This research was partially supported by the United States Navy through the Office of Naval Research under Contract Nonr-1202(17) Project NR 042 222.
1. INTRODUCTION

We shall omit introductory material and references which would duplicate those given by Draper and Stoneman (1966) and proceed directly to a statement of the problem. Suppose we wish to fit a response function of the form

\[ E(y) = \beta_0 + \sum_{i=1}^{p+q} \beta_i x_i + \sum_{i>p}^{p+q} \sum_{j \geq 1}^{p+q} \beta_{ij} x_i x_j \]  

(1.1)

to a set of observations \((y_u, x_{1u}, \ldots, x_{pu}, x_{(p+1)u}, \ldots, x_{(p+q)u})\) where factors \(x_1, x_2, \ldots, x_p\) can be set at only two levels (which we shall denote by \(-a\) and \(+a\)) and factors \(x_{p+1}, x_{p+2}, \ldots, x_{p+q}\) can be set at four levels (which we shall suppose are \(-d, -c, c,\) and \(d\)). How should the design points be selected so that (1.1) can be fitted and so that the design has certain desirable characteristics. We shall consider the following features to be desirable. The design should

1. provide a sufficient number of runs for the estimation of all coefficients in the polynomial of form (1.1),
2. allow separate estimation of all coefficients, that is, provide a non-singular moment matrix,  
   
   \[ (1.2) \]
3. allow for repeat runs for the estimation of pure error,
4. consistent with 1, 2, and 3, use as few experimental runs as possible,
5. make zero as many design moments as possible so that
   a. the estimates of the \(\beta\)'s are as little correlated as possible,
b. the estimated coefficients are biased as little as possible by coefficients which have been ignored (that is, are not included in the polynomial), and

c. the least square calculations are made as simple as possible.

We shall require that the $X^T X$ matrix (in the least squares estimation procedure $\mathbf{b} = (X^T X)^{-1} X^T \mathbf{y}$) obey the following conditions (where $N$ is the number of experimental runs):

1. $\sum_{u=1}^{N} x_{iu} = 0$  \hspace{1cm} i = 1, \ldots, p+q

2. $\sum_{u=1}^{N} x_{iu} x_{ju} = 0$  \hspace{1cm} i \neq j
   \hspace{1cm} i = 1, \ldots, p+q
   \hspace{1cm} j = 1, \ldots, p+q

3. $\sum_{u=1}^{N} x_{iu}^2 = \sum_{u=1}^{N} x_{ju}^2 > 0$  \hspace{1cm} i = 1, \ldots, p
   \hspace{1cm} j = 1, \ldots, p

4. $\sum_{u=1}^{N} x_{iu}^2 = \sum_{u=1}^{N} x_{ju}^2 > 0$  \hspace{1cm} i = p+1, \ldots, p+q
   \hspace{1cm} j = p+1, \ldots, p+q

5. $\sum_{u=1}^{N} x_{iu} x_{ju} x_{hu} = 0$  \hspace{1cm} i \neq j \neq h
   \hspace{1cm} i = 1, \ldots, p+q
   \hspace{1cm} j = p+1, \ldots, p+q
   \hspace{1cm} h = p+1, \ldots, p+q

6. $\sum_{u=1}^{N} x_{iu} x_{ju}^2 = 0$  \hspace{1cm} i \neq j
   \hspace{1cm} i = 1, \ldots, p+q
   \hspace{1cm} j = p+1, \ldots, p+q

7. $\sum_{u=1}^{N} x_{iu}^3 = 0$  \hspace{1cm} i \neq j \neq h \neq g
   \hspace{1cm} i = p+1, \ldots, p+q
   \hspace{1cm} j = p+1, \ldots, p+q
   \hspace{1cm} h = p+1, \ldots, p+q
   \hspace{1cm} g = p+1, \ldots, p+q

8. $\sum_{u=1}^{N} x_{iu} x_{ju} x_{hu} x_{gu} = 0$
9. \[ \sum_{u=1}^{N} x_{1u}^2 x_{ju} x_{hu} = 0 \]

10. \[ \sum_{u=1}^{N} x_{1u}^2 x_{ju}^2 = \sum_{u=1}^{N} x_{hu}^2 x_{gu} > 0 \]

11. \[ \sum_{u=1}^{N} x_{1u}^3 x_{ju} = 0 \]

12. \[ \sum_{u=1}^{N} x_{1u}^4 = \sum_{u=1}^{N} x_{ju}^4 > 0 \]

Of the conditions (1.3), parts 1, 2, 5, 6, 7, 8, 9, and 11 allow us to obtain an \( X'X \) matrix of satisfactory form which contains a large number of zero elements (see part 5 of conditions (1.2)). Parts 3, 4, 10, and 12 are not very restrictive, are easy to satisfy, and allow us to provide general inverses for the \( X'X \) matrices obtained.

