EXPERIMENTAL DESIGNS FOR MULTI-FACTOR EXPERIMENTS:
PRELIMINARY REPORT

Prepared Under Contract No. DA-36-034-ORD-1177 (RD)
(Experimental Designs for Industrial Research)

by

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Abstract

This report contains preliminary results of research on experimental design and statistical analysis of experiments whose purpose is to investigate functional relationships between a dependent and several independent variables. Background, largely contained in a paper by Box and Wilson (Journal of Royal Statistical Society Series B, 1951), is reviewed. An application in the field of chemistry is presented. Some useful matrix identities are developed and the solution of the design problem for first order surfaces is presented.
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1. INTRODUCTION

This report is intended to cover the background and initial phases of research work being done by the Institute of Statistics, North Carolina State College, under Contract No. DA-36-034-ORD-1177(RD) with the Office of Ordnance Research. The investigation is concerned with the design and analysis of experiments whose purpose is to explore functional relationships between a dependent or response variable, \( \eta \), and several independent variables or factors, \( x_1, x_2, \ldots, x_k \). It is supposed that the independent factors vary on a continuous scale and that they may be controlled at any pre-assigned value. It is further supposed that the response variable, also measured on a continuous scale, depends on the other variables according to an unknown function \( \eta = \phi(x_1 x_2 \ldots x_k) \). The experimenter selects several combinations of the \( x \) variables and carries out experiments leading to observed values of the response. These observed values, which differ from \( \eta \) due to experimental errors, we denote by \( y \). It is herein assumed that for any combination of factors the average or expected value of \( y \) is \( \eta \) and its variance is \( \sigma^2 \). The experimenter's object, of course, is to draw inferences about \( \phi(x_1 x_2 \ldots x_k) \) from the response pattern observed. The effect of the errors will be to introduce uncertainty into such inferences. It will be shown that this uncertainty may be materially reduced by a judicious selection of the several combinations of \( x_1, x_2, \ldots x_k \) to be tried in the experiment.

In a typical chemical experiment the factors \( x_1, x_2, x_3 \), etc. might be time, temperature, pressure, etc. of a reaction and \( \eta \) might be the yield, purity or cost of the product produced.
The values of $x_1, x_2, x_3 \ldots x_k$ for each experimental combination may be regarded as the coordinates of a point in $k$ dimensional space and the configuration of points given by the combinations used is called the design of the experiment. Designs heretofore recommended in the statistical literature for experiments of this character have been the so-called factorials or fractional factorials. In the factorial experiment a number of fixed levels are chosen for each factor and the design then consists of all combinations which may be made up by taking each of the factors at one of its fixed levels. If there are $a_1$ levels of the first factor, $a_2$ levels of the second, etc., then the number of possible combinations is $N = a_1 \cdot a_2 \cdot a_3 \ldots a_k$. It is easy to appreciate that the total number of combinations rapidly becomes prohibitively large. Thus far, efforts to reduce the amount of experimentation have taken the direction of fractional factorials in which a given fraction (e.g. $1/2$, $1/4$, etc.) of the $N$ are used. In so doing, certain factor comparisons become confounded with each other and care must be exercised to sacrifice only the least valuable information.

The fractional factorials have been of limited effectiveness in reducing multi-factor programs to manageable size. Moreover, the restriction to combinations of fixed levels of the variables has no apparent justification. In the work herein described this restriction has been dropped and designs are derived from more basic principles. It has been found that it is easily possible to construct designs which are more efficient per unit observation, in certain important respects, than are the traditional factorials.
2. ANALYSIS OF MULTI-FACTOR EXPERIMENTS

Experiments of the above mentioned multi-factor type have generally been analyzed by the analysis of variance techniques described in most modern statistical texts. We feel that from the experimenter's point of view this results in an inadequate interpretation of the data, and have chosen instead to work within the general framework of so-called regression analysis. Our method of analysis follows that set forth in the pioneer paper in this field by G.E.P. Box and K.B. Wilson "On the Experimental Attainment of Optimum Conditions", Journal of the Royal Statistical Society Series B Vol. XIII, No. 1, 1951. As the title indicates, this paper deals primarily with the strategy to be employed by an experimenter seeking the "best" combination of the several independent factors. The location of optimum is, however, only one aspect of the more general problem of drawing inferences about response surfaces from experimental data.

As pointed out earlier, the form of the function \( \varphi(x_1, x_2, \ldots, x_k) \) will, in general, be unknown. It will be assumed, however, that it can be represented by a Taylor series of some order. Naturally the order required will depend on the complexity of the true surface in the region over which we wish to use the approximation. For some purposes the first order terms alone will suffice. In three variables, for example, such a first order series is written as

\[
\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3
\]

* The variables \( x_1, x_2 \) and \( x_3 \) will usually be measured from the centroid of the design pattern.
Equation (2.0:1), of course, represents a plane and could be expected to provide a satisfactory approximation to the true surface only in regions of rather limited extent well removed from stationary points. In the Box and Wilson paper it is shown how the experimenter may use the estimates of the $\beta_i$ to determine the direction of steepest ascent on the local surface represented by (2.0:1). The direction of steepest ascent will, in fact, be along that line whose coordinates are proportional to the estimated $\beta_i$. Further experiments conducted along the indicated path can be expected to produce higher and higher responses. Eventually, however, an apparent stationary point will be reached. To determine the nature of the surface in the neighborhood of this stationary point it will generally be desirable to conduct a somewhat more intensive investigation using this time a second order (or higher, if necessary) Taylor series.

$$(2.0:2) \eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$

To estimate the coefficients in (2.0:2) it will be necessary to do a new series of experiments measuring the response, $y$, at each of several points $x_1, x_2, x_3$. The procedure for estimating the $\beta$'s will be that of least squares and will be described in detail in a subsequent section. It is customary to denote the estimates of the $\beta$'s by $b$'s and the estimate of $\eta$ by $Y$. Thus equation (2.0:2) becomes

$$(2.0:3) Y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + b_{11} x_1^2 + b_{22} x_2^2 + b_{33} x_3^2 + b_{12} x_1 x_2 + b_{13} x_1 x_3 + b_{23} x_2 x_3$$
Associated with this generalized quadratic surface are \( k \) dimensional contour surfaces on which the response is equal, say, to \( Y_c \). If we differentiate (2.0:3) with respect to \( x_1, x_2, \ldots x_k \) in turn and solve* the resulting set of \( k \) equations we get \( x_1^0, x_2^0, \ldots x_k^0 \), the coordinates of the stationary point which is the center of the system of contour surfaces. The response, \( Y^0 \), at this stationary point can be found by substituting \( x_1^0, x_2^0, \ldots x_k^0 \) back in (2.0:3).

