AD-A115 786 DESMATICS INC STATE COLLEGE PA F/G 12/2
INTERRUPTIBLE SUPERSATURATED TWO-LEVEL DESIGNS.(U)
JUN 82 J L ROSENBERGER, D E SMITH N00014-75-C-1054
UNCLASSIFIED TR-106-11 NL

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P. O. Box 618
State College, Pa. 16801
Phone: (814) 238-9621

Applied Research in Statistics - Mathematics - Operations Research

INTERRUPTIBLE SUPERSATURATED
TWO-LEVEL DESIGNS

by

James L. Rosenberger*

and

Dennis E. Smith

*Assistant Professor of Statistics, The Pennsylvania State University
(Research conducted at Desmatics, Inc. during Summer 1981.)

TECHNICAL REPORT NO. 106-11

June 1982

This study was supported by the Office of Naval Research
under Contract No. N00014-75-C-1054, Task No. NR 042-334.

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I. INTRODUCTION

To conserve time and money, saturated or nearly-saturated experiments are often designed, particularly in the early pilot phase of research projects where little is known about the priority of the factors to be investigated. Sometimes, an unanticipated supersaturated situation results when a saturated or nearly-saturated experiment is interrupted (and terminated) before its completion. Such a situation tends to be associated with a project which has tenuous funding or which is of uncertain length, such as occurs in operating a new plant under pilot protocols. This type of situation provides the rationale for investigating interruptible supersaturated designs.

Smith and Schmoyer (1982) defined interruptible designs as those which limit the adverse effects of an incomplete experimental program, and investigated the construction of such designs where a first-order model is assumed and factors at only two levels are considered. However, one of their assumptions was that any experiment would not be interrupted in the supersaturated stage.

In this paper, we extend their results by examining the case where the experiment is interrupted at a point where less runs have been made than there are parameters to be estimated. Specifically, we consider designs with $k = 4(1)9$ factors where each factor has exactly two levels. For convenience we code the factor levels as $\{-1, 1\}$ to represent the low and high level, respectively.

For each value of k we would like to determine a sequence of runs which at each step is best in some sense, and which leads to a D-optimal saturated design.

Thus, we want to lose the least if the experiment were interrupted, but wish to retain optimality if it were completed. The specific D-optimal designs we consider in this paper are the same ones considered by Smith and Schmoyer (1982). For $k = 4$, 5, and 6, we use the designs given by Box and Draper (1971); for $k = 7$, we use a Plackett-Burman design [Plackett and Burman (1946)]; for $k = 8$ and 9, we use the designs provided by Mitchell (1972, 1974).

II. OPTIMALITY CRITERIA

Optimality of designs is usually based on the variance-covariance matrix of the estimated parameters of the linear model. Let $\underline{y} = (y_1,\ldots,y_n)'$ be the n x 1 vector of observations from n independent and homoscedastic experiments with mean $\underline{X\beta}$, where the columns of the n x p matrix $\underline{X}$ specify the levels of $k = p - 1$ factors. From least squares theory, the variance-covariance matrix of the estimated $\underline{\beta}$ vector of effects is a constant times $(\underline{X}'\underline{X})^{-1}$.

D-optimality is defined by the minimum of the determinant of the $(\underline{X}'\underline{X})^{-1}$ matrix or equivalently, by the maximum of $|\underline{X}'\underline{X}|$. However supersaturated designs are characterized by having fewer runs (rows of $\underline{X}$) than parameters (columns of $\underline{X}$). Thus, for a supersaturated design, $\underline{X}'\underline{X}$ is not full rank, and $|\underline{X}'\underline{X}|$ is identically zero.

