Computer Aided Design of Experiments

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A computer oriented method which assists in the construction of response surface type experimental plans is described. It takes into account constraints met in practice that standard procedures do not consider explicitly. The method is a sequential one and each step covers the experimental region uniformly. Applications to well-known situations are given to demonstrate the reasonableness of the procedure. Application to a "messy" design situation is given to demonstrate its novelty.

0. INTRODUCTION

The studies which preceded the findings and conclusions reported in this paper were undertaken to meet some practical aspects of experimental planning that are not covered by many of the more commonly used experimental plans, especially in model building and response surface exploration. The ability to do reasonable smoothing of the results and to have plans as model-free as possible was of particular interest.

Considerable work has been done in deriving experimental plans for response surface exploration by first postulating a model and then deriving a plan based on one or more criteria of optimality. Excellent results have been achieved via this route and some of the derived plans have been used widely. However, there are a number of planning situations that present practical constraints that other approaches either ignore or compromise. The more important ones are:

(i) *Models are vague.*

At the time of the construction of the experimental plan, the relationships between the factors and the responses are difficult to put in specific mathematical form—either in terms of a given function or a class of functions. Sometimes detailed information is contained in the results of runs that have already been executed. These runs should be a part of the plan and the subsequent analysis. Prior information or assumptions on the response of the system may be available only in general terms, e.g. a set of candidate points for a four-factor experiment described as a $2 \cdot 3 \cdot 5^2$ limits the relationship of the first factor and the response to a linear one and the second one to a quadratic (without a transformation). It is doubtful if the two five-level factors reflect the desire to estimate up to a fourth degree polynomial; rather, they probably reflect hedges against complexity or uncertainties such as what transformations of the factors should be used, the possible existence of asymptotes, and the like. Of as much practical

importance as any other consideration is the fact that each experiment is a multiple response one—five to twenty responses are not uncommon. Hence, experimental plans based on postulated models really have to consider multiple models. So here we assume that the details of the model building come more after the execution of the experiment than before it.

(ii) *Practical factor spaces can be "messy".*

A standard design procedure is to assume that the factor space can be represented as a region bounded by a p-dimensional hypercube or hypersphere with any point on or inside the cube or sphere being a candidate design point. Simplification is often achieved by limiting the candidates to certain lattice points. However, practical problems of realizability, operability, and availability of the system being studied make it necessary to chop corners off the cubes, take slices off the spheres, or to dig holes in the region. In such cases, it can become difficult to obtain an explicit mathematical description of the region and the boundary enclosing it. "Messy" as these regions may be, the practical possibilities are usually lattice points and it is often possible to make a tabulation of these candidates. In the developments here we will assume that a tabulation of candidate design points exists.

(iii) *Replication is a separate design consideration.*

A primary constraint on the experimenter is the number of experimental runs that he can make; this number is small compared to the number that are conceptually possible. When this number is fixed and the model is fixed, almost all "optimum" allocation schemes lead to "uncomfortable" replication; that is, the number of distinctly different points to be observed is small and some are heavily replicated. The experimenter's model is usually vague and uncertain, so he wants to cover his region reasonably well. Having accomplished this, he will consider replication to assess the validity of his prior estimates of the control and reproducibility of his process. We focus on the primary problem of "covering the region" and leave replication as an important but secondary consideration.

1. Criteria for a Design

The conditions and restraints under which the experimental program is to be executed lead to the conclusion that the factorial design (when the factor space is the proper shape) is an ideal and the more levels per factor the better. The factorial gives good, uniform coverage of the factor space and it gives an opportunity to develop models of the observed phenomenon with a minimum of assumptions. Although we envision the use of any planning procedure that we develop to be used primarily in nonfactorial type situations, we establish a criterion that when the factor space is nice and round or square, the procedure should generate a factorial type structure or a reasonable facsimile. No explicit criterion for measuring coverage will be used, but we use these guide lines: (1) when the design is complete, no candidate point not included in the design should be "too far" from a design point, and (2) coverage should start on the boundary of the factor space. The latter seems reasonable as follows: If the

number of factors is p, the number of runs is n, and n is not much larger than p, then no amount of wishful thinking can produce a model that is other than linear and additive. The best way to learn about slopes is to go to the extremes of the factor space, so we start here. If prior information runs counter to this assumption, we incorporate this information into the design by forcing the appropriate points in the space to be in the design.