The nature of the fitted system is made more readily apparent by reduction of (2.0:3) to its canonical form

\[
(2.0:4) \quad Y - Y^0 = \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 x_3^2
\]

This consists essentially of shifting the origin to the stationary point \( x_1^0, x_2^0, \ldots x_k^0 \) and rotating the axes so that they correspond with the axes of the system of conic sections represented by the contour surfaces. Equation (2.0:4) then shows how the response changes as we move away from the stationary point. For example, if \( \lambda_1 \) is negative the change in response is negative as we move in the \( x_1 \) direction and the stationary point is therefore a maximum along this axis. As summarized in the Box and Wilson paper:

(i) If \( \lambda_1, \lambda_2, \ldots \lambda_k \) are negative, the fitted surface has a true maximum at the stationary point and the contour surfaces are ellipsoids.

(ii) If one or more of the \( \lambda_1 \) are positive there is a col or minimax and the contour surfaces are elliptical hyperboloids.

(iii) If one or more of the \( \lambda_1 \) approach zero, the curves are attenuated along the corresponding axes and the surface approaches an elliptic or hyperbolic cylinder. The surface may also be said to possess a ridge.

* Assuming a solution is possible.
\( \lambda_1, \lambda_2 \) of same sign

+ , unique minimum

-, unique maximum

\( \lambda_1 \) and \( \lambda_2 \) of different sign

Minimax

\( \lambda_2 \) small with respect to \( \lambda_1 \)

Rising Ridge

Extreme case of \( \lambda_2 = 0 \)

Stationary Ridge

Figure 1
Sometimes the stationary point will be remote from the center of the design, as is commonly the case when the steepest ascent technique leads the experimenter to a slowly rising ridge. One axis, say $x_1$, of the canonical form will lie along the ridge and the corresponding $\lambda$ will be small. The equation may then be referred to a local origin on $X_1$ and the contour surfaces then become

\[(2.0:5) \quad y - y^0 = B_1 x_1 + \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 x_3^2 \]

where $y^0$ is the response at the new origin.

When the nature of the surface has been reasonably well determined, the information may be used for whatever practical purpose is indicated. If a true maximum has not been arrived at, it may be desirable to proceed towards higher responses, e.g., up the ridge, if one has been found. Or, having located the contours of equal response, it may, for example, be possible to operate a chemical process in a region of the variables $x_1, x_2, x_3$ (time, temperature, reaction rate, etc.) for which an auxiliary response is favorable.

An example of the various steps mentioned above will be presented later in this report.

3. THE METHOD OF LEAST SQUARES

In this section we review briefly the matrix presentation of curve fitting by the method of least squares. For this purpose we first define the design matrix, $D$, as the $n \times k$ matrix of the coordinates of the $n$ experimental points:
Next let $Y$ be the $n \times 1$ matrix of observed responses at the $n$ experimental points, i.e.,

$$
Y = \begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_N 
\end{bmatrix}
$$

Suppose the equation to be fitted contains $L$ terms being of the form

$$(3.0.1) \quad \gamma_i = \sum_{i=1}^{L} \beta_i x_i$$

where $x_i$ is here used to represent not only individual $x_i$ but also powers and cross products of such $x_i$. Let $X$ be the $N \times L$ matrix of values of the $X_i$.

For example if the function to be fitted is

$$(3.0.2) \quad \gamma_i = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2,$$

with $x_0$ a dummy variable always equal to one* and $x_1$ and $x_2$ conventional variables, then the $X$ matrix is

* This device of a dummy variate, $x_0$, is merely a convenience in the matrix development.
The least squares estimates of the $\beta_i$ are found by taking

$$B = TY$$

where

$$T = (X'X)^{-1} X'$$

If the observations $y_i$ are subject to independent errors having common variance, $\sigma^2$, then it has been shown that the least squares procedure provides the "best" linear unbiased estimates of the $\beta_i$ in the sense that the $b_i$ so estimated have minimum variance.

An estimate of $\sigma^2$ itself, denoted by $s^2$, is available from

$$\begin{align*}
(N - L) s^2 &= Y'Y - Y'XB
\end{align*}$$

though it should be noted that this estimate is unbiased only if the surface is really described by the equation (3.0:1) i.e., only if higher order terms are non-existent.

The variances and covariances of the estimates $b_i$ are given by $\sigma^2$ times the elements of $C^{-1}$ where the matrix $C^{-1} = (X'X)^{-1}$. The precision matrix, $C^{-1}$, plays an extremely important role in this research as it provides one

For the design to be satisfactory, $X$ must have rank $L$ so that the inverse of $X'X$ exists.
means of comparing the relative merits of alternative design configurations.

4. EFFECT OF LACK OF FIT

A second criterion for comparing alternative designs is that of their relative sensitivity to higher order terms not included in the fitted equation. Suppose that the surface could be represented exactly by an equation involving \( L \) terms such as (3.0:1) of the preceding section. If now we fit an equation using only \( M \) \(<\) \( L \) then the resulting \( b_1 \) will be biased estimates of the corresponding \( \beta_1 \). The extent of such bias may be evaluated as follows: In matrix notation the set of equations representing the response at each of the experimental points is

\[
\eta = X_1\beta + X_2\beta_2
\]

where \( \beta_1 \) represents the \( M \times 1 \) matrix of coefficient actually fitted by the experimenter and \( \beta_2 \) the \( (L - M) \times 1 \) matrix of additional coefficients needed to describe the function exactly. The matrices \( X_1 \) and \( X_2 \) are those defined in the least squares section, \( X_1 \) for the included and \( X_2 \) for the omitted variables. The least square estimates will then be

\[
\hat{B}_1 = (X_1'X_1)^{-1} X_1'Y
\]

and it is shown in the Box and Wilson paper that the expected value is

\[
E(\hat{B}_1) = \beta_1 + T_1X_2\beta_2
\]
The $M \times (L-M)$ matrix $T_1X_2$ is called the alias matrix and denoted by $A$. It indicates the manner in which the omitted $\beta$'s bias the estimates of those included. The nature of this bias pattern depends on the design configuration used and thus provides a second criterion for comparing designs. Generally speaking one is most concerned about the bias introduced by the possible existence of terms of next higher order.

5. COMPARISON OF DESIGNS

As indicated above, design configurations will be compared primarily on the basis of their precision and alias matrices. In order to provide for the comparison of designs with unequal numbers of points we compare the precision on a per observation basis by comparing $N_1C_1^{-1}$ and $N_2C_2^{-1}$.

Both $C^{-1}$ and $A$ are dependent on scale factors and designs must therefore be brought to the same "size" before being compared. The measure of size here adopted is the marginal second moment of the design configuration. For the $t^{th}$ variable this is defined as

\[s_t^2 = \frac{1}{N} \sum_{i=1}^{N} (X_{ti} - \bar{X}_t)^2\]  

(5.011)

Two designs will be compared only after adjusting to the same $s_t^2$ in each of the several variables involved. To illustrate the process of comparing designs we compare the conventional three level factorial in two variables with a regular pentagon augmented by one point in its center. These two configurations are shown in Figure 2.
If the values of $x_1$ and $x_2$ in the factorial are taken as -1, 0, and +1 then the marginal second moments are $s_1^2 = s_2^2 = 2/3$ and it may be shown that in order for the pentagon to be of equal "size" the distance from the center to any point must be 1.265.