Booth and Cox (1962) suggested an optimality criterion based on a measure of the orthogonality of the columns of the matrix $\underline{X}$. If we let $\underline{X} = (\underline{x}_0, \underline{x}_1, \underline{x}_2,\ldots,\underline{x}_k)$ where $\underline{x}_0$ is the n-dimensional vector of 1's, and $\underline{x}_i$, $i = 1,\ldots,k$, are the design matrix n-vectors for the k factors, then the angle Θ_{ij} between any two column vectors, $\underline{x}_i$ and $\underline{x}_j$, is defined by

$$\text{Cosine } \Theta_{ij} = \underline{x}_i'\underline{x}_j / [(\underline{x}_i'\underline{x}_i)^{\frac{1}{2}}(\underline{x}_j'\underline{x}_j)^{\frac{1}{2}}].$$

Since all vectors $\underline{x}_i$ in the designs we consider only contain elements +1 or -1, they are of the same length, $\sqrt{n}$, and we measure the optimality of a supersaturated design by

$$\phi = \max_{i \neq j} |\underline{x}_i'\underline{x}_j|/n.$$

For two or more designs with the same value of ϕ, we rank them by the number of pairs of columns achieving that maximum. An optimal supersaturated design by this criterion minimizes the maximum$_{i \neq j}$ $|\underline{x}_i'\underline{x}_j|/n$ and within this set contains the smallest number of column pairs with ϕ_{min}, the minimax $|\underline{x}_i'\underline{x}_j|/n$.

Booth and Cox restricted their consideration to designs with even n, and an equal number of +1's and -1's in each column. Then the column $\underline{x}_0$ of all 1's was orthogonal to the remaining columns. Since in our investigation we allow for interruption after any run, we consider both odd and even numbers of runs, make no restrictions on the number of +1's and -1's in each column, and treat the $\underline{x}_0$ column the same as the $\underline{x}_1, \ldots, \underline{x}_k$ columns in our calculations.

III. INTERRUPTIBLE DESIGNS

We obtained interruptible designs by selecting a sequence of runs which optimize at each step the criterion presented in the previous section. The selection of runs was made without replacement from the set of k+1 runs comprising the D-optimal saturated designs for k factors referenced in the introduction. Computer evaluation of all possible run sequences guided the selection of the optimal order of runs.

We also obtained worst-case results for each number of runs. We define the worst case (for a given number of runs) as that set of runs which produces ϕ_{max}, the maximum value of ϕ. Further, if more than one set of runs corresponds to ϕ_{max}, we select as worst case that set having the largest number of pairs with ϕ equal to ϕ_{max}.

Tables 1 through 6 present the D-optimal designs we have considered and list the runs in the optimal sequence. These sequences are not necessarily unique. For each number of runs, the tables also provide ϕ_{min}, the minimum value of ϕ for this sequence, and the number of pairs for which the minimum occurs. Also, for each number of runs, ϕ_{max} and the number of pairs for which it occurs is given for the worst case. The runs where ϕ_{min} and ϕ_{max} differ indicate where the design would be suboptimal if interrupted without having used an optimal sequence.

IV. DISCUSSION

Except for the case $k=4$, the sequences of design runs reveal that at certain numbers of runs (asterisked in Tables 2 through 6), the design sequences specified are preferred to some other sequences. Therefore, for situations where it is likely the design may be interrupted, these sequences would be favorable in terms of the criterion used.

By deciding to use these optimal sequences to pursue a saturated design, unrestricted randomization would need to be forsaken. However, within subsets of runs where the optimality is not affected by choice of runs, the runs could be randomly ordered. In situations where it is possible that a supersaturated experiment may result, the experimenter should consider the use of our interruptible supersaturated designs, particularly if he or she feels that complete randomization may be foregone.

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Optimal Run Sequence	Factors x_0	x_1	x_2	x_3	x_4
1	1	1	-1	1	-1
2	1	1	1	-1	1
3	1	-1	-1	1	1
4	1	-1	-1	-1	-1
5	1	-1	1	1	-1

	Optimal Run Sequence		Worst Case	
Number of Runs	ϕ_{min}	No. of Pairs	ϕ_{max}	No. of Pairs
2	1.00	4	1.00	4
3	1.00	1	1.00	1
4	.50	4	.50	4
5	.20	10	.20	10

Table 1: Results for an optimal interruptible sequence of runs leading to a D-optimal saturated $k = 4$, $N = 5$ experiment.