2. GENERAL STATEMENT OF THE DESIGN PROCEDURE

There are p factors $(x_1, x_2, \cdots, x_p)$ that can be controlled. An experimental design is to be selected from a set of N points in the p-dimensional space defined by the factors. We denote these N points as candidates and represent them as follows:

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{p1} \\ x_{12} & x_{22} & \cdots & x_{p2} \\ & \cdots & & \\ x_{1\nu} & x_{2\nu} & \cdots & x_{p\nu} \\ & \cdots & & \\ x_{1N} & x_{2N} & \cdots & x_{pN} \end{bmatrix} \tag{2.1}$$

A design will be $n \leq N$ distinct points chosen from the candidates. The design points are chosen sequentially. At each stage in the choice sequence, the aim will be to have the points in the design "uniformly" spaced over the space defined by the candidates. We make this explicit. Let

$$D_{\nu\mu}^2 = ||\mathbf{x}_\nu - \mathbf{x}_\mu||^2 = \sum_{k=1}^{p} (x_{k\nu} - x_{k\mu})^2 \tag{2.2}$$

the squared distance from point ν to point μ.

Let $P_{1\bullet}, P_{2\bullet}, \cdots, P_{i\bullet}, \cdots, P_{k\bullet}, k* < n$, be k points that have been assigned to the design. Then define

$$\Delta_\nu^2(k) = \min_{i*} \{D_{1*\nu}^2, D_{2*\nu}^2, \cdots, D_{k*\nu}^2\} \nu \neq i* = 1, 2, \cdots, N \tag{2.3}$$

Thus $\Delta_\nu^2(k)$ defines the squared distance from candidate point ν, not yet in the design, to the nearest design point.

For the $(k + 1)$st point in the design, we choose from among the remaining $(N - k)$ candidates using the criterion

$$\Delta_{k+1}^2 = \max_{\nu \neq i*} \{\Delta_\nu^2(k)\} \tag{2.4}$$

Thus we choose the point among those remaining that is farthest from an existing design point.*

It remains to give a starting procedure. If a decision is made a priori that certain candidates must be included in the design, once these are specified the relations (2.2), (2.3), and (2.4) can be used repetitively to select the remaining

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* Note: The interpoint distances have to be calculated but once. The quantities $\Delta_\nu^2(k)$ can be obtained by simple summing in a vector generated from the interpoint distances.

points necessary to make a design of size n. Otherwise, to start we use

$$D^2_{\text{max}} = \max_{\substack{\nu, \mu \\ \nu < \mu}} ||\mathbf{x}_\nu - \mathbf{x}_\mu||^2 \tag{2.5}$$

That is, the first two points of the design P_{1*} and P_{2*} are selected by choosing the two candidate points that are farthest apart. Then max $\{\Delta^2_\nu(k)\}$ is used to select the remaining $(n - 2)$.

There is no guarantee of uniqueness of D^2_{max} or Δ^2_{k+1} for any of value of k. There may be more than one pair of points that are the same distance apart and there may be more than one candidate point whose minimum distance to a design point gives the same maximum. However, the procedure is aimed at aiding in the choice of a design and not mathematical uniqueness. The following is used to break ties: Each point is identified from its index in (2.1). If Δ^2_{k+1} is the same for points $\nu_1, \nu_2, \cdots, \nu_r$, then the $(k + 1)$st point is selected by choosing the point with the smallest index. The other $(r - 1)$ points are tabulated for reference. All pairs of points are labeled (ν, μ) with $\nu < \mu$. If $D^2_{\nu\mu}$ is the same for several pairs (ν, μ), the pair chosen to start is the one with the smallest ν index. This method of breaking ties may appear arbitrary and of doubtful rationale. However, in the "messy" space situations the probability of ties has been observed to be small. In spaces with a more regular structure, all the ties usually get into the design if n is large enough. If they are omitted by the size of n, substitution of tied points is always available.

Since the procedure outlined in (2.1) through (2.5) is based on the calculation of distances, it is sensitive to the metrics for the various factors. But this is a common problem in all quantitative factor design problems. Choice of the metrics is the choice of the experimenter. In the absence of any other criterion, it is recommended that a standardization step that will put $\mathbf{X}'\mathbf{X}$ is the form of a cosine (correlation) matrix be carried out first. That is, the elements of $\mathbf{X}$ are a result of the transformations

$$x_{i\nu} = (X_{i\nu} - X_{i.})/[\sum (X_{i\nu} - X_{i.})^2]^{\frac{1}{2}}$$
$$\text{where} \quad X_{i.} = \sum_\nu X_{i\nu}/N \tag{2.6}$$

and the $X_{i\nu}$ are thr raw coordinate values.