If the two designs of Figure 2 are now used to fit an equation

\[
y = b_0 x_0 + b_1 x_1 + b_2 x_2 + b_{11} x_1^2 + b_{22} x_2^2 + b_{12} x_1 x_2
\]

then the precision matrices are for the factorial and the pentagonal respectively

\[
\begin{bmatrix}
5.0 & 0 & 0 & -3.0 & -3.0 & 0 \\
0 & 1.5 & 0 & 0 & 0 & 0 \\
0 & 0 & 1.5 & 0 & 0 & 0 \\
-3.0 & 0 & 0 & 4.5 & 0 & 0 \\
-3.0 & 0 & 0 & 0 & 4.5 & 0 \\
0 & 0 & 0 & 0 & 0 & 2.25
\end{bmatrix}
\]

\[
\begin{bmatrix}
6.0 & 0 & 0 & -3.75 & -3.75 & 0 \\
0 & 1.5 & 0 & 0 & 0 & 0 \\
0 & 0 & 1.5 & 0 & 0 & 0 \\
-3.75 & 0 & 0 & 3.750 & 1.875 & 0 \\
-3.75 & 0 & 0 & 1.875 & 3.750 & 0 \\
0 & 0 & 0 & 0 & 0 & 3.75
\end{bmatrix}
\]

and the alias matrices, for terms of third order
The relative precisions of the two designs are not greatly different, however the alias pattern is somewhat more favorable in the case of the factorial design. The A matrices have been bordered with the $b$'s and $\beta$'s to which the elements apply, e.g., in $A_p$, $b_{11}$ estimates $\beta_{11} + .32\beta_{22} - .32\beta_{12}$ etc.

6. THE COMPOSITE DESIGN

Most of the preceding material is contained in the Box and Wilson paper previously referred to. This paper contains, in addition, a more detailed discussion, with several excellent examples, of the problems of locating an optimum point. Previous work in the field of fractional factorial designs is summarized and re-examined from the point of view of fitting surfaces. Shortcut systems of determining alias patterns are given. In a second paper by G.E.P. Box alone, the problem of "best" designs for fitting first order series is solved rather completely. This work will be summarized in the next section. Before doing so, however, we shall present the so-called "composite design" which was originally given in the Box and Wilson paper. It is basically a design for fitting second order series and, while work now in progress indicates
it is not the "best" design, it does appear to be extremely useful.

The composite design is illustrated for three variables in Figure 3. It consists of the corners of a cube

![Figure 3: Composite Design in Three Variables](image)

(which would form a conventional $2^3$ factorial) plus a point exactly at the center of the cube plus six points outside of the cube, two points equally spaced along each of the three major axes. The design matrix is

$$
D = \begin{bmatrix}
1 & 1 & 1 \\
1 & 1 & -1 \\
1 & -1 & 1 \\
1 & -1 & -1 \\
-1 & 1 & 1 \\
-1 & 1 & -1 \\
-1 & -1 & 1 \\
-1 & -1 & -1 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
$$
where \( \alpha \) is the distance from the center to each of the "outside" points. The pattern lends itself rather well to two stage experimentation. One would first run the experiments corresponding to the corners of the cube. From this pattern the first order series may be fitted and coefficients of mixed terms, i.e., \( b_{12}, b_{13}, b_{23}, b_{123} \) determined as well. If the latter are judged to be appreciable in size it is a good indication that a higher order series will be necessary. The additional seven points may then be added and a second order series fitted to the entire fifteen. If the experimenter is satisfied with the first order approximation he can conveniently stop after running the first set.

In comparing composite designs with the conventional three level factorial which ordinarily is proposed to estimate second order terms it should first be noted that for the factorial it can be shown that the variance of estimated quadratic derivatives, i.e., \( 2b_{st} \), is eight times as large as that for mixed derivatives such as \( b_{st} \). This would not appear to be a desirable property of the design. It seems reasonable to determine all second order effects with about the same precision. This may be accomplished in the composite designs by an appropriate choice of \( \alpha \) (see Appendix (4) of the Box and Wilson paper).

It should also be pointed out that if the conventional three level factorial is used to fit a second order series \( 3^3 = 27 \) experiments (for a three variable system) are being used to fit only 10 constants in the series. The composite design requires only 15 experiments to estimate the 10 constants. When precision is expressed on a per observation basis the composite design can be at least as efficient on all the estimates as the factorial or alternatively much more efficient on some estimates and less efficient on others depending
on the choice of \( \alpha \). The factorial design does provide information on certain mixed effects of higher order but it does not seem particularly useful for the experimenter to get these and not have the pure cubic derivatives, for example.

When \( k = 4 \) the composite design requires \( 2^4 = 16 \) plus \( 2k + 1 = 9 \) experiments for a total of 25. The number of constants estimated will be 15. For \( k = 5 \) and above, it seems desirable to use the device of fractional factorials to reduce the number of experiments contained in the "cube" stage of the composite design. A five factor experiment would otherwise require \( 2^{5} + (2)(5) + 1 = 43 \). This may be reduced to 27 by taking only one half of the \( 2^5 \) part. The particular half selected should be taken according to a split on the five factor interaction.

7. AN APPLICATION

The following example concerns a reaction of the type \( A + B \rightarrow C + D \). The object was to obtain the maximum yield of \( C \), subject to the condition that the yield of \( D \) should not exceed 20%. The factors varied were temperature \( (x_1) \), concentration of \( A \) \( (x_2) \), and time of reaction \( (x_3) \), the starting quantity of B being kept constant throughout. A \( 2^3 \) factorial experiment was run first, the levels of the factors being taken as

<table>
<thead>
<tr>
<th>Factor Levels</th>
<th>Temperature °C</th>
<th>Concentration of A</th>
<th>Time of Reaction hours</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-1</td>
<td>+1</td>
<td>Base Level</td>
</tr>
<tr>
<td>Temperature</td>
<td>142</td>
<td>152</td>
<td>147</td>
</tr>
<tr>
<td>Concentration of A</td>
<td>35</td>
<td>40</td>
<td>37.5</td>
</tr>
<tr>
<td>Time of Reaction</td>
<td>7</td>
<td>10</td>
<td>8.5</td>
</tr>
</tbody>
</table>
Letting

\[ x_1 = \frac{\text{Temp} - 147}{5} \]
\[ x_2 = \frac{\text{Conc} - 37.5}{2.5} \]
\[ x_3 = \frac{\text{Time} - 8.5}{1.5} \]

the \( 2^3 \) part of the experiment had the design matrix

\[
D = \begin{bmatrix}
-1 & -1 & -1 \\
-1 & -1 & 1 \\
-1 & 1 & -1 \\
-1 & 1 & 1 \\
1 & -1 & -1 \\
1 & -1 & 1 \\
1 & 1 & -1 \\
1 & 1 & 1 \\
\end{bmatrix}
\]

The matrix of experimental results was

\[
Y = \begin{bmatrix}
55.9 \\
63.3 \\
67.5 \\
68.8 \\
70.6 \\
68.0 \\
68.6 \\
62.4 \\
\end{bmatrix}
\]

At this stage it is possible to obtain estimates of the coefficients \( \beta_0, \beta_1, \beta_2, \beta_3, \beta_{12}, \beta_{13}, \beta_{23}, \beta_{123} \). For this purpose the matrix \( X'X \) is
Its inverse, $C^{-1}$, is clearly a matrix with $1/8$ down the main diagonal and zeros elsewhere. The $T$ matrix is therefore

$$T = C^{-1}X' = 1/8$$

Therefore

$$B = TY = \begin{bmatrix} 65.64 \\ 1.76 \\ 1.19 \\ -0.01 \\ -3.09 \\ -2.19 \\ -1.21 \\ 0.31 \end{bmatrix}$$

The magnitude of the "mixed" coefficients, i.e. $b_{12}$, $b_{13}$, etc., relative to the linear coefficients indicates that the surface would not be adequately described by a plane and the design must therefore be expanded to enable a
complete second order representation to be constructed. This expansion was done by adding seven further points to form a composite design with $\alpha = 2$.