Optimal Run Sequence	Factors x_0	x_1	x_2	x_3	x_4	x_5
1	1	1	1	1	1	1
2	1	1	-1	-1	1	-1
3	1	1	1	1	-1	-1
4	1	-1	-1	1	-1	1
5	1	-1	1	1	1	-1
6	1	-1	1	-1	-1	1

Number of Runs	Optimal Run Sequence ϕ_{min}	No. of Pairs	Worst Case ϕ_{max}	No. of Pairs
2	1.000	6	1.000	7 **
3	1.000	2	1.000	3 **
4	.500	8	1.000*	1
5	.600	2	.600	2
6	$.33\overline{3}$	6	$.33\overline{3}$	6

* $\phi_{max} > \phi_{min}$ for some suboptimal sequence of runs.

** $\phi_{max} = \phi_{min}$, but the number of pairs attaining the maximum is greater.

Table 2: Results for an optimal interruptible sequence of runs leading to a D-optimal saturated $k = 5$, $N = 6$ experiment.

Optimal Run Sequence	Factors x_0	x_1	x_2	x_3	x_4	x_5	x_6
1	1	-1	1	1	-1	-1	1
2	1	-1	1	-1	1	1	-1
3	1	-1	-1	-1	1	-1	1
4	1	1	1	-1	-1	-1	-1
5	1	1	-1	1	1	1	1
6	1	-1	-1	-1	-1	1	1
7	1	-1	-1	1	-1	-1	-1

Number of Runs	Optimal Run Sequence ϕ_{min}	No. of Pairs	Worst Case ϕ_{max}	No. of Pairs
2	1.000	9	1.000	11**
3	1.000	3	1.000	4**
4	.500	12	1.000*	2
5	.600	4	1.000*	1
6	$.66\overline{6}$	1	$.66\overline{6}$	1
7	.429	3	.429	3

* $\phi_{max} > \phi_{min}$ for some suboptimal sequence of runs.

** $\phi_{max} = \phi_{min}$, but the number of pairs attaining the maximum is greater.

Table 3: Results for an optimal interruptible sequence of runs leading to a D-optimal saturated $k = 6$, $N = 7$ experiment.

Optimal Run Sequence	Factors x_0	x_1	x_2	x_3	x_4	x_5	x_6	x_7
1	1	1	1	1	1	1	1	1
2	1	1	1	-1	1	-1	-1	-1
3	1	1	-1	1	-1	1	-1	-1
4	1	-1	1	1	-1	-1	1	-1
5	1	1	-1	-1	-1	-1	1	1
6	1	-1	1	-1	-1	1	-1	1
7	1	-1	-1	1	1	-1	-1	1
8	1	-1	-1	-1	1	1	1	-1

Number of Runs	Optimal Run Sequence ϕ_{min}	No. of Pairs	Worst Case ϕ_{max}	No. of Pairs
2	1.000	12	1.000	12
3	1.000	4	1.000	4
4	.500	16	1.000*	4
5	.600	4	.600	4
6	$.33\overline{3}$	12	$.33\overline{3}$	12
7	.143	28	.143	28
8	0	28	0	28

* $\phi_{max} > \phi_{min}$ for some suboptimal sequence of runs.

Table 4: Results for an optimal interruptible sequence of runs leading to a D-optimal saturated $k = 7$, $N = 8$ experiment. (Resolution III 2^{7-4} design.)

Optimal Run Sequence	Factors x_0	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8
1	1	1	-1	1	1	1	1	1	-1
2	1	1	1	-1	1	1	-1	-1	-1
3	1	-1	1	-1	1	-1	1	1	-1
4	1	1	-1	-1	-1	-1	-1	1	1
5	1	-1	1	1	-1	1	-1	1	-1
6	1	-1	-1	1	1	-1	-1	-1	1
7	1	-1	1	-1	1	1	1	1	1
8	1	-1	-1	-1	-1	1	1	-1	-1
9	1	1	1	1	-1	-1	1	-1	1

Number of Runs	Optimal Run Sequence ϕ_{min}	No. of Pairs	Worst Case ϕ_{max}	No. of Pairs
2	1.000	16	1.000	22**
3	1.000	6	1.000	9**
4	1.000	1	1.000	6**
5	.600	8	1.000*	3
6	$.66\overline{6}$	2	1.000*	1
7	.429	9	1.000*	1
8	.500	1	.750	1
9	$.55\overline{5}$	1	$.55\overline{5}$	1

*$\phi_{max} > \phi_{min}$ for some suboptimal sequence of runs.