The transformation (2.6) will suffice to produce reasonable designs if the factor space does not deviate "too much" from a hypercube or hypersphere. On the other hand, a study of the maximum-minimum distance procedure will show that it will tend to follow the shape of the space too faithfully, especially for the smaller values of n which are those of interest. To circumvent this difficulty and to get designs that have more uniform coverage, the distance calculations are proceeded by an orthonormalizing transformation. Using a Choleski variant of Gaussian elimination, make the decomposition

$$\mathbf{X}'\mathbf{X} \to \mathbf{T}'\mathbf{T} \tag{2.7}$$

where $\mathbf{T}$ is upper triangular.

This assumes that $\mathbf{X}$ is of rank p, a not unreasonable assumption. If rank $(\mathbf{X}) < P$, then it seems that the process under investigation has not been well defined. Using $\mathbf{T}$ next make the transformation

$$W = XT^{-1} \tag{2.8}$$

Then $W'W = I_p$ and we have tended to give the points a more spherical orientation. The distance calculations and the point choices are made using the elements of W rather than X.

3. Examples of the Design Procedure

A. Factorial Structure of the Form 5^2

The operation of the design procedure can be demonstrated with a simple two-factor situation with $N = 25$ candidate points as shown in Figure 1.
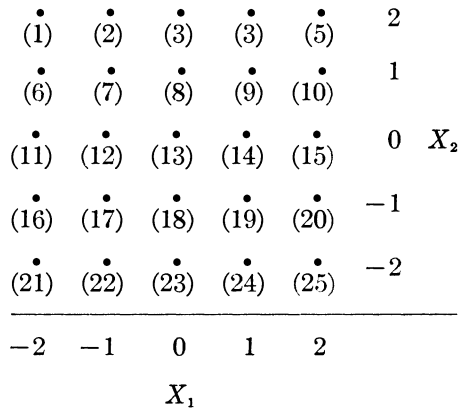
Figure 1—5^2

The step-by-step build-up of the design will go as follows:

Start: The pairs of points (1, 25) and (5, 21) are tied for the points being farthest apart. Choosing the pair having the point with the smallest index, viz. 1, the pair (1, 25) is chosen. Hence, the first two design points are:

$$\text{Point } 1 - \#(1) - (-2, 2)$$

$$\text{Point } 2 - \#(25) - (2, -2)$$

Choice: There are now $(N - 2) = 23$ of the candidate points not in the design. For each of these points we compute its squared distance to each point in the design, that is, points (1) and (25). For example, take point (2) with coordinates $(-1, 2)$. Its squared distance to point (1) is 1 and to point (25) is 25. Hence

$$\min \{D^2_{2,1}, D^2_{2,25}\} = \min \{1, 25\} = 1.$$

The same calculation is made for each point. It is clear that the points (5) and (21) are tied for being farthest from the design points (1) and (25) with a minimum squared distance of 25. Choosing the one with the smaller index, the third point is:

$$\text{Point } 3 - \#5 - (2, 2).$$

Choice: The procedure outlined for choosing point number three in the design is now applied sequentially. The next two obtained are:

$$\text{Point } 4 - \#(21) - (2, -2)$$
$$\text{Point } 5 - \#(13) - (0, 0).$$

Each of these points is unique and is not tied with another when it is a candidate to be chosen. Thus the procedure has produced a 2^2 using ± 2 as the levels for the first four points; then the center point is added. There are four candidates for the sixth point in the design, they are (3), (11), (15), and (23). Continued application of the procedure shows that each of these will be selected to fill out the 3^2 factorial. Four more selections give:

$$\text{Point } 6 - \#(3) \ \ - (0, 2)$$
$$\text{Point } 7 - \#(11) - (-2, 0)$$
$$\text{Point } 8 - \#(15) - (2, 0)$$
$$\text{Point } 9 - \#(23) - (0, -2)$$

This serves to demonstrate that the procedure is reasonable in a small, well-structured situation.

B.   *Factorial Structure of the Form* 4^4

The reasonableness of the design procedure and its usefulness in "discovering" designs can be further demonstrated by its performance in the four-factor situation with four levels for each factor denoted as $(-3, -1, 1, 3)$ in the raw units. This array is not one that fits directly into many standard design schemes, although one can generate certain candidates by association of the levels of the factors with those of a 2^8 system.

