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Response Surface Designs for Factors at Two and Three Levels

by

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1. INTRODUCTION

Suppose we have a response $\eta$ which depends on a finite number of factors $\xi_1, \xi_2, \ldots, \xi_k$ through an unknown response relationship

$$\eta = f(\xi_1, \xi_2, \ldots, \xi_k).$$

Since an exact determination of a general relationship may be impossible, techniques for empirical examination of the response surface are often employed. A basic method of examining such a surface is through the $s_1 \times s_2 \times \ldots \times s_k$ factorial design (Fisher, 1935, Yates, 1935), in which the $i$-th factor is examined at $s_i$ levels, and the various main effects and interactions are evaluated (Davies, 1960, Chapters 7 and 8).

It is often difficult to guarantee that the basic experimental units will be homogeneous. For example if each run involves a fertilizer trial on a plot of ground, the physical location of one plot might lie in an extremely fertile region, while that of another plot might be in a region considerable less fertile. When differences of this type are known to occur, it is sensible to block the experiment so that such differences do not affect the more important estimates and are associated (or confused, of confounded) with estimates of small importance. (See Fisher, 1935, Barnard, 1936, Yates, 1937, Nair, 1938, Bose and Kishen, 1940, Fisher, 1942, Li, 1944, Rao, 1946, Finney, 1947, Kempthorne, 1947, Nair and Rao, 1948, Zelen, 1958, and Kurkjian, 1959.)

In many experimental situations full factorials, confounded or not, require too many experimental runs and fractional factorial designs must be used. The economy obtained in reducing the number of runs is balanced by a corresponding loss of information since either some or all of the estimated effects are associated or aliased with other estimates. Part of the art of
fractionating a factorial design lies in aliasing estimates believed, a priori, to be important with those believed to be unimportant so that any estimates can be tentatively associated with the "important" effect.

One of the first such designs was developed by Tippett (1934) and Finney (1945) was the first to introduce the theory for their selection. (See Brownlee, Kelly, and Loraine, 1948, Kitogawa and Mitome, 1953, Clatworthy, Connor, Deming, and Zelen, 1957, and Connor and Zelen, 1959, for catalogues of designs.) The very important class of two level fractional factorial designs appear in Plackett and Burman (1946) and Box and Hunter (1961a, b). The method of selection of a subset of runs from asymmetric full factorial designs has been developed by several authors, including Chakravarti, 1956, Morrison, 1956, Connor, 1960, Connor and Young, 1961, Fry, 1961, and Addelman, 1962a, b.

2. GRADUATING FUNCTIONS

As an alternative to evaluating factorial effects and interactions or perhaps as a subsequent investigation, we can fit, to a set of experimental results, a mathematical model which will grade or approximate the true but unknown response function \( n = f(\xi_1, \xi_2, \ldots, \xi_k) \) over some region of interest \( R \). Often, for example, a response function can be represented quite closely by a fitted polynomial equation over a limited region. In practice, the variables \( \xi_i \) are usually transformed to standardized or coded variables \( x_i, i = 1, 2, \ldots, k \), which are easier to manipulate than the original variables.

The region \( R \) is often of such a size that it is possible to obtain a good approximation to the true response function by use of a reasonably simple polynomial, perhaps one involving just first order terms or one involving all possible first order and second order terms in \( x_i \). (See, for example, Davies, 1960, Chapter 11.)
When data are not yet available, a suitable experimental design is required. (The center of the design is usually taken at the \( x \)-origin, incidentally.) In order to decide on one we need to be more specific about the desirable properties the design should possess. Box (1964) has given a list of twelve desirable features for response surface designs of any order. A specific design may not necessarily have all of these desirable features. However, there are a number of types of designs (some of which are rotatable designs which provide equal information in all directions of the factor-space) which do display many of them. (See, for example, Box, 1952, Box and Wilson, 1951, Box and Hunter, 1957, and Box and Behnken, 1960b. See also related papers by Box and Draper, 1959, and 1963, Bose and Draper, 1959, Hartley, 1959, DeBaun, 1959, Box and Behnken, 1960a, Draper, 1960a, Dykstra, 1959, and 1960, Das and Narasimham, 1962, and Das, 1963.)

If a first or second order polynomial is inadequate to represent the response surface, we might wish to use a third order polynomial. (See Gardiner, Grandage, and Hader, 1959, Draper, 1960b, c, 1961, and 1962, and Herzberg, 1964, for experimental designs.) Alternatively we can apply transformations (see Box and Tidwell, 1962, and Box and Cox, 1964) which may eliminate entirely the need for third order terms (and perhaps even second order terms as well.)
3. SPECIFIED DESIGN LEVELS

In choosing the runs of an experimental design, we may be restricted in various ways. Possible restrictions are that the design should be rotatable or require a minimal number of runs. Another possible restriction is the specification of the number of levels permitted for each factor. Two papers by DeBaun (1959) and Box and Behnken (1960b) consider the construction of second order designs when only three levels of each factor are to be used. DeBaun provides designs for three factors and Box and Behnken provide designs for 3, 4, 5, 6, 7, 9, 10, 11, 12, and 16 factors. These designs, which are effectively subsets or fractions of the $3^k$ factorial series, are used to fit a second order polynomial and are economical in that their redundancy factors (defined by Box and Behnken as the ratio N/L where N runs are employed to separately estimate L coefficients) are low.