These further experiments and the resulting yields are shown below:

<table>
<thead>
<tr>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>$y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>66.9</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>65.4</td>
</tr>
<tr>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>56.9</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>0</td>
<td>67.5</td>
</tr>
<tr>
<td>0</td>
<td>-2</td>
<td>0</td>
<td>65.0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>2</td>
<td>68.9</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>-2</td>
<td>60.3</td>
</tr>
</tbody>
</table>

The new $T$ matrix, using all fifteen points, is now

$$T = \begin{bmatrix} 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 56 & -8 & -8 & -8 & -8 & -8 & -8 \\ -4.5 & -4.5 & -4.5 & -4.5 & 4.5 & 4.5 & 4.5 & 4.5 & 0 & 9 & -9 & 0 & 0 & 0 & 0 \\ -4.5 & -4.5 & 4.5 & 4.5 & -4.5 & -4.5 & 4.5 & 4.5 & 0 & 0 & 0 & 9 & -9 & 0 & 0 \\ -4.5 & 4.5 & -4.5 & 4.5 & -4.5 & 4.5 & -4.5 & 4.5 & 0 & 0 & 0 & 0 & 0 & 9 & -9 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -16 & 10 & 10 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -16 & 1 & 10 & 10 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -16 & 1 & 1 & 1 & 10 & 10 & 10 \\ 9 & 9 & -9 & -9 & -9 & -9 & 9 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 9 & -9 & 9 & -9 & -9 & 9 & -9 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 9 & -9 & -9 & 9 & 9 & -9 & -9 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Multiplying the augmented $Y$ matrix by $T$ we get the new estimates of the $\beta$'s as
An estimate of the residual mean square based on 5 degrees of freedom was
2.20 which was slightly larger than prior knowledge had indicated, but not
enough so to indicate that a still higher order series would be necessary.

The fitted equation is

\[(7.0:1) \quad Y = 67.714 + 1.944x_1 + 0.906x_2 + 1.069x_3 - 1.539x_1^2 - 0.264x_2^2 - 0.676x_3^2
\]
\[-3.088x_1x_2 - 2.188x_1x_3 - 1.212x_2x_3\]

7.1 Determination of Canonical Form

The position of the center of the system of contours represented by (7.0:1)
is found by differentiating the equation with respect to \(x_1, x_2\) and \(x_3\) in
turn and equating the results to zero. The set of equations so obtained is
The solution is $x_1^0 = 0.061$, $x_2^0 = 0.215$, $x_3^0 = 0.499$ and by substituting these values back in (7.0.1) we find the response at this stationary point to be $Y^0 = 68.14$. In terms of the original experimental variables the stationary point is at Temp = 147.3 °C, Concentration = 38.04% and Time = 9.25 hours.

The canonical form of (7.0.1) is found by setting up the determinatal equation

$$
\begin{vmatrix}
 b_{11} - \lambda & \frac{1}{2} b_{12} & \frac{1}{2} b_{13} \\
 \frac{1}{2} b_{12} & b_{22} - \lambda & \frac{1}{2} b_{23} \\
 \frac{1}{2} b_{13} & \frac{1}{2} b_{23} & b_{33} - \lambda
\end{vmatrix} = 0
$$

The resulting cubic equation has three roots $\lambda_1$, $\lambda_2$ and $\lambda_3$. In the present example these are $\lambda_1 = -3.189$, $\lambda_2 = -0.068$, $\lambda_3 = 0.781$. In canonical form then the equation is

$$
(7.1.3) \quad Y - Y^0 = \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 x_3^2
$$

or

$$
(7.1.4) \quad Y - 68.14 = -3.189x_1^2 - 0.068x_2^2 + 0.781x_3^2
$$
The canonical form essentially shifts the origin to the stationary point and rotates the axes to line up with those of the system of generalized conic sections represented by the fitted second degree surface. The relation between the canonical variables and the \( x \)'s is of the form

\[
7.15 \quad x_i = m_{11}(x_1 - x_1^0) + m_{12}(x_2 - x_2^0) + m_{13}(x_3 - x_3^0)
\]

The \( m \)'s may be obtained by solving three sets of three simultaneous linear equations

\[
\begin{align*}
(b_{11} - \lambda_1) m_{11} + \frac{1}{2} b_{12} m_{12} + \frac{1}{2} b_{13} m_{13} &= 0 \\
\frac{1}{2} b_{12} m_{11} + (b_{22} - \lambda_1) m_{12} + \frac{1}{2} b_{23} m_{13} &= 0 \\
\frac{1}{2} b_{13} m_{11} + \frac{1}{2} b_{23} m_{12} + (b_{33} - \lambda_1) m_{13} &= 0
\end{align*}
\]

Letting \( \lambda_1 = \lambda_1, \lambda_2 \) and \( \lambda_3 \) in turn and solving these equations we get the transformation

\[
7.17
\begin{align*}
x_1 &= 0.7511(x_1 - x_1^0) + 0.4884(x_2 - x_2^0) + 0.4443(x_3 - x_3^0) \\
x_2 &= 0.3066(x_1 - x_1^0) + 0.3383(x_2 - x_2^0) - 0.8897(x_3 - x_3^0) \\
x_3 &= 0.5848(x_1 - x_1^0) - 0.8044(x_2 - x_2^0) - 0.1044(x_3 - x_3^0)
\end{align*}
\]
An important property of this transformation is that the reciprocal transformation by means of which the $x$'s are expressed in terms of the $\lambda$'s is of exactly similar form with rows substituted for columns. For the above example

$$x_1 - x_1^0 = 0.7511x_1 + 0.3066x_2 + 0.5846x_3$$

$$x_2 - x_2^0 = 0.4884x_1 + 0.3383x_2 - 0.8044x_3$$

$$x_3 - x_3^0 = 0.6433x_1 - 0.8897x_2 - 0.1044x_3$$

Examination of the canonical form reveals that two of the $\lambda$ coefficients are close to zero relative to the third. In these two directions the response change is very small. For $x_1$, however, there is a substantial decrease in response as we move away from the stationary point in either the positive or negative direction. This indicates that the system of contour surfaces is roughly speaking a series of parallel planes, the response changing from one plane to the next but not in the planes themselves. An approximate plane of maxima exists on either side of which the response falls off. In this example the experimenters were able to pick out combinations of temperature, concentration and reaction time along the plane of maxima in such a way that the yield of the auxiliary product D was always less than the specified 20%.