The indexing scheme used was to start with the point $(-3, -3, -3, -3)$, indexing through the levels of factors four, three, two, and one, in that order, to generate a total of 256 candidates.

The results of the procedure given in Section 2 are as follows:

1. *First two points*

$$\text{Point } 1 - \#(1) \ \ \ - (-3, -3, -3, -3)$$
$$\text{Point } 2 - \#(256) - (3, 3, 3, 3)$$

There are eight pairs of points tied with the greatest distance between them. They are readily seen to be the points corresponding to a 2^4 if the levels are ± 3. This pair is used to start as a result of the application of the tie-breaking procedure.

Based on the ties that occur in subsequent choices using the max-min algorithm, there appear to be "natural" designs of size $n = 8, 16, 18,$ and 26 in the smaller sizes that would be of interest.

2. *Up to* $n = 8$

After the points (1) and (256) are in the design, there are six points tied for inclusion. The next six iterations of the procedure bring them into the design. The points and their coordinates are:

$$
\begin{aligned}
&\text{Point 3} - (16) \quad - (-3, -3, 3, 3) \\
&\text{Point 4} - (52) \quad - (-3, 3, -3, 3) \\
&\text{Point 5} - (61) \quad - (-3, 3, 3, -3) \\
&\text{Point 6} - (196) - (3, -3, -3, 3) \\
&\text{Point 7} - (205) - (3, -3, 3, -3) \\
&\text{Point 8} - (241) - (3, 3, -3, -3)
\end{aligned}
$$

These are recognized as completing the one-half replicate of the 2^4 using the levels ± 3.

3. *Up to n = 16*

Once there are eight points in the design, there are eight points tied. The procedure includes them in their index order for the next eight points. Their indices and coordinates are:

$$
\begin{aligned}
&\text{Point 9} \;\; - (4) \quad\; - (-3, -3, -3, 3) \\
&\text{Point 10} - (13) \quad - (-3, -3, 3, -3) \\
&\text{Point 11} - (49) \quad - (-3, 3, -3, -3) \\
&\text{Point 12} - (64) \quad - (-3, 3, 3, 3) \\
&\text{Point 13} - (193) - (3, -3, -3, -3) \\
&\text{Point 14} - (208) - (3, -3, 3, 3) \\
&\text{Point 15} - (244) - (3, 3, -3, 3) \\
&\text{Point 16} - (253) - (3, 3, 3, -3)
\end{aligned}
$$

The first 16 points thus constitute the full 2^4 factorial using the levels ± 3 and all the starting point ties have been included.

4. *Up to n = 18*

The next two points (ties) included are:

$$
\begin{aligned}
&\text{Point 17} - (86) \quad (-1, -1, -1, -1) \\
&\text{Point 18} - (171) \quad (1, 1, 1, 1)
\end{aligned}
$$

These two points together constitute a center point since the center of gravity $(0, 0, 0, 0)$ is not a candidate point.

5. *Up to n = 26*

The next eight points (ties) included are:

$$
\begin{aligned}
&\text{Point 19} - (43) \quad\; - (-3, 1, 1, 1) \\
&\text{Point 20} - (88) \quad\; - (-1, -1, -1, 3) \\
&\text{Point 21} - (94) \quad\; - (-1, -1, 3, -1) \\
&\text{Point 22} - (118) - (-1, 3, -1, -1) \\
&\text{Point 23} - (139) - (1, -3, 1, 1) \\
&\text{Point 24} - (163) - (1, 1, -3, 1) \\
&\text{Point 25} - (169) - (1, 1, 1, -3) \\
&\text{Point 26} - (214) - (3, -1, -1, -1)
\end{aligned}
$$

The build-up of the design points is shown in Figure 2. A number in a block indicates that the point is included, the number giving the step in the the procedure at which it was chosen.

4^4 FACTORIAL STRUCTURE

X_3	X_4	-3				-1				1				3			
		-3	-1	1	3	-3	-1	1	3	-3	-1	1	3	-3	-1	1	3
-3	-3	2		11										13		8	
	-1																
	1											24					
	3	9		4										6		15	
-1	-3																
	-1					17	22								26		
	1																
	3					20											
1	-3									25							
	-1																
	1		19							23	18						
	3																
3	-3	10		5										7		16	
	-1					21											
	1																
	3	3		12										14			1

X-axis: X_1, X_2 (top)

NUMBERS GIVE THE ORDER IN WHICH THE POINTS ENTER THE DESIGN

FIGURE 2

Altogether the procedure develops three reasonable designs in addition to the obvious factorials.