In some experimental situations it may not be possible to fit a full second order polynomial in all variables or such a polynomial may not be necessary. Suppose, for example, that some factors are to be examined at two levels and some at three levels. Then we cannot fit a polynomial which includes squared terms in the two-level variables since these coefficients cannot be estimated. To elaborate this point consider the case where we are examining $k = 4$ variables, $p = 2$ of which ($x_1$ and $x_2$, say) are examined at two levels and $q = k-p = 2$ of which ($x_3$ and $x_4$, say) are examined at three levels. A full $2^2 3^2$ factorial design would contain 36 runs and would allow us to fit the polynomial

$$E(y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4$$

$$+ \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{14} x_1 x_4 + \beta_{23} x_2 x_3$$

$$+ \beta_{24} x_2 x_4 + \beta_{34} x_3 x_4 + \beta_{33} x_3^2 + \beta_{44} x_4^2$$

(3.1)
2. allow separate estimation of non-singular moment matrix,

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 β'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.

Suppose the coded levels in standardized units are such that the two values taken by each of the variables $x_1, x_2, \ldots, x_p$ are $-a, a$ and the three values taken by each of the variables $x_{p+1}, x_{p+2}, \ldots, x_k$ are $-b, 0, b$. We shall require that the moment matrix obey the following conditions (where $N$ is the number of experimental runs):

1. $\sum_{u=1}^{N} x_{iu} = 0 \quad i = 1, \ldots, k$

2. $\sum_{u=1}^{N} x_{iu} x_{ju} = 0 \quad i \neq j \quad i = 1, \ldots, k \quad j = 1, \ldots, k$

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

4. $\sum_{u=1}^{N} x_{iu}^2 = \sum_{u=1}^{N} x_{ju}^2 > 0 \quad i = p+1, \ldots, k \quad j = p+1, \ldots, k \quad (4.2)$

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

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

7. $\sum_{u=1}^{N} x_{iu}^3 = 0 \quad i = p+1, \ldots, k$
8. $\sum_{u=1}^{N} x_{iu} x_{ju} x_{hu} x_{gu} = 0$

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

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

11. $\sum_{u=1}^{N} 3 x_{iu} x_{ju} = 0$

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

$i \neq j \neq h \neq g$

$i = p+1, \ldots, k$

$j = p+1, \ldots, k$

$h = p+1, \ldots, k$

$g = p+1, \ldots, k$

$i \neq j \neq h$

$i = p+1, \ldots, k$

$j = p+1, \ldots, k$

$h = p+1, \ldots, k$

$g = p+1, \ldots, k$

$i \neq j$

$h \neq g$

$i = p+1, \ldots, k$

$j = p+1, \ldots, k$

$h = p+1, \ldots, k$

$g = p+1, \ldots, k$

$i \neq j$

$i = p+1, \ldots, k$

$j = p+1, \ldots, k$

$\begin{equation}
(4.2)
\end{equation}$
Of the conditions (4.2), 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 (4.1)). 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.

5. CONSTRUCTION OF DESIGNS

We now introduce the method of design construction we propose in order to select a suitable subset of points from a \( 2^p3^q \) factorial design. In this discussion we shall use the \( 2^43^3 \) design as an example throughout.

When 4 variables, \( x_1 \) through \( x_4 \), are at two levels and 3 variables, \( x_5 \), \( x_6 \), \( x_7 \), are at three levels we shall wish to fit the polynomial

\[
E(y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6 + \beta_7 x_7 + \beta_{55} x_5^2 + \beta_{66} x_6^2 + \beta_{77} x_7^2 + \beta_{56} x_5 x_6 + \beta_{57} x_5 x_7 + \beta_{67} x_6 x_7 \tag{5.1}
\]

In the \( 2^43^3 \) design there are 432 runs which consist of all possible combinations of levels of \( \pm a \) for variables \( x_1, x_2, x_3 \), and \( x_4 \) and levels \((-b, 0, b)\) for variables \( x_5, x_6, \) and \( x_7 \). It is convenient to arrange these runs into eight sets on the basis of the positions and numbers of zero levels in the variables \( x_5, x_6, \) and \( x_7 \) as shown in Table 1.
Table 1  $2^4 \cdot 3^3$ Full Factorial Design

<table>
<thead>
<tr>
<th>Set</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>$x_4$</th>
<th>$x_5$</th>
<th>$x_6$</th>
<th>$x_7$</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>b</td>
<td>128</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>b</td>
<td>64</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>b</td>
<td>64</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>b</td>
<td>64</td>
</tr>
<tr>
<td>5</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>0</td>
<td>32</td>
</tr>
<tr>
<td>6</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>0</td>
<td>32</td>
</tr>
<tr>
<td>7</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>0</td>
<td>32</td>
</tr>
<tr>
<td>8</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>0</td>
<td>15</td>
</tr>
</tbody>
</table>

