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We, the members of the Committee appointed to examine the Thesis submitted by Walter Zayachkowski, B.A. (Sask.), in partial fulfillment of the requirements for the Degree of Master of Arts, beg to report that we consider the thesis satisfactory both in form and content.

Subject of Thesis: An Analysis of Certain Composite Designs and Their Response Surfaces.

We also report that Walter Zayachkowski has successfully passed an oral examination on the general field of the subject of his thesis.

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AN ANALYSIS OF CERTAIN COMPOSITE DESIGNS AND THEIR RESPONSE SURFACES

A Thesis
Submitted to the Faculty of Graduate Studies
in Partial Fulfilment of the Requirements
for the Degree of
Master of Arts
in the Department of Mathematics
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by
Walter Zayachkowski
Written under the Supervision of
Professor N. Shklov
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Abstract

Use of factorial experiments and factorial designs in experimental design work to obtain optimum results is the gist of the thesis. A treatment, both descriptive and mathematical, of experimental designs, response surfaces, and optimum conditions, based on the greater portion of the bibliography, is given.

The problem dealt with is the exploration and exploitation of response surfaces for the attainment of optimum conditions. A descriptive account and representation of a response surface by a response function is given. Methods of finding an optimum response on the response surface employing certain experimental strategy in the experimental region, using the method of steepest ascent to approach a near-stationary point, and local exploration of the surface in a near-stationary region are treated. Types of surfaces encountered in such a region are indicated.

Experimental and composite designs are described and several examples given. The matrix theory applicable to experimental designs for the estimation of coefficients of the response surface equation is presented. It applies to both orthogonal and non-orthogonal designs.

The second degree equation representing a response surface is discussed. Contours generated in both two and three dimensions, with surfaces and hypersurfaces represented by the respective contours, are discussed. The canonical analysis of the second degree equation, consisting of the determination of stationary points, of the canonical form of the equation, and of the new axes in terms of the original axes, is carried out.

Next, several examples of surfaces met in actual experimental research are presented. The 2^2 and 2^3 composite, pentagonal, and cubic-octahedral designs are used. All their corresponding matrices necessary for the estimation of the coefficients of the response surfaces, are tabulated. Hypothetical experiments are planned to indicate the possible variety of response surfaces. Each experimental design presents a different type of response surface. There are surfaces giving ellipses for contours, surfaces containing a rising ridge, surfaces giving ellipsoids for contours, and surfaces containing a stationary plane ridge in three variables. Calculations and computations, based on the theory in Chapter II, are carried out and the results are stated. The cubic-octahedral design, incidentially, is a more compact design than the 2^3 composite, and its required matrices are more conveniently determined.

A statement of how the study of this thesis topic may be extended is given in Chapter V.

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CHAPTER I

INTRODUCTION

In experimental design work, situations occur in which it is necessary to study the effects of varying several factors. The term factor is used here to denote any feature of the experimental conditions which may be deliberately varied from trial to trial. It could happen that in a thorough investigation of such a situation it is not sufficient to vary one factor at a time. An examination of all possible combinations of the different factor levels may have to be carried out in order to discern the effect of each factor and the ways in which each factor is modified by the variations of the others. In the analysis, not only is the effect of each factor determined just as accurately as if only one factor had been varied at a time, but the interaction effects are also evaluated. This technique can be easily extended to experiments in which the factors are to be investigated at more than two levels. For measurable factors the experiment results in a series of points to which may be fitted a curve or surface which expresses the results in terms of the factor levels. Combinations of factor levels correspond to points in space. For any set of trials the levels will be represented by a group of such points, and it is the configuration of these points which is called the experimental design.

Experiments carried out by research workers and experimenters are usually intended to determine the effects of several factors on the yield or quality of a product, the resistance of material to corrosive action, and so on. There is a great advantage in designing an experiment so that the effect of changing the level of any one variable can be assessed quite independently of changes in the levels of the others. This can be achieved by choosing a set of values for the factors involved, and carrying out trials of the process with all possible combinations of the levels of the factors. Such an experiment is called a <u>factorial experiment</u>, and the most efficient method of studying such an experiment is to use a <u>factorial design</u>. An efficient method is one which obtains the required information with the desired degree of precision and with the minimum amount of effort. Factorial designs estimate the main effects of every factor independently of one another and determine the interaction effects, both with maximum precision. They also supply an estimate of the experimental error for assessing the significance of the effects. The classical field in which the theory of factorial designs has evolved is that of agricultural experimentation.