(i) *26 Point Design*

This balanced. All levels are covered. For each factor the levels -3 and 3 are observed nine times each and the levels -1 and 1, four times each. The design vectors are nearly orthogonal.

(ii) *18 Point Design*

Two reasonable designs are evident. Either of the one-half replicates (1 through 8 or 9 through 16) augmented by the last ten points. Again, there is balance and near orthogonality.

C. *Factorial Structure with Inoperable Regions*

This last example is in the category of messy factor spaces. It is an example of a design situation for which the procedure should give real assistance. The structure of this problem is best shown in Figure 3. It is of the form $3^4.4$. How-

MESSY DESIGN PROBLEM

ORTHONORMALIZED VECTORS
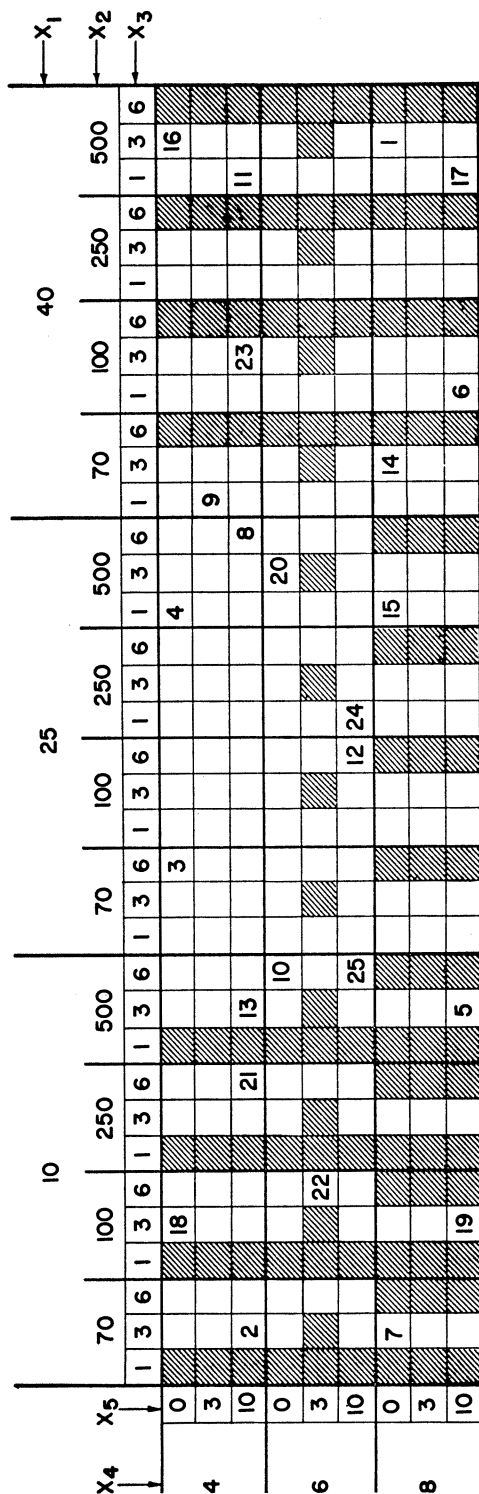
SHADED AREAS ARE NOT REALIZABLE

n = 25

FIGURE 3

ever, the shaded blocks represent factor combinations that are not available or not operable so that $N = 216$, rather than the 324 that it would be if the complete factorial structure were available. An assessment of the imbalance caused by the elimination of the 108 factor combinations can be obtained from the eigenvalues of $X'X$ in correlation form. For the full factorial $\lambda = 1$ $i = 1, 2, \cdots, 5$; for the $N = 216$ points, they are 1.577, 1.000, 1.000, 0.924, 0.499. Because of this imbalance, the orthonormalizing procedure was used prior to the execution of the max-min algorithm.