8. SOME USEFUL MATRIX IDENTITIES

Frequently, after a surface has been estimated and its contours examined, an experimenter may wish to supplement the original design with further experiments in regions of special interest. The coefficients will, of course, be modified by the inclusion of new data. On other occasions, the experimenter
may wish to augment the original model by adding additional variables, usually higher order terms of the variables already used. Finally, new experiments and additional terms may be desired simultaneously. To alleviate the heavy computing labor involved in making these modifications, particularly in inverting the variance-covariance matrix $C = X'X$, certain known matrix identities have been recorded, and others are developed, in this section.

In matrix notation the linear model may be written as

$$Y = X\beta + \epsilon$$

where $Y$ is a column vector of $N_1$ observations, $X$ an $N_1 \times L_1$ matrix (i.e., $N_1$ rows and $L_1$ columns) of the $L_1$ independent variables, $\beta$ a column vector of $L_1$ coefficients, and $\epsilon$ a column vector of $N_1$ errors assumed to be normally distributed with zero mean and variance $\sigma^2$. As mentioned previously the least squares estimates of the coefficients $\beta$ based on $N_1 \geq L_1$ observations are given by the formula

$$\beta_1 = C^{-1}_1 X'Y$$

where

$$C^{-1}_1 = \begin{bmatrix} X'X \end{bmatrix}^{-1},$$

the precision matrix of full rank $L_1$. In addition the estimate of $\sigma^2$ can be obtained from

$$S = Y'Y - Y'XB = (N_1 - L_1) s^2$$

where $S$, a scalar, is the residual sum of squares based on $N_1 - L_1$ degrees of freedom.
8.1 Additional Experiments

If the original estimates of $\beta$ have been obtained and more points are added to the experimental region a recalculation of the inverse $C^{-1}$ is required. To avoid re-inverting this matrix, Plackett (1950, *Biometrika* V 37 p. 149) derived formulas that utilize the original labor involved in calculating $C^{-1}$, and require only the additional inverting of a matrix equal in rank to $N_2$ the number of new observations. Let

$$W = (N_2 \times L) \text{ matrix of independent variables based on the new points.}$$

$$Z = (N_2 \times 1) \text{ column vector of new observations.}$$

In addition let

$$C_0^{-1} = \text{the new precision matrix based on } N_1 + N_2 \text{ observations}$$

$$B_0 = \text{the new estimates of the } \beta \text{ coefficients based on all } N_1 + N_2 \text{ observations}$$

$$S_0 = \text{the new residual sum of squares based on } N_1 + N_2 - L_1 \text{ degrees of freedom.}$$

Then

\[ (8.1:1) \quad C_0^{-1} = C^{-1} - J'GJ \quad (LxL) \]

\[ (8.1:2) \quad B_0' = B' + A'GJ \quad (Lx1) \]

\[ (8.1:3) \quad S_0 = S + A'G \quad (1x1) \]
where

\[(8.1:4) \quad J = WC^{-1} \quad (N_2 \times L)\]

\[(8.1:5) \quad G = (1+R)^{-1} \quad (N_2 \times N_2)\]

\[(8.1:6) \quad R = WC^{-1}W' \quad (N_2 \times N_2)\]

\[(8.1:7) \quad \Delta = Z - WB \quad (N_2 \times 1)\]

It is well to remember that the major saving in computation occurs in getting the new inverse \(C_0^{-1}\). To secure \(C_0^{-1}\) it is necessary only to invert a matrix of size \(N_2 \times N_2\) rather than completely recalculate the inverse of \(C = X'X\) of rank \(L\) based on all \(N_1 + N_2\) observations. However, Plackett's method for getting the new inverse is helpful only when the rank of \(C\) is appreciably greater than the number of new observations. Obviously, if \(N_2 \geq L\), no saving in the labor of inversion is accomplished, and much time wasted in additional matrix multiplications and additions.

8.2 Additional Terms in Model

Frequently, after observing how well the original model fits the observations, the experimenter may wish to add, say, \(L_2\) additional variables to the model. Under these circumstances the model becomes

\[(8.2:1) \quad y = \sum_{i=1}^{L_1} \beta_i x_i + \sum_{i=L_1+1}^{L_2} \beta_i x_i + \epsilon\]
or in matrix form

\[(8.2.2) \quad Y = \begin{bmatrix} X_1 & X_2 \end{bmatrix} \cdot \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \varepsilon\]

where \(\begin{bmatrix} X_1 & X_2 \end{bmatrix}\) is the matrix of independent variables \(X\), now partitioned into two sub-matrices \(X_1\), the original \((N \times L_1)\) matrix of independent variables, and \(X_2\), representing the new \((N \times L_2)\) matrix of independent variables. Similarly, \(\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}\) is the new column vector of coefficients partitioned to indicate \(\beta_1\) the original \((L_1 \times 1)\) column vector of coefficients, and \(\beta_2\) the \((L_2 \times 1)\) vector of the new coefficients.

The direct approach towards getting estimates of the coefficients \(\beta_1\) and \(\beta_2\) is to form the product matrix of the independent variables \(X'X\) and invert this matrix, now of rank \(L_1 + L_2\). Call this new matrix \(C_{1,2}\).

The inversion of matrices of high order, however, is very laborious, the time required increasing approximately with the cube of the rank. To reduce this work, advantage can be taken of the original inverse \(C^{-1}\) of rank \(L_1\), and the inverse of an additional matrix of rank \(L_2\). The matrix \(C_{1,2}\) can be written in partitioned form as

\[(8.2.3) \quad C_{1,2} = \begin{bmatrix} X_1' X_1 & X_1' X_2 \\ X_2' X_1 & X_2' X_2 \end{bmatrix} = \begin{bmatrix} C_1 & P \\ - & - \end{bmatrix} \begin{bmatrix} P' & C_2 \end{bmatrix}\]

\(C_{1,2}: (L_1 + L_2) \times (L_1 + L_2)\)
\(C_1: (L_1 \times L_1)\)
\(C_2: (L_2 \times L_2)\)
\(P: (L_1 \times L_2)\)
Let
\[ C_{1,2}^{-1} = \begin{bmatrix} C_1^{-1} & E \\ E' & F \end{bmatrix} \]

Since \( C_1^{-1} \) has already been determined, the sub-matrices of \( C_{1,2}^{-1} \) can be obtained using the formulas

\[(8.2:4) \quad F = \left[ C_2 - P'C_1^{-1} P \right]^{-1} \quad F: (L_2 \times L_2)\]

\[(8.2:5) \quad E = -C_1^{-1} PP' \quad E: (L_1 \times L_2)\]

\[(8.2:6) \quad G = C_1^{-1} \cdot \left[ I - PE' \right] \quad G: (L_1 \times L_1)\]