By writing the design in this way we can regard each of eight sets of Table 1 as a two-level full factorial design in certain variables with the levels of the other variables fixed at their zero levels. For example, set 5 is a $2^5$ full factorial design with variables $x_1$, $x_2$, $x_3$, and $x_4$ at levels ±a, variable $x_5$ at levels ±b, and variables $x_6$ and $x_7$ at their zero levels. It follows that

A. set 1 is a $2^7$ full factorial with 128 runs,
B. sets 2, 3, and 4 are each $2^6$ full factorials each with 64 runs,
C. sets 5, 6, and 7 are each $2^5$ full factorials each with 32 runs,
D. set 8 is a $2^4$ full factorial with 16 runs.

A further property of the 432 design points is that they can be divided into the four groups A, B, C, and D defined above in such a way that the points of each group lie on a hypersphere in seven dimensional space (see Fry, 1961). The center of each hypersphere is at $(x_1, x_2, \ldots, x_7) = (0, 0, \ldots, 0)$. 
If a group contains runs in which three level variables are at the zero level, the points of the group lie on a hypersphere with radius \(\sqrt{\frac{1}{4a^2 + (3-v)b^2}}\).

The outer hypersphere, hypersphere 1, of radius \(\sqrt{\frac{1}{4a^2 + 3b^2}}\) contains the points of set 1, that is, of group A; hypersphere 2 of radius \(\sqrt{\frac{1}{4a^2 + 2b^2}}\) contains the points of sets 2, 3, and 4, that is, of group B; hypersphere 3 of radius \(\sqrt{\frac{1}{4a^2 + b^2}}\) contains the points of sets 5, 6, and 7, that is, of group C; and hypersphere 4 of radius \(\sqrt{\frac{1}{4a^2}}\) contains the points of set 8, that is, of group D.

One possibility for choosing a subset of points 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. As can be shown (Stoneman, 1966) the runs of a single hypersphere provide a singular \(X'X\) matrix (in the least squares estimation procedure \(b = (X'X)^{-1}X'y\)) and thus will not allow separate estimation of all parameters in (2.3). A singular \(X'X\) matrix can also be obtained from some pairs of hyperspheres, for example hyperspheres 1 and 4. We can, however, select other pairs of hyperspheres and also any three hyperspheres. For example we can use hyperspheres 2 and 4 to obtain a \(64 + 64 + 64 + 16 = 208\) run response surface design consisting of the sets 2, 3, 4, and 8 of Table 1.

In the general case any subset of hyperspheres which does not give rise to a singular \(X'X\) matrix will provide a design. As in the example above, however, it will usually have an unreasonably large number of runs. Thus some method of reducing the number of runs is needed.

As mentioned above each set of 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, 1961a, b) to fractionate these sets.

In order to achieve the conditions (4.2), 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 three-level factors. (Note that the conditions (4.2) 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 three-level factors,
5. any two-factor interaction of two three-level factors with any other two-factor interaction of two three-level factors,
6. any two-factor interaction of two three-level factors with any quadratic effect of the three-level factors.

This can be achieved by fractionation of the sets, which make up the full design, as follows. Suppose the lower case letters r, s, t, and u represent two-level factors and the capital letters W, X, and Y represent three-level factors.

Then, in the standard notation used by Box and Hunter (1961a, b), fractionation of each set is possible using words of several types, for example, I = rst, I=rsw, I = rstu, I = rstW, I = rsWX, I = rWXY, or any word with five or more letters.

For our example of the $2^3$ case a subset of 56 design points can be obtained in several ways: two examples are shown below. (We recall that variables $x_1, x_2, x_3,$ and $x_4$ are two-level variables and variables $x_5, x_6,$ and $x_7$ are three-level variables.)
<table>
<thead>
<tr>
<th>Example</th>
<th>Set</th>
<th>Defining Relations</th>
<th>Type Fraction</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>2</td>
<td>I = 1235 = 1346 = 2456</td>
<td>$2^{6-2}$</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>I = 1235 = 1347 = 2457</td>
<td>$2^{6-2}$</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>I = 1236 = 1347 = 2467</td>
<td>$2^{6-2}$</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>I = 1234</td>
<td>$2^{4-1}$</td>
<td>8</td>
</tr>
<tr>
<td>II</td>
<td>2</td>
<td>I = 125 = 346 = 123456</td>
<td>$2^{6-2}$</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>I = 125 = 347 = 123457</td>
<td>$2^{6-2}$</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>I = 126 = 347 = 123467</td>
<td>$2^{6-2}$</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>I = 123</td>
<td>$2^{4-1}$</td>
<td>8</td>
</tr>
</tbody>
</table>

To provide an estimate of pure error we can repeat the 8 runs of set 8. We thus obtain two subsets of 56 (or 64 with set 8 repeated) design points which can be used as response surface designs to estimate the 14 coefficients in the polynomial (5.1). While the number of points in designs of this type shows a great reduction from the original number, an even greater reduction is often possible. We now describe the method by which this is achieved.