In this example ties are few. Two pairs of points are tied for the starting pair. In the succeeding 23 steps using max-min, pairs of points are tied at four steps and both points in the pair enter the design. In Figure 3, the numbers in the blocks again give the points that are included in the design and the order in which they are chosen. A design of size $n = 25$ is shown to assist in an assessment of the procedure. Table 1 gives a cross tabulation of the number of times pairs of factor levels appear both as candidates and as elements of design points. The design points are well distributed over the factor space. The design vectors are nearly orthogonal; the correlation matrix for these vectors is:

$$X'X_{25} = \begin{bmatrix} 1.000 & .036 & .129 & -.103 & .022 \\ & 1.000 & -.007 & -.049 & -.082 \\ & & 1.000 & -.110 & .004 \\ & & & 1.000 & .138 \\ \text{Symmetric} & & & & 1.000 \end{bmatrix}$$

Its eigenvalues are: 1.266, 1.103, .961, .861, .809.

Figure 4 shows another 25-point design and another use of the design procedure. Note that the numbered blocks go from 1 to 14. The other 11 points in

TABLE 1

TABLE 1 *Messy Design Problem Cross Tabulation of Candidate & Design Points M = 25.*

x_2

Totals	70	100	250	500	
68 (8)	17 (2)	17 (2)	17 (0)	17 (4)	40
92 (7)	23 (1)	23 (1)	23 (1)	23 (4)	25 x_1
56 (10)	14 (2)	14 (3)	14 (1)	14 (4)	10
216 (25)	54 (5)	54 (6)	54 (2)	54 (12)	Totals

Totals	1	3	6	
68 (8)	36 (4)	32 (4)	----	40
92 (7)	36 (3)	32 (1)	24 (3)	25 x_1
56 (10)	----	32 (6)	24 (4)	10
(25)	72 (7)	96 (11)	48 (7)	Totals

x_4

Totals	4	6	8	
68 (8)	24 (4)	20 (0)	24 (4)	40
92 (7)	36 (3)	32 (3)	24 (1)	25 x_1
56 (10)	24 (4)	20 (3)	12 (3)	10
(25)	84 (11)	72 (6)	60 (8)	Totals

x_5

Totals	0	3	10	
68 (8)	24 (3)	20 (1)	24 (4)	40
92 (7)	32 (4)	28 (0)	32 (3)	25 x_1
56 (10)	20 (3)	16 (1)	20 (6)	10
(25)	76 (10)	64 (2)	76 (13)	Totals

x_3

Totals	1	3	6	
54 (12)	18 (4)	24 (5)	12 (3)	500
54 (2)	18 (1)	24 (0)	12 (1)	250 x_2
54 (6)	18 (1)	24 (3)	12 (2)	100
54 (5)	18 (1)	24 (3)	12 (1)	70
(25)	72 (7)	96 (11)	48 (7)	Totals

x_4

Totals	4	6	8	
54 (12)	21 (5)	18 (3)	15 (4)	500
54 (2)	21 (1)	18 (1)	15 (0)	250 x_2
54 (6)	21 (2)	18 (2)	15 (2)	100
54 (5)	21 (3)	18 (0)	15 (2)	70
(25)	84 (11)	72 (6)	60 (8)	

x_5

Totals	0	3	10	
54 (12)	19 (6)	16 (0)	19 (6)	500
54 (2)	19 (0)	16 (0)	19 (2)	250 x_2
54 (6)	19 (1)	16 (1)	19 (4)	100
54 (5)	19 (3)	16 (1)	19 (1)	70
(25)	76 (10)	64 (2)	76 (13)	Totals

x_4

Totals	4	6	8	
48 (7)	24 (3)	24 (4)	----	6
96 (11)	36 (5)	24 (1)	36 (5)	3 x_3
72 (7)	24 (3)	24 (1)	24 (3)	1
(25)	84 (11)	72 (6)	60 (8)	Totals

x_5

Totals	0	3	10	
48 (7)	16 (1)	16 (1)	16 (4)	6
96 (11)	36 (6)	24 (0)	36 (5)	3 x_3
72 (7)	24 (2)	24 (1)	24 (4)	1
(25)	76 (10	64 (2)	76 (13)	Totals