Expanding these submatrices of the inverse \( C_{1,2}^{-1} \) in terms of the submatrices of the original matrix yields

\[(8.2:7) \quad C_{1,2}^{-1} = \begin{bmatrix} \frac{C_1^{-1} \left( I + PF(C_2 - P'C_1^{-1} P)^{-1} \cdot P'C_1^{-1} \right)}{-\left( C_2 - P'C_1^{-1} P \right)^{-1} P'C_1^{-1}} & -C_1^{-1} P \left( C_2 - P'C_1^{-1} P \right)^{-1} \\ \frac{-\left( C_2 - P'C_1^{-1} P \right)^{-1} P'C_1^{-1}}{(C_2 - P'C_1^{-1} P)^{-1}} & \left( C_2 - P'C_1^{-1} P \right)^{-1} \end{bmatrix} \]

An important application of these formulas for adding more constants to the model arises in considering the effects of bias on the original estimates of the coefficients. If the experimenter fits the model

\[(8.2:8) \quad y = X_1 \beta_1 + \epsilon\]

when, in order to fully describe the response surface he should be using the model

\[(8.2:9) \quad Y = \begin{bmatrix} X_1 \end{bmatrix} \cdot \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \epsilon \]
the estimates of $\beta_1$ obtained from (8.2:8) will be biased by his failure to include in the model the additional independent variables $X_2$.

Actually, $\hat{B}_1$ will estimate $\beta_1 + AB_2$

where

$$A = \left[ X_1'X_1 \right]^{-1}X_1'X_2 \quad (L_1 \times L_2)$$

has been called the alias matrix (Box & Wilson 1951).

It is of interest to note that the sub-matrices of $C_{1,2}$ can be written in terms of the alias matrix $A$ as follows

$$F = \left[ C_2 - A'C_1A \right]^{-1}$$

$$E = -AF$$

$$G = C_1^{-1} + AFA'$$

Now denote by $B_1(2)$ the $B_1$ constants recalculated after including additional terms. Then $B_1(2)$ would be an unbiased estimate of $\beta_1$ if the response surface were fully explained by (8.2:9).

Then

(8.2:10) $\quad B_1(2) = B_1 + EH_Y$,

where

(8.2:11) $\quad H = X_2' - P'C_1^{-1}X_1$.

Thus

(8.2:12) $\quad B_1(2) = B_1 - APH_Y$. 
Equation (8.2:12) indicates that the $b_1$ among the original set of $L_1$ are modified by the inclusion of additional terms in the model, only if they have previously had alias connections with any of these new terms. Thus in most factorial and composite designs only isolated coefficients are affected by the addition of higher order terms.

If we denote additional constants by the matrix $B(1)2$ then

$$B(1)2 = FHY$$

and therefore

$$B(1)2 = B_1 - AB(1)2 .$$

8.3 Additional Experiments and Terms

If additional experiments and additional terms to the model are desired simultaneously it appears that the most expeditious procedure is

1. Use Plackett's formulae to find the new inverse matrix for the original $L_1$ constants.
2. Then use the formulae for additional terms working, of course, with the modified $C^{-1}$ found in (1).

9. MULTI-FACTOR DESIGNS OF FIRST ORDER

The design problem for fitting first order series was completely solved by G.E.P. Box (Biometrika V 39, April 1952 p. 49). Since this paper is extremely fundamental to later phases of this research project we shall present the pertinent sections verbatim.
9.1 Suppose that the effect of \( k \) quantitative variables or factors \( X_1, \ldots, X_i, \ldots, X_k \) (such as time, temperature, concentration) on some measurable response (such as yield of product) is being studied in a region of the response surface that can be represented to a sufficient degree of accuracy by a polynomial equation of degree \( d \). We define a design of order \( d \) as an arrangement of experiments which will allow all the coefficients in this polynomial to be separately determined. In this paper it is assumed that \( d \) is equal to 1, i.e., that a planar approximation is adequate. It is also assumed that the variables can be controlled exactly at levels decided in advance and that the observed response \( y \) differs from \( \eta \) due to experimental error having variance \( \sigma^2 \).

\[
(9.1:1) \quad \text{E}(y) = \eta, \quad \text{E}(y-\eta)^2 = \sigma^2.
\]

We can perform \( N > k \) trials; the problem is to decide which \( N \) combinations of levels to use so that the constants defining the plane are estimated with maximum accuracy. We shall not apply the usual limitation that the design is to consist of combinations of a few fixed levels of the factors, but as a means of specifying the extent of variation for a given factor \( X_i \) we define the unit \( S_i \) for this variable as

\[
S_i = \left\{ \frac{1}{N} \sum_{u=1}^{N} \frac{(X_{iu} - \bar{X}_i)^2}{2} \right\}^{1/2},
\]

and write the design in terms of the standardized variables \( x_{iu} = (X_{iu} - \bar{X}_i)/S_i \).
It will be noted, therefore, that for the standardized variables

\[ \sum_{u} x_{iu} = 0, \]

\[ \sum_{u} x_{iu}^2 = N. \]

A discussion of the problem of scaling and comparing experimental designs will be found in a recent paper (Box & Wilson, 1951), where there is an account of the planning of experiments to attain maxima in connexion with which this investigation was undertaken. The design matrix \( D \) is an \( N \times k \) matrix providing a programme of experiments to be performed. The \( k \) elements \( x_{1u}, \ldots, x_{iu}, \ldots, x_{ku} \) of the \( u \)th row are the levels of the standardized variables to be used in the \( u \)th trial. They can also be regarded as defining the \( k \) co-ordinates of the \( u \)th experimental point in the \( k \)-dimensional factor space. To use the design the experimenter must decide on suitable average levels \( \bar{x}_1, \bar{x}_2, \ldots, \bar{x}_k \) and units \( S_1, S_2, \ldots, S_k \) for the variables. The level to be used for the \( i \)th variable in the \( u \)th trial will then be \( x_{iu} = \bar{x}_i + s_i x_{iu} \).

9.2 Suppose the true regression plane in the region considered is

\[ \eta_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_k x_{ik}. \]

In an obvious matrix notation the \( N \) equations (9.2:1) at the \( N \) experimental points may be written

\[ \eta_i = \bar{x}_1 \beta_1. \]

* Henceforth in this section, matrices will be indicated by underlined quantities.
where $X_1 = [U; D]$ and each element of the column vector $U$ is unity. If $Y$ is a column vector of observations $y_1, \ldots, y_u, \ldots, y_N$ made at these experimental points, then providing $X_1$ is of rank $k + 1$ (which implies that $D$ is of rank $k$), separate linear estimates $b_0, b_1, \ldots, b_k$ of each of the $\beta$'s may be calculated. For a particular design $D$, linear estimates having smallest variances are provided by the method of least squares and are given by $B_1 = (X_1'X_1)^{-1}X_1'Y = T_1Y$, and it is well known that the matrix of variances and covariances for the estimates is $(X_1'X_1)^{-1}\sigma^2$. We have then to choose $D$ so that the diagonal elements of $(X_1'X_1)^{-1}$ are minimized.