6. IMPROVED METHOD OF FRACTIONATING DESIGNS

Above we stated the conditions which must be observed in the bias relationships (5.2) of the final design and in deriving two design examples, we maintained these conditions in each fractionated set. However a violation of these relationships 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 way we must observe the following rules:
1. For any pair of selected sets a violating word must not include a three-level variable which takes the zero level in either set. (Since, when a set is regarded as a two-level design, this particular variable is absent.) (For example, we cannot use the word 17 in set 2 because the variable \( x_7 \) takes the zero level.)

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 (3.3). (For example, we can use the word 14 since \( \beta_{14} \) does not appear in (3.3).)

or, (b) if an associated coefficient does appear in (3.3), will subsequently not be confounded with an effect corresponding to any other coefficient also appearing in (3.3). (For example, we can use 56 if, in the subsequent design, 56 is not aliased with any effect corresponding to any other coefficient in (3.3).)

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. (For example, if in set 2 \( I = 26 \) then \( I = -26 \) in set 4.)

4. The final design must contain the same number of design points from each of the two selected sets. (For example, if we use \( I = 12 \) in set 2 and \( I = -12 \) in set 3 the final design must contain the same number of design points from both sets.)
As an example in the $2^{4 \times 3}$ case, consider the word 15 and the sets 2 and 3. The word 15

(a) is a violating word because it confounds the main effect of variable 1 with the main effect of variable 5,

(b) does not contain any letter (1 or 5) which represents a variable at the zero level in either set,

(c) and does not represent a two-factor interaction corresponding to a coefficient appearing in polynomial (5.1).

Thus if in the final design the same number of design points are selected from sets 2 and 3, we can use 15 in the defining relation for either set and -15 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 use $I = 15$ for set 2 and $I = -15$ for set 3; $I = 26$ for set 1 and $I = -26$ for set 4; and $I = 37$ for set 3 and $I = -37$ for set 4. We must also place, in the final design, the same number of design points from sets 2, 3, and 4 and so must fractionate accordingly. Using these generators we can obtain a response surface design with 32 experimental runs which is shown as Design I in Table 2. This particular subset of 32 design points from the full $2^{4 \times 3}$ factorial design does not violate the bias relationships (5.2) and will allow the separate estimation of the 14 coefficients in polynomial (5.1). To provide for the estimation of pure error we could repeat the 8 runs from set 8, if desired.

An alternative subset of 32 design points can be obtained using the defining relations listed in Design II of Table 2. Again we could repeat the 8 runs in set 8 to allow for the estimation of pure error.
Table 2 Two Design Examples

<table>
<thead>
<tr>
<th>Design</th>
<th>Set</th>
<th>Defining Relations</th>
<th>Type Fraction</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>2</td>
<td>I = 15 = 26 = 1234 = 1256 = 2345 = 1346 = 3456</td>
<td>$2^{6-3}$</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>I = -15 = 37 = 1234 = -1357 = -2345 = 1247 = -2457</td>
<td>$2^{6-3}$</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>I = -26 = -37 = 1234 = 2367 = -1346 = -1247 = 1467</td>
<td>$2^{6-3}$</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>I = -1234</td>
<td>$2^{4-1}$</td>
<td>8</td>
</tr>
<tr>
<td>II</td>
<td>2</td>
<td>I = 12 = 36 = 1345 = 1236 = 2345 = 1456 = 2456</td>
<td>$2^{6-3}$</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>I = -12 = 47 = 1345 = -1247 = -2345 = 1357 = -2357</td>
<td>$2^{6-3}$</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>I = -36 = -47 = 1234 = 3467 = -1246 = -1237 = 1267</td>
<td>$2^{6-3}$</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>I = -1234</td>
<td>$2^{4-1}$</td>
<td>8</td>
</tr>
</tbody>
</table>

There are many other possible ways of obtaining similar designs with 32 runs which allow the separate estimation of the 14 coefficients in polynomial (5.1). Specific selection among such designs can be made by considering other design properties such as the biases due to unestimated coefficients of second order and the number of additional interaction-type coefficients the design will allow to be estimated uncorrelated with estimates of coefficients in (3.3). We now discuss these points.