x_5

Totals	0	3	10	
60 (8)	20 (4)	20 (0)	20 (4)	8
72 (6)	28 (2)	16 (1)	28 (3)	6 x_4
84 (11)	28 (4)	28 (1)	28 (6)	4
(25)	76 (10)	64 (2)	76 (13)	Totals
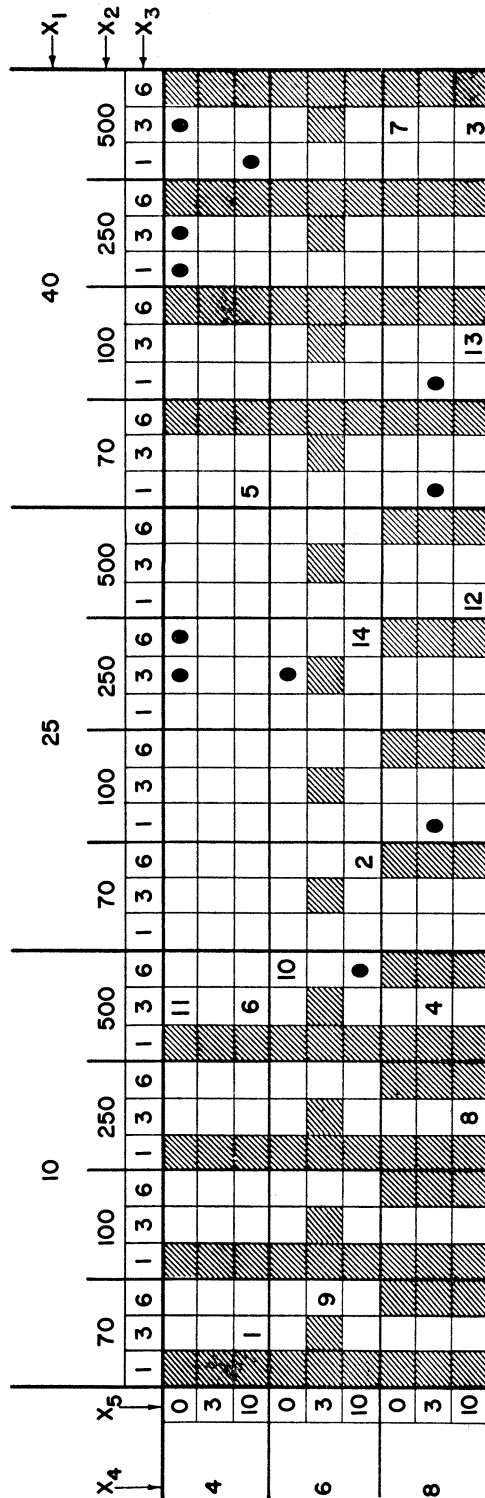
FIGURE 4

the design are represented by the blocks with dots; they correspond to factor combinations that had been executed prior to the design. Hence the procedure started with $k = 11$ and iterated to $n = 25$. Again, the coverage is reasonably uniform, indicating a "good" design.

4. Using the Method

The algorithm, as outlined in Section 2, has been used in a large number of nonstandard design situations and in each case has been able to produce a practical design. However, its spirit is not that of a cookbook, but that of an assistant. Those who have used it have found a number of ways to vary the parameters of the algorithm to give information on the structure of the factor space that make it possible to construct small designs that are not obvious by inspection. Especially attractive has been the "boss option," the ability to include points specified by authority without sacrificing the overall objectives of the exploration.

Although no examples were given, the procedure has been found to do a creditable job for mixture systems and for cases in which a nonlinear model has been specified, without the combinatorial problems inherent in some other approaches. Of course, if there is a model that one wants to use to fit the data, the design vectors can be expanded to generate the vectors appropriate to the model, and these generated vectors used as input to the procedure. Candidate designs can then be evaluated by looking at variance contours, determinant of $(\mathbf{X}'\mathbf{X})^{-1}$, and the like. However, building models in constrained spaces such as in the "messy" design example is a problem in itself. All parameters in the usual response surface smoothing function are not always estimable, either mathematically or practically.

One obvious limitation of a method based on interpoint distances is the computer memory necessary to store the distances, and this is true for even the largest computers. For problems having a very large number of candidate points, it has been found that a workable procedure is to first calculate the radius for each point, sort the radii, choose radii bands, and then have only points in these bands as input to the selection procedure.

The algorithm has also been applied in post-mortem data analyses for situations in which the data collection procedure has resulted in pseudo-replication and, hence, a poorly conditioned $\mathbf{X}'\mathbf{X}$ matrix.

5. Computer Program

CADEX-I, a computer program to implement the procedure, has been written in FORTRAN IV for the UNIVAC 1107 or 1108 and makes extensive use of the high-speed drum of these machines. A large number of auxiliary parameters, not described in the text, are computed to assist the user. Operating instructions and a program deck are available from the authors.