**$\phi_{max} = \phi_{min}$, but the number of pairs attaining the maximum is greater.

Table 5: Results for an optimal interruptible sequence of runs leading to a D-optimal saturated $k = 8$, $N = 9$ experiment.

Optimal Run Sequence	Factors x_0	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9
1	1	1	-1	1	1	1	1	1	-1	-1
2	1	1	-1	-1	1	-1	-1	-1	1	-1
3	1	1	1	1	1	1	-1	-1	-1	1
4	1	-1	1	-1	1	1	-1	1	-1	-1
5	1	-1	1	1	-1	1	1	-1	1	-1
6	1	1	1	1	-1	-1	-1	1	-1	-1
7	1	-1	-1	-1	-1	-1	1	-1	-1	1
8	1	-1	-1	1	1	-1	-1	1	1	1
9	1	1	-1	-1	-1	1	-1	1	1	1
10	1	1	1	-1	1	-1	1	1	1	1

Number of Runs	Optimal Run Sequence ϕ_{min}	No. of Pairs	Worst Case ϕ_{max}	No. of Pairs
2	1.000	20	1.000	21**
3	1.000	8	1.000	9**
4	1.000	2	1.000	8**
5	.600	12	1.000*	5
6	$.66\overline{6}$	2	1.000*	2
7	.429	12	.714*	2
8	.500	2	.500	8**
9	$.33\overline{3}$	8	$.33\overline{3}$	8
10	.200	20	.200	20

*$\phi_{max} > \phi_{min}$ for some suboptimal sequence of runs.

**$\phi_{max} = \phi_{min}$, but the number of pairs attaining the maximum is greater.

Table 6: Results for an optimal interruptible sequence of runs leading to a D-optimal saturated $k = 9$, $N = 10$ experiment.

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REPORT DOCUMENTATION PAGE

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1. REPORT NUMBER: 106-11
2. GOVT ACCESSION NO.: AD-A115 786
3. RECIPIENT'S CATALOG NUMBER:
4. TITLE (and Subtitle): INTERRUPTIBLE SUPERSATURATED TWO-LEVEL DESIGNS
5. TYPE OF REPORT & PERIOD COVERED: Technical Report
6. PERFORMING ORG. REPORT NUMBER:
7. AUTHOR(s): James L. Rosenberger and Dennis E. Smith
8. CONTRACT OR GRANT NUMBER(s): N00014-75-C-1054
9. PERFORMING ORGANIZATION NAME AND ADDRESS: Desmatics, Inc., P. O. Box 618, State College, PA 16801
10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: NR 042-334
11. CONTROLLING OFFICE NAME AND ADDRESS: Office of Naval Research, Arlington, VA 22217
12. REPORT DATE: June 1982
13. NUMBER OF PAGES: 13
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office):
15. SECURITY CLASS. (of this report): Unclassified
15a. DECLASSIFICATION/DOWNGRADING SCHEDULE:
16. DISTRIBUTION STATEMENT (of this Report): Distribution of this report is unlimited.
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report):
18. SUPPLEMENTARY NOTES:
19. KEY WORDS (Continue on reverse side if necessary and identify by block number):
D-optimality
Interruptible Designs
Two-Level Designs

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Interruptible designs possess a robustness against possible premature termination of an experiment. We consider such two-level designs for a first-order model and present interruptible sequences which lead to the D-optimal saturated design for four to nine factors. Premature termination of the experiment at any stage results in a supersaturated design with minimum loss of information about the factors. The loss for these designs which is measured by the pairwise orthogonality between columns, is compared with that of the worst case for randomly ordered sequences.

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