7. BIASES DUE TO UNESTIMATED COEFFICIENTS

Suppose we are interested in fitting a polynomial of the form (3.3) (which can for convenience be written as $E(\mathbf{y}) = \mathbf{X} \beta$ where $\mathbf{X}$ is the matrix of independent variables and $\beta$ is the vector of unknown coefficients). The least
squares estimate of \( \hat{\beta} \), that is, \( \hat{b} = (X'X)^{-1}X'y \), is such that \( E(\hat{b}) = \beta \) if (3.3) is an adequate representation of the response surface. Suppose this is not true and in fact the correct polynomial which should have been fitted contains \( S \) extra terms \( x_1\beta_1 \), so that the correct polynomial is of the form

\[
E(y) = X\beta + x_1\beta_1.
\]

Then (see Box, 1952) \( \hat{b} \) would no longer provide an unbiased estimate of \( \beta \) since now

\[
E(\hat{b}) = \beta + A\beta_1
\]

where \( A \) is a \((k+q/2) (q+1) +1\)x\( S \) matrix of coefficients of the biases given by

\[
A = (X'X)^{-1}X'x_1.
\]

We now apply this result to our \( 2^{33} \) examples. Let us suppose that the assumed polynomial (5.1) is not adequate because of the 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. Then if we express (5.1) in the form \( E(y) = X\beta \), the true model will take the form

\[
E(y) = X\beta + x_1\beta_1
\]

where

\[
\beta_1 = (\beta_{11}, \beta_{22}, \beta_{33}, \beta_{44}, \beta_{12}, \beta_{13}, \beta_{14}, \beta_{23}, \beta_{24}, \beta_{34}, \beta_{15}, \ldots, \beta_{25}, \beta_{35}, \beta_{45}, \beta_{16}, \beta_{26}, \beta_{36}, \beta_{46}, \beta_{17}, \beta_{27}, \beta_{37}, \beta_{47})
\]

and \( x_1 \) is the matrix which has, for its columns, the values of

\[
x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4, x_2x_3, x_2x_4, x_3x_4, x_1x_5, x_2x_5,
\]

\[
x_3x_5, x_4x_5, x_1x_6, x_2x_6, x_3x_6, x_4x_6, x_1x_7, x_2x_7, x_3x_7, x_4x_7 \text{ appropriate to the } N \text{ design points listed in the design matrix. For a given design we can}
then form the 14x22 matrix $A$ and calculate the bias relationships $E(b) = \beta + A\beta_1$.

We can also determine groups of coefficients not in the fitted polynomial which are uncorrelated with coefficients in the polynomial and which could be estimated if suitable terms were inserted.

Design I of Table 2 provides the following relationships:

$$E(b_0) = \beta_0 + a^2(\beta_{11} + \beta_{22} + \beta_{33} + \beta_{44})$$

$$E(b_i) = \beta_i, \ i = 1, \ldots, 7$$

$$E(b_{55}) = \beta_{55} + (a/b)(\beta_{26} + \beta_{37})$$

$$E(b_{66}) = \beta_{66} + (a/b)(\beta_{15} - \beta_{37})$$

$$E(b_{77}) = \beta_{77} - (a/b)(\beta_{15} + \beta_{26})$$

$$E(b_{56}) = \beta_{56} + (a^2/b^2)(\beta_{12} + \beta_{34}) + (a/b)(\beta_{16} + \beta_{25})$$

$$E(b_{57}) = \beta_{57} - (a^2/b^2)(\beta_{13} + \beta_{24}) + (a/b)(\beta_{35} - \beta_{17})$$

$$E(b_{67}) = \beta_{67} + (a^2/b^2)(\beta_{23} + \beta_{14}) - (a/b)(\beta_{27} + \beta_{36})$$

In addition if terms $\beta_{45}x_5^2$, $\beta_{46}x_6^2$, $\beta_{47}x_7^2$ were added to (5.1) estimates could be obtained of the quantities on the right hand side of the following equations:

$$E(b_{45}) = \beta_{45} + \frac{1}{2}(\beta_{36} - \beta_{27})$$

$$E(b_{46}) = \beta_{46} + \frac{1}{2}(\beta_{35} + \beta_{17})$$

$$E(b_{47}) = \beta_{47} + \frac{1}{2}(\beta_{16} - \beta_{25})$$
Similarly for design II of Table 2 we obtain

\[
\begin{align*}
E(b_0) &= \beta_0 + a^2 (\beta_{11} + \beta_{22} + \beta_{33} + \beta_{44}) \\
E(b_i) &= \beta_i, \quad i = 1, \ldots, 7 \\
E(b_{55}) &= \beta_{55} + (a/b) (\beta_{36} + \beta_{47}) \\
E(b_{66}) &= \beta_{66} + (a^2/b^2) \beta_{12} - a/b \beta_{47} \\
E(b_{77}) &= \beta_{77} - (a^2/b^2) \beta_{12} - a/b \beta_{36} \\
E(b_{56}) &= \beta_{56} + (a^2/b^2) (\beta_{14} + \beta_{24}) + (a/b) \beta_{35} \\
E(b_{57}) &= \beta_{57} + (a^2/b^2) (\beta_{15} - \beta_{25}) + (a/b) \beta_{46} \\
E(b_{67}) &= \beta_{67} + (a^2/b^2) (\beta_{34} + \beta_{12}) - (a/b)(\beta_{37} + \beta_{46})
\end{align*}
\]