Sometimes it may be necessary to confuse deliberately unimportant comparisons in order to assess the more important comparisons with greater accuracy. This process is called <u>confounding</u>, and it is required in factorial experiments in which it is impractical to carry out the number of observations for the complete design. In a complete factorial experiment, all possible combinations of all the levels of the different factors are investigated. This involves a large number of tests when the number of factors is five or more. However, in certain cases it may be sufficient to investigate the main effects of the factors and only their more important interactions. This is accomplished by using a fraction of the number of tests required for a complete factorial experiment, and gives rise to <u>fractional factorial</u> experiments with corresponding designs.

The subject of this dissertation is the mathematical analysis of the problem of finding the best operating conditions for a process by maximizing a feature such as the yield of a product, or minimizing a feature such as the cost. Equations of the corresponding response surfaces are derived. If the initial conditions are quite different from those giving an optimum result, the path of steepest ascent is used to determine new levels which are nearer the optimum ones. Near the optimum, the technique of local exploration is used to determine this optimum more precisely. The most practical physical conditions for obtaining it are also set up. Composite designs are invaluable in this problem. The 2^2 and 2^3 composite, pentagonal, and cubic-octahedral designs are dealt with separately. Their response surfaces are analyzed and the desired information obtained. Several original designs and their corresponding matrices are presented.

It should be mentioned that, in certain cases, both the empirical surface, based on the factor levels and experimental results, and the theoretical surface, based on the factor levels and the mechanism of the system, can be derived and compared with one another to notice how close an agreement there is between the general characteristics of the two surfaces. This is possible only if the mechanism of the system is not a very complicated one. Otherwise, an empirical approach is the better choice.

CHAPTER II

COMPOSITE DESIGNS AND THE EXPLORATION AND EXPLOITATION OF THEIR RESPONSE SURFACES FOR THE ATTAINMENT OF OPTIMUM CONDITIONS

A. Response Surfaces.

1. Descriptive Account.

The object of this chapter is to find the levels of the factors which give an optimum response. To any particular combination of factor levels corresponds a true level of the response, actually a hypothetical value which would be obtained in the absence of experimental error. It is denoted by η, and it is this η which is optimized in the problem. Due to the experimental error, which is supposed to be distributed as $N(0,\sigma^2)$, the observed response for a particular combination of factor levels differs from η and is denoted by y.

Thus, the levels of k quantitative factors or variables, $x_1, x_2, \ldots x_k$, capable of measurement and control, determine a response η. In other words, there exists a mathematical function of $x_1, x_2, \ldots x_k$, the value of which for the u^{th} combination of factor levels ($u = 1,2,\ldots,n$) supplies the corresponding value of η:

$$\eta_u = \varphi(x_{1u}, x_{2u}, \ldots, x_{ku}) \tag{1}$$

This function φ is called the response function. Owing to unavoidable uncontrollable items, as intimated above, the observed response y_u varies in repeated observations having mean η_u and variance σ^2.

The relation between response and factor levels may be conveniently visualized geometrically when the number of factors is not greater than three. The relation between η and a single factor x_1 may be represented by a response curve; that between η and two factors x_1 and x_2 may be represented by a surface called the <u>response surface</u>. Such a surface, in which x_1 is the concentration of one of the reactants, x_2 the reaction time, and η the yield, is shown in Figure 1.

