	-	-	-	-	-	-	-	+	-	+	+	+	-	193
-	-	-	-	-	+	+	-	-	-	+	+	-	-	+	+	+	-	-	-	-	+	+	32
+	+	+	+	-	+	+	+	-	-	-	+	-	+	+	+	-	+	-	+	-	-	+	53
-	+	-	+	+	-	-	+	+	-	+	-	-	+	-	-	+	+	-	-	-	+	+	276
+	-	-	-	+	+	+	-	+	+	+	+	+	-	-	-	-	+	-	+	+	+	+	145
+	+	+	+	+	-	+	-	+	-	-	+	-	-	-	-	+	-	+	+	-	+	-	130
-	-	+	-	-	-	-	-	-	-	+	+	-	+	-	-	-	-	+	-	+	-	-	127

3.1 **Least Squares Estimation Methods**

Most often data analysis techniques are borrowed from regression analysis. Satterthwaite (1959) suggested a graphical method that is essentially equivalent to producing the least squares estimates from each simple linear regression. For example, in the data in Table 2, the effect of factor 1 is estimated by fitting $Y_i = \beta_0 + \beta_1 x_{1i} + e_i$ and so on, giving the results in Table 3. Chen and Lin (1998) showed that, if there is a single active factor with true magnitude greater than σ and if all other factors have exactly zero effect, then this procedure gives a high probability of the active factor having the largest estimated main effect. Lin (1995) suggested plotting these simple linear regression estimates on normal probability paper, although the lack of orthogonality makes the interpretation of such a plot difficult. Kelly and Voelkel (2000) showed that the probabilities of type-II errors resulting from this method are very high and recommended instead that all sub-sets selection be used, which involves fitting all estimable sub models of the main effects model. Holcomb et al. (2003) studied the method of using the simple linear regression estimates in more detail. They described it as a contrast-based method obtained by using X'Y from the full model, but these are the simple linear regression estimates multiplied by n.

They tried several procedures for separating the active from the inactive factors based on these estimates. In a large simulation study they found that resampling methods to control the type-II error rate worked best and better than stepwise selection. However, they also concluded that none of the methods worked very well. Lin (1993) suggested using stepwise variable selection and Wu (1993) suggested forward selection or all (estimable) subsets selection. Lin (1993) gave an illustrative analysis by stepwise selection of the data in Table 2. He found that this identified factors 15,12,19,4,and10 as the active factors, when their main effects are entered into the model in this order. Wang (1995) analyzed the other half of the Williams experiment and identified only one of the five factors that Lin had identified as being non negligible, namely, factor 4. Abraham et al. (1999) studied forward selection and all subsets selection in detail. They showed, by simulating data from several different experiments, that the factors identified as active could change completely if a different fraction was used and that neither of these methods could reliably find three factors which have large effects. However, they concluded that all subsets selection is better than forward selection. Kelly and Voelkel (2000) showed more generally that the probabilities of type-II errors from stepwise regression are high. The first paper to concentrate on the analysis of data from supersaturated designs was by Westfall et al. (1998).
They suggested using forward selection with adjusted p-values to control the type-I error rate. They showed how to obtain good approximations to the true p-values using resampling methods, but concluded that control of type-I and type-II errors in supersaturated designs is fundamentally a difficult problem. Applying their adjusted p-values to the data in Table 2, they found that only the effect of factor 15 is significantly different from zero.

Table 3. Estimates of main effects obtained from the data of Table 3 using linear regressions

Factors	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Effect	-14.2	23.2	2.8	-8.6	9.6	-20.2	-16.8	20.2	18.5	-2.4	13.2	-14.2
Factor	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	
Effect	-19.8	-3.1	-53.2	-37.9	-4.6	19.2	-12.4	-0.2	-6.4	22.5	9.1	

3.2 Biased Estimation Methods

The methods described above all use ordinary least squares to fit several different sub models of the main effects model. Biased estimation methods attempt to fit the full main effects model by using modifications of the least squares method. Lin (1995) suggested using ridge regression, that is, replacing X'X with X'X +λI for some λ and then inverting this matrix instead of X'X in the least squares equations. However, he reported that ridge regression seems to perform poorly when the number of factors, *f*, is considerably greater than the number of runs, *n*.
Li and Lin (2002) used a form of penalized least squares with the smoothly clipped absolute deviation penalty proposed by Fan and Li (2001). This method estimates the parameters, β, by minimizing not the usual residual sum of squares, but

$$\frac{1}{2n}\sum_{i=1}^{n}(y_i - x_i^{'}\beta)^2 + \sum_{j=1}^{f+1}\phi(\beta_j),\qquad(8)$$

where the penalty, φ(βj), shrinks small estimated effects towards zero. It is defined by its first derivative,

$$\frac{\partial\phi}{\partial\beta} = \lambda\left\{I(\beta \le \lambda + \frac{3.7\lambda - \beta}{2.7\lambda} I(\beta > \lambda)\right\}, \beta = 0,\qquad(9)$$

and φ(0) = 0, where I(·) is an indicator function and λ is a tuning constant chosen from the data by cross-validation. Li and Lin also showed that a good approximation to this method is given by iterated ridge regression. They showed that this method greatly outperformed stepwise variable selection in terms of finding the true model from simulated data. In the data set considered here, it identified 15, 12, 19, and 4 as the active factors.

Comparing the results from different methods of analyzing the data in Table 2, it can be seen that they generally agree on the ordering of effects, namely, 15, 12, 19, 4, and 10, but that they lead to different decisions about which factors should be declared active and which should not.

3.3 Recommendations and Future Research

Several methods for analyzing data from supersaturated designs have been proposed, but none of them seem very convincing. Designs are usually built to optimize the $E(s^2)$ criterion, but this appears to be unrelated to the way in which the data are analyzed. The potential user of supersaturated designs needs to know the answers to three questions.

1. Should supersaturated designs ever be used? If so, in what circumstances? If not, what should be used instead?

2. How should data from supersaturated designs be analyzed and interpreted?
3. How should supersaturated designs be constructed?

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