In addition if terms \( \beta_{15} x_1 x_5, \beta_{25} x_2 x_5, \beta_{16} x_1 x_6, \beta_{17} x_1 x_7 \) were added to (5.1) estimates could be obtained of the quantities on the right hand side of the following equations:

\[
\begin{align*}
E(b_{15}) &= \beta_{15} + (a/b) \beta_{34} + \frac{1}{2} (\beta_{45} + \beta_{37}) \\
E(b_{25}) &= \beta_{25} + \frac{1}{2} (\beta_{46} - \beta_{37}) \\
E(b_{16}) &= \beta_{16} + (a/b)(\beta_{23} - \beta_{24}) + \frac{1}{2} (\beta_{26} + \beta_{45} + \beta_{27}) \\
E(b_{17}) &= \beta_{17} - (a/b)(\beta_{23} + \beta_{24}) + \frac{1}{2} (\beta_{27} + \beta_{35} + \beta_{26})
\end{align*}
\]

We see that there is little to choose between the two designs. In design II there is one less coefficient biased with estimates \( b_{56} \) and \( b_{47} \). In the bias relationships for \( b_{66} \) and \( b_{77} \) the coefficients, of terms other than \( b_{66} \) and \( b_{77} \), on the right hand side are either plus or minus \( a/b \) in design I where as in design II some coefficients are plus or minus \( a^2/b^2 \). The effect of \( a^2/b^2 \) as opposed to \( a/b \) depends on the relative magnitude of \( a \) and \( b \). For example, if we choose \( a \) and
b such that

\[ \sum_{u=1}^{N} x_{i u}^2 = \sum_{u=1}^{N} x_{j u}^2 \quad i = 1, \ldots, p; \quad j = p+1, \ldots, k \]

that is, \( 2a^2 = b^2 \), then \( a^2/b^2 = \frac{1}{2} = 0.5 \) and \( a/b = \sqrt{2}/2 = 0.707 \). In design I there are, in addition to the estimates of the coefficients in polynomial (5.1), three additional estimates available which are uncorrelated with the coefficients in (5.1). If these estimates were observed to be large, large biases would be indicated. In design II there are four such estimates.

8. A MORE COMPLICATED EXAMPLE (\( 2^{4}3^{5} \); A SUBSET OF 48 RUNS)

Suppose \( k = 9 \) variables are being investigated and \( p = 4 \) of these can be examined at two levels and \( q = k-p = 5 \) can be examined at three levels. We then wish to choose a subset of design points from the \( 2^{4}3^{5} \) full factorial design which will allow the estimation of the 25 coefficients in the polynomial

\[ E(y) = \beta_0 + \sum_{i=1}^{9} \beta_i x_i + \sum_{i=5}^{9} \sum_{j>i}^{9} \beta_{ij} x_i x_j \quad (8.1) \]

where \( x_1, x_2, x_3, \) and \( x_4 \) are two-level variables and \( x_5, x_6, x_7, x_8, \) and \( x_9 \) are three-level variables.

The 3888 experimental runs of the \( 2^{4}3^{5} \) full factorial design can be divided into 32 sets which belong to 6 hyperspheres. We can now select a subset of these 6 hyperspheres from which to generate a suitable response surface design. More than one hypersphere must be selected since otherwise the resulting \( X'X \) matrix will be singular. For the same reason certain pairs of hyperspheres cannot be chosen. We can, however, select certain other pairs, for example those given in Table 3 which contain
656 design points - far more than are necessary for the estimation of the 25 coefficients in (8.1). We now search for a group of defining relations which will generate as small a subset of design points as we can find and yet which will provide the types relationships (5.2) required for the complete design as well as allow satisfaction of (4.2). Rather remarkably we can achieve this by selecting only four runs out of the 64 runs in each of sets 1 - 10, namely by choosing ten $2^{6-4}$ designs of resolution only I. By careful balancing of the selected generators as well as of all violating cross-products of generators, and by adding half of set 11 (8 points) a very useful design can be constructed which satisfies (4.2), contains only 48 runs out of the original 3888 runs and allows estimation of the 25 coefficients in the polynomial (8.1). (If the 8 runs of set 32 are repeated for pure error estimation a 56 run design is obtained.) The defining relations for this design appear in Table 4.
### Table 3  List of Sets