2. CONSTRUCTION OF DESIGNS

The method of constructing designs in this case is similar to the method of construction developed for the \( 2^p q \) case but the non-availability of a zero level for factors at more than two levels creates some additional difficulties. We shall present the method via the following example.
Suppose we have \( p+q = 8 \) variables to investigate and of these \( p = 5 \), denoted by \( x_1, x_2, x_3, x_4, x_5 \), must be examined at two levels, \(-a\) and \( a\), and the remaining \( q = 3 \), denoted by \( x_6, x_7, x_8 \), must each be examined at four levels, \(-d, -c, c, d\). The response surface design will then be chosen from the 2048 runs of the \( 2^{5.4.3} \) full factorial. We wish to estimate the 15 coefficients of the polynomial

\[
E(y) = \beta_0 + \sum_{i=1}^{8} \beta_i x_i + \sum_{i=6}^{8} \sum_{j=1}^{8} \beta_{ij} x_i x_j.
\]

(2.1)

The 2048 design points can be divided into the eight sets shown in Table 1 where, for example, set 1 consists of the 256 runs obtained by placing either a plus or a minus sign before the numbers \( a \) and \( d \). By dividing

<table>
<thead>
<tr>
<th>Table 1</th>
<th>( 2^{5.4.3} ) Full Factorial Design</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variable</td>
<td>( x_1 \ x_2 \ x_3 \ x_4 \ x_5 \ x_6 \ x_7 \ x_8 )</td>
</tr>
<tr>
<td>Set</td>
<td>( a \ a \ a \ a \ a \ d \ d \ d )</td>
</tr>
<tr>
<td>Hypersphere 1</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>( a \ a \ a \ a \ a \ d \ d \ d )</td>
</tr>
<tr>
<td>Hypersphere 2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>( a \ a \ a \ a \ a \ d \ d \ c )</td>
</tr>
<tr>
<td>3</td>
<td>( a \ a \ a \ a \ a \ d \ c \ d )</td>
</tr>
<tr>
<td>4</td>
<td>( a \ a \ a \ a \ a \ c \ d \ d )</td>
</tr>
<tr>
<td>Hypersphere 3</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>( a \ a \ a \ a \ a \ c \ c \ d )</td>
</tr>
<tr>
<td>6</td>
<td>( a \ a \ a \ a \ a \ c \ d \ c )</td>
</tr>
<tr>
<td>7</td>
<td>( a \ a \ a \ a \ a \ d \ c \ c )</td>
</tr>
<tr>
<td>Hypersphere 4</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>( a \ a \ a \ a \ a \ c \ c \ c )</td>
</tr>
</tbody>
</table>
the design into sets in this manner, we can regard each of the eight sets of Table 1 as a $2^8$ full factorial design. For example, set 3 is a $2^8$ full factorial design with variables $x_1, x_2, x_3, x_4,$ and $x_5$ at levels $-a$ and $a$, variables $x_6$ and $x_8$ at levels $-d$ and $d$, and variable $x_7$ at levels $-c$ and $c$. A further property of the 2048 design points is that they can be divided into the four groups or hyperspheres shown in Table 1 in such a way that the points of each group lie on a hypersphere in eight dimensional space. The center of each hypersphere is at $(x_1, x_2, \ldots, x_8) = (0, 0, \ldots, 0)$. If a group contains runs in which $w (=0,1, \text{or} \ 2)$ of the four level variables have levels $-d$ and $d$, the points of the group lie on a hypersphere with radius $(5a^2 + wd^2 + (3-w)c^2)^{1/2}$.

One possibility for choosing a subset of runs for a response surface design is to make use of the points in one or more hyperspheres and delete the points in all other hyperspheres. Selection of a single hypersphere does not provide a suitable design, however, since (Stoneman, 1966), the runs of a single hypersphere give rise to a singular $X'X$ matrix and thus will not allow separate estimation of all parameters in (2.1). A singular $X'X$ matrix can also arise from some pairs of hyperspheres, for example hyperspheres 1 and 4. We can, however, select other pairs of hyperspheres (for example hyperspheres 2 and 4) and also any three hyperspheres.

In the general case, any subset of hyperspheres which does not give rise to a singular $X'X$ matrix will provide a design. However, it will usually have an unreasonably large number of runs and thus some method of reducing the number of runs is needed.
As mentioned above, each hypersphere can be considered as a full two level factorial design and thus we can reduce the number of runs by using standard methods (see Box and Hunter, 1961 a, b) to fractionate these sets.

In order to achieve the conditions (1.3), the final design must be such that the factorial fractionation does not confound

1. any main effect with the mean,
2. any main effect with any other main effect,
3. any main effect with any two-factor interaction of the four-level factors. (Note that the conditions (1.3) do not forbid the confounding of any main effect with any two-factor interaction of the two-level factors.),
4. any main effect with any quadratic effect of the four-level factors,
5. any two-factor interaction of two four-level factors with any other two-factor interaction of two four-level factors,
6. any two-factor interaction of two four-level factors with any quadratic effect of the four-level factors.