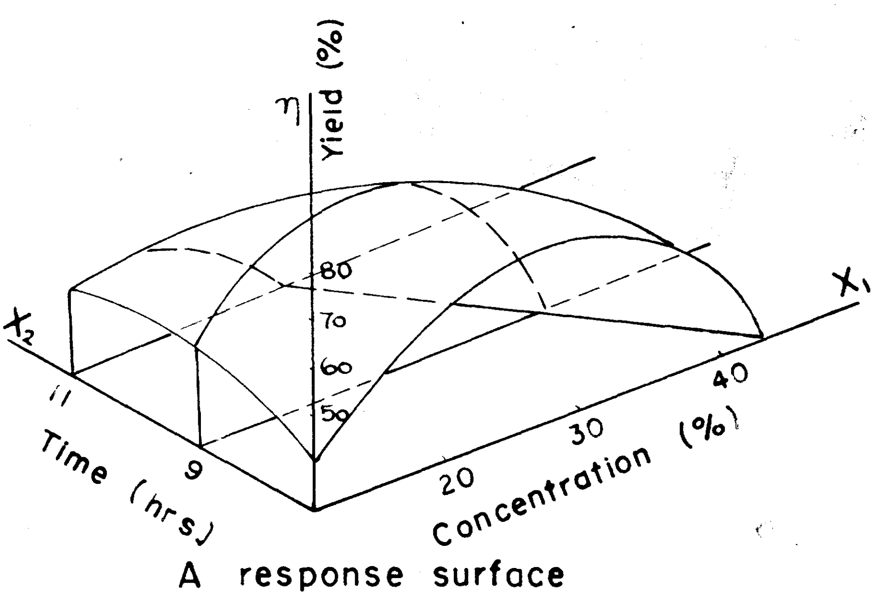
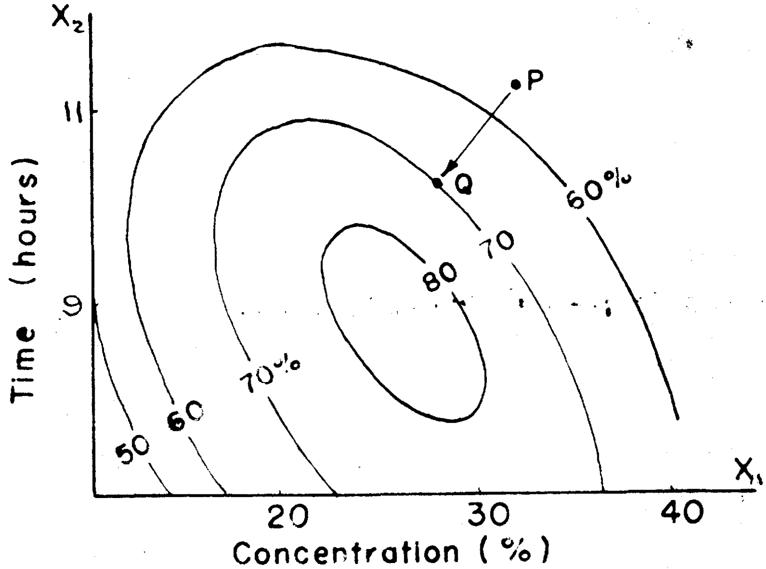


Fig. 1

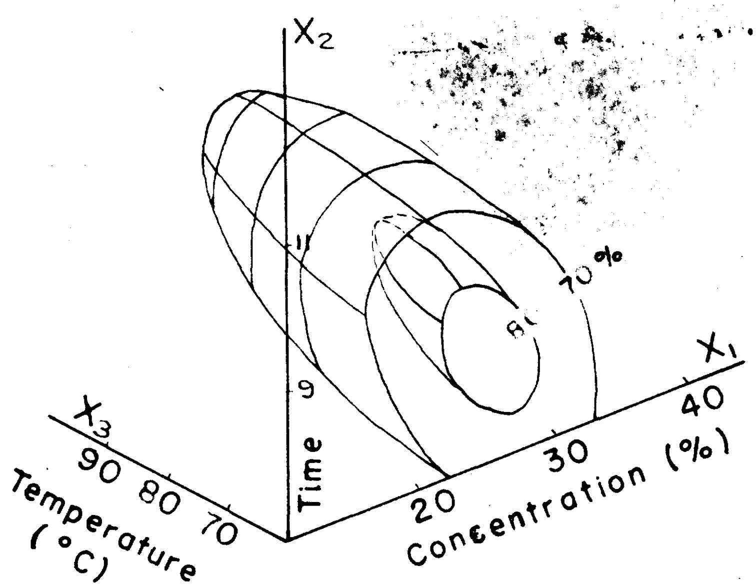
If lines of equal response are drawn on a graph whose co-ordinates denote the levels of the factors, response contours for the surface are obtained. Figure 2 shows the yield contours for the surface of Figure 1. This happens to be a useful alternative representation of a response surface.



Yield contours for the surface of Figure 1

Fig. 2

Furthermore, geometrical representation is possible with as many as three factors. The third dimension, not required for the representation of the response, may be used to accommodate an extra factor. The methods developed may be applied to k dimensions; however, a geometrical illustration is no longer possible. If, in addition to the concentration x_1 and the time x_2, a third factor, the temperature of reaction x_3, is added, it is then possible to study the contour surfaces of equal yield in a three-dimensional factor space, as in Figure 3.



Contour Surfaces in Three-dimensional Factor Space

Fig. 3

It is usually possible for the experimenter, at the beginning of his experimental work, to define the region of the factor space corresponding to factor combinations of major interest. This is called the experimental region. The problem is to find the point or points of optimum response in this experimental region.