Consider the symmetrical determinant of sums of squares and products $\Delta = |c_{ij}| = |X_1'X_1|$, and denote by $C_{hh}$ the cofactor of $c_{hh}$ in $\Delta$ and by $C_{ij,hh}$ the cofactor of $c_{ij}$ in $C_{hh}$. Using Cauchy's expansion we have

$$
\Delta = c_{hh}C_{hh} - Q,
$$

where $Q$ is a quadratic form in the $k$ variables $c_{hi} (i = 0, 1, \ldots, h-1, h+1, \ldots, k)$ and

$$
Q = \sum_{ij,h} c_{hi}c_{hj}C_{ij,hh}.
$$

Now since $X_1$ is of rank $k + 1$, $Q$ is necessarily positive definite and $\Delta$ is positive. Also $c_{hh} = N$ (from (9.1:3)) and $V(b_h) = \sigma^2 c_{hh}/\Delta$, where $V(b_h)$ is the variance of $b_h$. Consequently, rearranging (9.2:3),

$$
V(b_h) = N^{-1} \sigma^2 \left\{ 1 + \Delta^{-1} \right\} (\text{positive definite quadratic form in the } c_{hi}).
$$
Thus $V(b_h)$ is a minimum only when each of the $c_{hi}$ (the $k$ sums of products of the $h$th variable with each of the remaining variables) is zero. When this is so all the $c_{hi}$ must be zero also, and consequently $b_h$ is uncorrelated with each of the other estimates and has variance $\sigma^2/N$. For maximum efficiency for all the coefficients then $c_{ij} = NJ$ and a suitable design $D$ is supplied by any $k$ columns after the first, of a matrix $N_{ij}Q$, where $Q$ is orthogonal with the elements of its first column all equal. This result was arrived at by Plackett & Burman (1946). They postulated, however, that the $x$'s in their first-order optimum designs should take only the values $+1$ and $-1$. With this limitation designs existed only when $N$ was a multiple of 4 and they obtained arrangements for $k = 3, 7, 11, \ldots, 99$ factors using $N = 4, 8, 12, \ldots, 100$ trials. Such designs may be used with qualitative or quantitative variables; in our case where the variables are essentially quantitative this restriction is not introduced and $N$ can have any value.

9.3 For our problem, therefore designs of optimum precision for up to $k = N - 1$ factors in $N$ experiments may be obtained from any orthogonal matrix $Q$ with elements in the first column all equal and $Q_{ij} = N_{ij}Q$. We now assume $k = N - 1$ and consider the geometrical implications of the above result. Since $D$ is of rank $k = N - 1$, the $N$ experimental points are the vertices of an $N - 1$ dimensional simplex. Write the $u$th row of $Q_{ij}$ as $x_u'$ and denote the angle which the $u$th and $s$th experimental points make with the origin by $\theta_{us}$, then since $Q_{ij} = \frac{[u':D]}{Q}$, the distance of each experimental point from the origin is $(N - 1)^{1/2}$ and

\[(9.3:1)\]

\[x'_u x'_s = 0 = 1 + (N - 1) \cos \theta_{us}\]

i.e.

\[(9.3:2)\]

\[\cos \theta_{us} = - (N - 1)^{-1} \text{all } u \text{ and } s, u \neq s.\]
Consequently this design is formed by the vertices of the regular $N-1$ dimensional simplex. If two factors are tested in three trials the experimental points should be at the vertices of an equilateral triangle; for three factors tested in four trials the experimental points should form a regular tetrahedron and so on. It should be noted that no restriction is necessary on the orientation of the design. We can turn the regular figure in any direction; this will correspond simply to a different choice of the orthogonal matrix $Q$, and the variance covariance matrix for the b's will remain unchanged.

As an example, Figure 1 shows two particular orientations of the optimum design for $N = 4$, $k = 3$.

Figure 1. Orientations of the optimum design for $N = 4$, $k = 3$.

The design matrices are

\[
\begin{align*}
D_a &= \begin{pmatrix}
    1 & -1 & -1 \\
    2 & 1 & -1 \\
    3 & -1 & 1 \\
    4 & 1 & 1
\end{pmatrix}, \\
D_b &= \begin{pmatrix}
    1 & -1 & -1 \\
    2 & 1 & -1 \\
    3 & 2 & -1 \\
    4 & . & 3
\end{pmatrix}
\end{align*}
\]

\[
\begin{pmatrix}
    x_1 \\
    x_2 \\
    x_3
\end{pmatrix} = \begin{pmatrix}
    \sqrt{2} \\
    \sqrt{2}/3 \\
    1/\sqrt{3}
\end{pmatrix}
\]
\( D_a \) is the familiar half-replicate of the \( 2^3 \) factorial; the other half replicate is obtained by rotation of the first and completes the cube. \( D_b \) is also obtained by orthogonal rotation of \( D_a \), so that the line joining the points (1) and (2) is parallel to the axis of \( x_1 \) and (1), (2) and (3) fall on a plane parallel to the plane of \( x_1 \) and \( x_2 \). \( D_b \) is seen to have elements proportional to Helmert's orthogonal matrix (for clarity the elements are given as whole numbers with the necessary multiplier shown below). This latter design has rather a curious property, for it is a 'one factor at a time design' although not of the orthodox pattern. To use it the experimenter would first perform a 'blank' experiment with all factors at the lower levels; in the second experiment the level of the first factor only would be changed; in all subsequent experiments this would then be held at the average of these two levels. In the third experiment the level of a second factor would be raised, and in all subsequent experiments this factor would be held at the average level of the three experiments. This procedure could be continued for any number of experiments and factors. The estimates would be uncorrelated, and on the convention we have adopted concerning the units for the factors, the variance of the estimates would be the same with both designs.

9.4 Although the variances and covariances under orthogonal rotation of the design remain constant, the magnitude and arrangement of the possible biases which might occur if the planar approximation was inadequate do not. Suppose that, contrary to assumption, to obtain a perfect fit it was necessary to include \( S \) extra terms \( x_2 \beta_2 \), so that instead of (9.2:2) we had

\[
\eta = x_1 \beta_1 + x_2 \beta_2,
\]
then (Box & Wilson, 1951) \( B_1 \) would no longer supply unbiased estimates of \( \beta_1 \) but instead

\[
E(B_1) = \beta_1 + AB_2,
\]

where \( A \) is a \((k = 1) \times 5\) matrix of coefficients of the biases called the alias matrix and given by \( A = (X'X)^{-1} X_1X_2 \). With the orthogonal designs discussed here this simplifies to \( A = N^{-1} X_1X_2 \). In judging first-order designs we shall consider possible biases due to terms of second order. Now there are two varieties of second-order terms: those which are coefficients of square terms \( x_1^2, x_2^2, \) etc., sometimes called quadratic effects, and those which are the coefficients of product terms \( x_1x_2, x_1x_3, \) etc., sometimes called linear \( \times \) linear interactions. In what follows it is mathematically convenient to define the effect \( \beta_{11} \) as the coefficient of \( x_1^2 \) whilst \( \beta_{12} \) is defined as the coefficient of \( x_1x_2 \). Equation (9.4:1) may then be written