Direct fractionation of the sets in Table 1 can be carried out, making sure that the requirements 1, ..., 6 above are not violated for each set. However a more economical design can be achieved if the improved method of fractionation given by Draper and Stoneman (1966) is applied. In this improved method, a violation of the relationships (2.2) can be tolerated within a set provided that a compensating violation occurs in another set so that, in the final design, no violation occurs.
This is not always possible and is sometimes difficult to find. In dividing sets in this manner we must observe the following general rules.

1. For any pair of selected sets, a violating word must be balanced in two or more comparable sets.
   (In our specific example, we could use the word 16 if, in both sets, variable $x_6$ takes either the levels $\pm c$ or $\pm d$, for example, we could use the word 16 in sets 2 and 3 because variable $x_6$ takes the levels $\pm d$ in both of these sets. Also we could use the word 167 if, in both sets, the 67 column of the $X$ matrix has levels $\pm c^2$ or $\pm cd$ or $\pm d^2$, for example, we could use the word 167 in sets 3 and 4 because the 67 column of the $X$ matrix has levels $\pm cd$ in both of these sets.)

2. The violating word must represent a main effect or an interaction which either
   (a) is not associated with a coefficient to be estimated in (1.1). (In our example, we could use the word 18 since $\beta_{18}$ does not appear in (2.1).

   or (b) if an associated coefficient does appear in (1.1), will subsequently not be confounded with an effect corresponding to any other coefficient also appearing in (1.1).

   (In our example, we could use 67 if, in the subsequent design, 67 is not aliased with any effect corresponding to any other coefficient in (2.1).)
3. The violating word must appear as a positive word in the defining relation for one of the two chosen fractional sets and as a negative word in the defining relation for the other set.

(In our example, if we chose sets 2 and 3 and the word 26 then, if we used I = 26 in set 2, we must use I = -26 in set 3.)

4. The final design must contain the same number of design points from each of the two selected sets.

(In our example, if we used I = 12 in set 2, and I = -12 in set 3, the final design must contain the same number of design points from both sets 2 and 3.)

Rules 2, 3, and 4 also applied in the $2^{p_3}q$ case (Draper and Stoneman, 1966). Rule 1 is necessarily different since, in the $2^{p_4}q$ case, no zero level exists.

As an example in the $2^{5_4^3}$ case, consider the word 16 and the sets 2 and 3. The word 16

(a) is a violating word because it confounds the main effect of variable 1 with the main effect of variable 6,

(b) contains the letter 6 which represents a variable at the levels ±d in both sets, and

(c) does not represent a two-factor interaction corresponding to a coefficient appearing in polynomial (2.1).

Thus if in the final design the same number of design points are selected from sets 2 and 3, we can use 16 in the defining relation for either set and -16 in the defining relation for the other set.
In choosing the final design, more than one violation and compensation can be allowed, provided all rules are observed for each violation. For example, we can obtain a $2^{5\times 3}$ response surface design which satisfies our requirements and contains only 32 experimental runs, by using the defining relations shown in Table 2. In Table 2, the generators appear in the first row of each defining relation and all five letter words are omitted from the defining relations, since they will not be required for the alias relationships to be found in the next section.

**Table 2  Defining Relations**

<table>
<thead>
<tr>
<th>Set</th>
<th>Defining Relations</th>
<th>Number of Runs</th>
</tr>
</thead>
</table>
| 2   | $I=-16=26=-37=47=-58$  
    | $=-12=1367=-2367=1237=-1467=2467=-34$  
    | $=-1247=1346=-2346=1234=1568=-2568$  
    | $=3578=-4578=1258=3458$ | $2^{8-5}=8$ |
| 3   | $I=16=-26=-37=-47=58$  
    | $=-12=-1367=2367=1237=-1467=2467=34$  
    | $=1247=1346=-2346=-1234=1568=-2568$  
    | $=-3578=-4578=-1258=3458$ | $2^{8-5}=8$ |
| 4   | $I=-16=26=37=-47=-58$  
    | $=-12=-1367=-2367=1237=1467=2467=-34$  
    | $=-1247=1346=2346=-1234=1568=2568$  
    | $=-3578=4578=-1258=3458$ | $2^{8-5}=8$ |
| 8   | $I=16=26=37=47=58$  
    | $=12=1367=2367=1237=1467=2467=34$  
    | $=1247=1346=2346=1234=1568=2568$  
    | $=3578=4578=1258=3458$ | $2^{8-5}=8$ |