<table>
<thead>
<tr>
<th>Hypersphere</th>
<th>Set</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>$x_4$</th>
<th>$x_5$</th>
<th>$x_6$</th>
<th>$x_7$</th>
<th>$x_8$</th>
<th>$x_9$</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
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<td>a</td>
<td>a</td>
<td>a</td>
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<td>b</td>
<td>0</td>
<td>0</td>
<td>$2^6 = 64$</td>
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<td></td>
<td>2</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>0</td>
<td>b</td>
<td>0</td>
<td>$2^6 = 64$</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>0</td>
<td>0</td>
<td>b</td>
<td>$2^6 = 64$</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$2^6 = 64$</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>b</td>
<td>b</td>
<td>0</td>
<td>$2^6 = 64$</td>
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<td>0</td>
<td>b</td>
<td>$2^6 = 64$</td>
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<td>b</td>
<td>0</td>
<td>0</td>
<td>$2^6 = 64$</td>
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<td>b</td>
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<td>a</td>
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<td>0</td>
<td>b</td>
<td>0</td>
<td>$2^6 = 64$</td>
</tr>
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<td></td>
<td>10</td>
<td>a</td>
<td>a</td>
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<td>0</td>
<td>b</td>
<td>$2^6 = 64$</td>
</tr>
<tr>
<td>B</td>
<td>11</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$2^4 = 16$</td>
</tr>
<tr>
<td>Set</td>
<td>Defining Relations</td>
<td>Type Fraction</td>
<td>Number of runs</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----</td>
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<td>---------------</td>
<td>----------------</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| 1   | $I = 15 = 26 = 35 = 4 = 1256 = 13 = 145$  
     | = 2356 = 246 = 345 = 1236 = 12456  
     | = 134 = 23456 = 12346 | $2^{-4}$ | 4 |
| 2   | $I = -15 = 27 = 35 = 4 = -13 = -1257 = -145$  
     | = 2357 = 247 = 345 = -12347 = -1237  
     | = -12457 = -134 = 23457 | $2^{-4}$ | 4 |
| 3   | $I = 15 = 28 = -35 = -4 = -13 = 1258 = -145$  
     | = -2358 = -248 = 345 = 12348 = -1238  
     | = -12458 = 134 = 23458 | $2^{-4}$ | 4 |
| 4   | $I = -15 = 29 = -35 = -4 = 13 = -1259 = 145$  
     | = -2359 = -249 = 345 = -12349 = 1239  
     | = 12459 = -134 = 23459 | $2^{-4}$ | 4 |
| 5   | $I = 17 = -26 = 36 = -4 = -23 = -1267 = 1367$  
     | = -147 = 246 = -346 = 12347 = -1237  
     | = 12467 = -13467 = 234 | $2^{-4}$ | 4 |
| 6   | $I = 16 = -28 = 38 = 4 = -23 = -1268 = 1368$  
     | = 146 = -248 = 346 = -12346 = -1235  
     | = -12468 = 13468 = -234 | $2^{-4}$ | 4 |
| 7   | $I = -16 = -29 = -36 = -4 = 13 = 1269 = 146$  
     | = 2369 = 249 = 346 = 12349 = -1239  
     | = -12469 = -134 = -23469 | $2^{-4}$ | 4 |
| 8   | $I = 18 = -27 = -38 = -4 = -13 = -1278 = -148$  
     | = 2378 = 247 = 348 = -12347 = 1237  
     | = 12478 = 134 = -23478 | $2^{-4}$ | 4 |
| 9   | $I = -17 = 29 = 39 = 4 = 23 = -1279 = -1379$  
     | = -147 = 249 = 349 = -12347 = -1237  
     | = -12479 = -13479 = 234 | $2^{-4}$ | 4 |
| 10  | $I = -18 = -29 = -39 = 4 = 23 = 1289 = 1389$  
     | = -148 = -249 = -349 = -12348 = -1238  
     | = 12489 = 13489 = 234 | $2^{-4}$ | 4 |
| 11  | $I = 1234$ | $2^{-1}$ | 8 |
9. AN EXTENSION OF THE METHOD

The method of choosing a violating word in one set and a compensating word in another set can be extended. For example, if a single set is fractionated in such a way that a violating word is in the defining relation, the violation can be partially compensated in each of several other sets so that over the whole design no violation occurs. As an example of this consider the $2^{5.4}$ situation. The polynomial of form (3.3) contains 20 coefficients. We can select five sets and fractionate them so that one fractionated set contains 16 runs and the violation $I = 15$ and the other four fractional sets each contain 4 runs and the compensation $I = -15$. We thus obtain a 32 run design which satisfies all requirements. This design is summarised in Table 5. Note that for a given set the generators appear on the first line of the defining relation and (since they are not needed to determine alias relationships of the type desired) words of the defining relation which contain five or more letters have been omitted.

Table 5 $2^{5.4}$ Design

<table>
<thead>
<tr>
<th>Set</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>$x_4$</th>
<th>$x_5$</th>
<th>$x_6$</th>
<th>$x_7$</th>
<th>$x_8$</th>
<th>$x_9$</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>$2^9 = 512$</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>b</td>
<td>0</td>
<td>0</td>
<td>$2^5 = 64$</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>b</td>
<td>0</td>
<td>0</td>
<td>$2^5 = 64$</td>
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<tr>
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<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>0</td>
<td>b</td>
<td>0</td>
<td>$2^5 = 64$</td>
</tr>
<tr>
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<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
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<td>0</td>
<td>0</td>
<td>b</td>
<td>$2^5 = 64$</td>
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</tbody>
</table>
Table 5 cont'd