\[
\eta = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k + \beta_{11} x_1^2 + \ldots + \beta_{kk} x_k^2 + \beta_{12} (x_1x_2)^2 + \ldots + \beta_{kk-k} (x_{k-k}x_k)^2,
\]

and the matrices of bias coefficients corresponding to \( D_a \) and \( D_b \) are found to be

\[
A_a = \begin{bmatrix} 0 & 1 & 1 & 1 & \ldots & \ldots & 33 & 22 & 11 & 12 & 13 & 23 \\ 0 & 1 & 1 & 1 & \ldots & \ldots & 1 & 1 & 1 & \ldots & \ldots & \ldots \\ 2 & \ldots & \ldots & \ldots & \sqrt{2} & \ldots & \ldots & \sqrt{2} & \ldots & \ldots & \sqrt{2} & \ldots \\ 3 & \ldots & \ldots & \ldots & \ldots & \ldots & \sqrt{2} & \ldots & \ldots & \ldots & \sqrt{2} & \ldots \\ \end{bmatrix}, \quad A_b = \begin{bmatrix} 0 & 1 & 1 & 1 & \ldots & \ldots & 33 & 22 & 11 & 12 & 13 & 23 \\ 0 & 1 & 1 & 1 & \ldots & \ldots & 1 & 1 & 1 & \ldots & \ldots & \ldots \\ 2 & \ldots & \ldots & \ldots & \sqrt{2} & \ldots & \ldots & \sqrt{2} & \ldots & \ldots & \sqrt{2} & \ldots \\ 3 & \ldots & \ldots & \ldots & \ldots & \ldots & \sqrt{2} & \ldots & \ldots & \ldots & \sqrt{2} & \ldots \\ \end{bmatrix}
\]

The figures in brackets are multipliers of the rows of \( A_b \). Using \( D_b \), for example, the expected value of \( b_3 \) when second-order terms were not all zero would be
9.5 If we could, we would choose to orient the optimum design so that the bias coefficients were as small as possible. In this way both random and systematic errors might be simultaneously minimized. Consider the \((k+1) \times (k+1)\) matrix \(A^\dagger\). The sums of squares of bias coefficients for the \(k+1\) estimates \(b_0, b_1, \ldots, b_k\) are given by the diagonal elements, and the magnitude of these would provide one indication of the efficacy of any particular orientation. We find somewhat unexpectedly, however, that for these optimum first-order designs \(A^\dagger\) is invariant for any orthogonal rotation of the design. This is proved as follows. Denote by \(x'_1, \ldots, x'_N\) the \(N\) rows of the matrix \(X_1\) and by \(X_3\) a matrix whose \(N\) rows are \((x'^1_1) [2], \ldots, (x'^1_N) [2], \ldots, (x'^N_1) [2]\), the derived power vectors of degree 2 (Aitken, 1948). Then \(X_3 = \begin{bmatrix} U & D & E \end{bmatrix} \begin{bmatrix} x_1 \end{bmatrix}\) and \(N^2 \begin{bmatrix} x'_1 X_1 X'_1 \end{bmatrix} = AA^\dagger + J\), where \(J\) is a diagonal matrix in which the first diagonal element is 1 and each of the remaining \(k\) diagonal elements is 2.

Now suppose the design is submitted to orthogonal rotation and denote the new matrices by \(\tilde{D}, \tilde{X}_1, \tilde{X}_3\) and \(\tilde{A}\). Then \(\tilde{D} = DQ\), where \(Q\) is some \(k \times k\) orthogonal matrix, and \(\tilde{X}_1 = X_1H\), where \(H\) is a \((k+1) \times (k+1)\) orthogonal matrix consisting of \(G\) bordered by a first row \(r' = (100 \ldots 0)\) and a first column \(r\). Now \(H\) transforms the vector \(x'^1u\); denote by \(H [2]\) the matrix which correspondingly transforms the vector \((x'^1u) [2]\).

Then

\[
(9.5:1) \quad AA^\dagger + J = N^{-2} H' X_1 X_3 H [2] H'[2] X_3 X_1 H,
\]

and since \(H\) is orthogonal so is \(H [2]\). Now the \(j\)th diagonal element of \(X_3 X_3'^1\) is

\[
(x'_j [2]) (x'_j [2]) = (x_j x'_j)^2 = N^2
\]
and the $i_j$th non-diagonal element is $(x_i)^2(x_j)^2 = (x_i x_j)^2 = 0$. Consequently the right-hand side of (9.5:1) reduces to $N$. We find in consequence that $AA' = N - J$, whatever the orientation of the design. That is, the sum of squares of the coefficient of the biases for $b_0$ is $N - 1$, and for each of the effects $b_1 \ldots b_k$ it is $N - 2$. The result is of course only true for the particular relative weighting of quadratic and interaction terms which has been adopted. This relative weighting is, however, a reasonable one, and the important conclusion emerges that if we have no prior knowledge concerning the relative importance of particular second-order terms no arrangements which are dramatically worse or better than others can be expected to arise as a result of rotation of the designs. In particular, if $k = N - 1$, it is not possible to keep a selected estimate clear of bias.

9.6 When, on the other hand, something is known of the type of approximating second-degree equation to be expected it might be possible to reduce bias by suitable rotation of the design. Consider a particular class of designs which are such that only $b_0$ is biased by quadratic terms. For this to happen each of the $N - 1$ column vectors in $x_1$ corresponding to first-order effects must have zero inner product with the $N - 1$ column vectors in $x_2$ corresponding to quadratic effects. This can only happen if the latter have all elements equal to $+1$ which in turn implies that elements in $D$ consist entirely of $+1$'s and $-1$'s. These designs are those obtained by Plackett & Burman. Now the response contours generated by the second degree approximating equation are a set of conics. Suppose the direction of the principal axes of the system were known. Then because of the property mentioned above, if any of the designs of Plackett & Burman were rotated so that their axes were parallel to these...
principal axes the effects $b_1, \ldots, b_k$ would be unbiased, since in the new variables the second-degree equation contains no product terms. This may have practical application in the exploration of 'ridge' systems. Such systems occur, for example, when a line or plane of near maxima rather than a single point maximum is found. The probable existence and direction of such systems can sometimes be deduced from theoretical considerations, in which case it might be an advantage to rotate axes of the design so as to be parallel to these suspected 'ridges'.

It is worth noting (Box & Wilson, 1951) that by replication of any design with change of signs a design of 'Type B' is obtained. That is to say, one in which the first-order estimates are unbiased by terms of second order. This of course applies to all the designs discussed here.

10. FURTHER RESEARCH

Considerable progress has been made in obtaining designs for fitting second order and higher series, however, the results are not yet sufficiently complete to include in this report. In the second order case the condition of orthogonality is a necessary condition but does not yield a unique solution. The further criterion of "rotability" is being investigated. This criterion essentially requires that the efficiency of a design should be independent of how it happens to be oriented with respect to the contours of the unknown response surface.