**3. BIASES DUE TO UNESTIMATED COEFFICIENTS**

If we use designs of the type given above, we are tentatively entertaining the model (1.1). Suppose this model is inadequate; how would the estimates be affected? To examine
this question for the example above we shall suppose that the assumed polynomial (2.1) is inadequate because of failure to include second order terms such as the pure quadratic coefficients of the two-level variables, the crossproduct coefficients between two two-level variables, and the crossproduct coefficients between a two-level variable and a three-level variable. In other words, we suppose that the true model is the full, second order expression in all eight variables. (Other specified types of model inadequacy can be treated in exactly the same manner as below, of course.) The correct model then contains 30 extra terms of the form:

$$\sum_{i=1}^{5} \sum_{j=1}^{8} \beta_{ij} x_i x_j.$$  \hspace{1cm} (3.1)

Using the formula \( E(b) = \beta + A \beta_1 \) given by Box (1952) for evaluation of bias terms, we obtain the following relationships:

\[
\begin{align*}
E(b_{o}) & = \beta_0 + 4\beta_{11} + \beta_{22} + \beta_{33} + \beta_{44} + \beta_{55} - (a(c^2-d^2)/(c^2-d^2))[(a(\beta_{12} + \beta_{34}) + c(\beta_{16} + \beta_{26} + \beta_{37} + \beta_{47} + \beta_{58})] \\
E(b_{1}) & = \beta_1, \hspace{1cm} i=1, \ldots, 8 \\
E(b_{66}) & = \beta_{66} + (2a^2/(c^2-d^2))\beta_{12} + a/(c^2-d^2)[(c-d)(\beta_{47} + \beta_{58}) + (c+d)\beta_{37}] \\
E(b_{77}) & = \beta_{77} + (2a^2/(c^2-d^2))\beta_{34} + a/(c^2-d^2)[(c-d)\beta_{26} + (c+d)(\beta_{16} + \beta_{58})] \\
E(b_{88}) & = \beta_{88} + a/(c^2-d^2) [ (c+d)(\beta_{26} + \beta_{47}) + (c-d)(\beta_{16} + \beta_{37}) ] \\
E(b_{67}) & = \beta_{67} + (a^2/(c^2-d^2)) [(c-d)^2\beta_{13} + (c^2-d^2)(\beta_{14} + \beta_{23}) + (c+d)^2 \beta_{24}] \\
& + a/(c^2-d^2)/(c^2-d^2) [(c+d)(\beta_{17} + \beta_{36}) + (c-d)(\beta_{27} + \beta_{46})] \\
E(b_{68}) & = \beta_{68} + (a^2/(c^2-d^2))^2 [(c+d)^2\beta_{15} + (c^2-d^2) \beta_{25}] \\
& + a/(c^2-d^2)^2 [(c^2-d^2)(c-d)(\beta_{18} + \beta_{56}) + (c^2-d^2)(c+d)\beta_{28}] \\
E(b_{78}) & = \beta_{78} + (a^2/(c^2-d^2))^2 [(c^2-d^2)\beta_{35} + (c-d)^2 \beta_{45}] + a/(c^2-d^2)^2 [(c^2-d^2)(c-d)\beta_{38} \\
& + (c^2-d^2)(c+d)\beta_{48} + (c^2-d^2)(c+d)\beta_{57}) .
\end{align*}
\]
Relationships of this type and complexity occur whenever a highly fractionated design (here a \((1/64)\)-th fraction of the full \(2^54^3\) design) is employed, of course.

4. FURTHER DESIGNS

Many additional designs can be obtained through the application of the methods above. For a complete listing of designs for cases \(2^p4^q\) where \(1 \leq p \leq 9\) and \(1 \leq q \leq 9\) and \(p + q \leq 10\), see Stoneman (1966). For each listed design is given the number of runs, the number of coefficients to be estimated, the sets used, the defining relation for each set, the elements of the \((X'X)^{-1}\) matrix, and the biases arising from second order coefficients not estimated. Many of the designs listed do not contain repeat runs as given. However, in general, all fractional sets belonging to one hypersphere can be repeated for pure error estimation if, for every violating set in the hypersphere, there is a compensating set in the same hypersphere.

ACKNOWLEDGEMENT

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REFERENCES


3. RESPONSE SURFACE DESIGNS FOR FACTORS AT TWO AND FOUR LEVELS.

5. Norman R. Draper and David M. Stoneman

6. May, 1966

8a. Nonr-1202

8b. NR 042 222

10. Distribution of this document is unlimited.

13. Abstract: In a previous paper (Draper and Stoneman, 1966) we considered the construction of response surface designs for situations where p factors could be examined at two levels and q factors could be examined at three levels. These designs consisted of portions of the corresponding $2^p3^q$ factorial designs. In this paper we extend the construction method to situations where p factors are at two, and q factors are at four levels.

14. 1. Experimental design

2. Response surfaces

3. $2^p4^q$ fractions

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Security Classification