<table>
<thead>
<tr>
<th>Set</th>
<th>Defining Relations</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>I = 1249 = 1369 = 2379 = 1238 = 15</td>
<td>$2^{9-5} = 16$</td>
</tr>
<tr>
<td></td>
<td>= 2346 = 1347 = 1267 = 4679 = 3489 = 2689 = 1789</td>
<td></td>
</tr>
<tr>
<td></td>
<td>= 1468 = 2478 = 3678 = 2459 = 3569 = 2358 = 3457</td>
<td></td>
</tr>
<tr>
<td></td>
<td>= 2567 = 5789 = 4568</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>I = 12 = 34 = 136 = -15</td>
<td>$2^{6-4} = 4$</td>
</tr>
<tr>
<td></td>
<td>= 1234 = 236 = 146 = 246 = -25 = -1345 = -356</td>
<td></td>
</tr>
<tr>
<td></td>
<td>= -2345 = -456</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>I = 12 = 34 = 137 = -15</td>
<td>$2^{6-4} = 4$</td>
</tr>
<tr>
<td></td>
<td>= 1234 = 237 = 147 = 247 = -25 = -1345 = -357</td>
<td></td>
</tr>
<tr>
<td></td>
<td>= -2345 = -457</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>I = -12 = -34 = 138 = -15</td>
<td>$2^{6-4} = 4$</td>
</tr>
<tr>
<td></td>
<td>= 1234 = -238 = -148 = 248 = 25 = 1345 = -358</td>
<td></td>
</tr>
<tr>
<td></td>
<td>= -2345 = 458</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>I = -12 = -34 = 139 = -15</td>
<td>$2^{6-4} = 4$</td>
</tr>
<tr>
<td></td>
<td>= 1234 = -239 = -149 = 249 = 25 = 1345 = -359</td>
<td></td>
</tr>
<tr>
<td></td>
<td>= -2345 = 459</td>
<td></td>
</tr>
</tbody>
</table>

10. USING PARTIAL HYPERSPHERES

The examples given previously in this paper have made use of all sets in a hypersphere and all the sets were then fractionated. In certain cases, however, it is possible to begin with a restricted selection of the sets of a hypersphere (which provides an immediate reduction in the number of runs) and then to fractionate these selected sets. This can be done in cases where sets of a hypersphere can be chosen which provide a certain balance in the placings of the b's and the zeros for the three-level variable positions. To satisfy the restrictions (4.2) in fact, the balance must be that of a balanced incomplete block design (see Cochran and Cox, 1957, Chapter 11) where, in the layout of the sets selected from the hypersphere, each set represents a block, the b's represent
treatments that are present and the zeros represent treatments that are absent. As an example of this consider the $2^{3 \times 7}$ situation.

The 17496 experimental runs of the $2^{3 \times 7}$ full factorial design can be divided into 128 sets each of which belong to one of eight hyperspheres. To generate a response surface design which will allow the estimation of the 37 coefficients in the polynomial of form (3.3), we could select the hypersphere containing the 35 sets each having four three-level variables at the zero level. (Of course another hypersphere must also be chosen so that $X'X$ is not singular.) Instead of using all 35 sets we can select (in many possible ways) a subset of only seven sets which satisfies the balance described above by making use of the balanced incomplete block design for seven treatments in seven blocks of block size three. We can then fractionate these seven sets (and at least one set from a different hypersphere) to obtain an appropriate response surface design. This design is summarised in Table 6. Again note that for a given set the generators appear on the first line of the defining relation.
### Table 6: $2^3 \times 3^7$ Design

<table>
<thead>
<tr>
<th>Set</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>$x_4$</th>
<th>$x_5$</th>
<th>$x_6$</th>
<th>$x_7$</th>
<th>$x_8$</th>
<th>$x_9$</th>
<th>$x_{10}$</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>0</td>
<td>$2^6 = 64$</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>b</td>
<td>$2^6 = 64$</td>
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<td>3</td>
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<td>a</td>
<td>a</td>
<td>0</td>
<td>b</td>
<td>0</td>
<td>0</td>
<td>b</td>
<td>0</td>
<td>0</td>
<td>$2^6 = 64$</td>
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<td>a</td>
<td>a</td>
<td>b</td>
<td>b</td>
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<td>0</td>
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<td>0</td>
<td>$2^6 = 64$</td>
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<tr>
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<td>a</td>
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<td>0</td>
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<td>b</td>
<td>b</td>
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11. FURTHER DESIGNS

Many additional designs can be obtained through the application of the methods above. For a complete listing of designs for cases $2^{p+q}$ 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.

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.

12. ACKNOWLEDGEMENT

This research was partially supported by the United States Navy through the Office of Naval Research under Contract Nonr-1202, Project NR 042 222.
REFERENCES


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

5. Norman R. Draper and David M. Stoneman

10. Distribution of this document is unlimited.

13. Abstract: The choice of an experimental design suitable for fitting a graduating polynomial can be made according to a number of criteria, depending on the problem involved. Difficulties arise when, although the factors are continuous in nature, the number of levels is specified by some external considerations. For example, if some factors can be examined at only two levels, the graduating function cannot include quadratic terms in those variables, but all second order terms for variables to be examined at three or more levels can be permitted. For such cases, a restricted model and special experimental designs are needed. This paper considers the problem when there are some factors at two levels and some factors at three levels.

14. 1. Experimental design
     2. Response surfaces
     3. $2^{P-3}q$ fractions