2. Representation of the Response Curve or Surface.

First of all, the experimenter is assumed to be studying the effect of the response η of changing the level x_1 of a single variable. If the locus of the functional relation $\eta = \varphi(x_1)$ is continuous, it is possible to represent it to any degree of approximation by taking a sufficient number of terms of the series

$$\eta = \beta_0 + \beta_1 x_1 + \beta_{11} x_1^2 + \beta_{111} x_1^3 + \cdots\cdots, \qquad (2)$$

and suitably choosing the constants $\beta_0, \beta_1, \beta_{11}$, etc. If the range of values of x_1 is wide, more terms will be necessary to obtain a suitable fit. If the range is quite narrow and does not include a turning point of the curve, the straight line $\eta = \beta_0 + \beta_1 x_1$ usually supplies a good approximation.

For two factors, the corresponding polynomial is

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \beta_{111} x_1^3 + \cdots \qquad (3)$$

Assume that the origin of the co-ordinate system is taken at some point in the region in which an approximation is required. If the polynomial (3) exactly represents the response function $\varphi(x_1, x_2)$ in this region, the level of response at the origin is β_0; the values at the origin of the first order differential coefficients $\partial\varphi/\partial x_1$, $\partial\varphi/\partial x_2$, referred to as <u>first order effects</u>, are given by β_1 and β_2. The <u>second order effects</u>, multiples of the second order differential coefficients and equal to $\frac{1}{2}\partial^2\varphi/\partial x_1^2$, $\frac{1}{2}\partial^2\varphi/\partial x_2^2$, $\partial^2\varphi/\partial x_1\partial x_2$, are given by β_{11}, β_{22}, and β_{12} respectively. It is now quite obvious how the analysis may be extended.

As terms of higher degree are added to the series, a closer approximation to the response surface is obtained. If terms of degree 2 and higher are ignored in equation (3), the function is approximated by

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 \ . \qquad (4)$$

This is the equation of a plane, $-\beta_1$, $-\beta_2$ and 1 being the direction numbers of any normal to it. If the sub-region of the surface is small and does not include a turning point, the above equation might provide an adequate approximation. For a larger region, a polynomial of higher degree would be necessary for a reasonable approximation. If the surface were like that of Figure 1, terms of higher degree would be needed for a larger region in order to take into account the curvature of the surface.

In general, it has been assumed that the response at a point $(x_1, x_2, \ldots x_k)$ in the factor space can be represented by a regression equation of the form

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdot\ \cdot + \beta_{11} x_1^2 + \cdot\ + \beta_{12} x_1 x_2 + \cdot\cdot + \beta_{111} x_1^3 + \cdots \quad (5)$$

Here, the coefficient of $x_1^{\alpha} x_2^{\gamma} \ldots x_k^{\pi}$ is given by $\beta_{1\,2\,\cdot\cdot\,k}^{\alpha\,\gamma\,\pi}$, where subscript 1 is to be repeated α times, subscript 2, γ times, etc.

Suppose that all terms of degree d and less are included and a perfect fit is obtained within a given region. Equation (5) then corresponds to the Taylor expansion of the response function $\varphi(x_1, x_2, \ldots, x_k)$ about the origin 0 and the derivatives at 0 are simple multiples of the β's [3, p.5]. That is, $\varphi_0 = \beta_0$, $\varphi_1 = \beta_1$, $\varphi_{11} = 2\beta_{11}$, $\varphi_{12} = \beta_{12}$, $\varphi_{111} = 6\beta_{111}$, and in general

$$\varphi_{1\,2\,\ldots\,k}^{\alpha\,\gamma\,\ldots\,\pi} = \alpha!\gamma!\ldots\pi!\beta_{1\,2\,\ldots\,k}^{\alpha\,\gamma\,\ldots\,\pi}. \quad (6)$$

The quantity on the left is the value at the origin 0 of the derivative obtained by differentiating the function α times with respect to x_1, γ times with respect to x_2, etc.

Furthermore, estimates b_0, b_1, b_2, etc. of β_0, β_1, β_2, etc. can be obtained by fitting the regression equation, provided that the responses are observed at a set of points numerous enough and suitably placed within the region concerned. From relationship (6) the appropriate multiplier may be obtained and the b's used to provide estimates f_0, f_1, f_2, etc. of the derivatives φ_0, φ_1, φ_2, etc. at the origin 0.

B. Methods of Finding an Optimum Response.

1. Experimental Strategy.

In the entire k-dimensional factor space, there exists a region R, whose boundary depends on the practicability of the factor level selections, which is called the experimental region. In the smallest number of experiments, it is required to find the point $(x_1^0, x_2^0, .. x_k^0)$ within R at which η is an optimum. In experimental work, responses optimized are yield, purity, or cost; factors affecting them are variables such as temperature, pressure, and time.

The strategy of the experimenter will be influenced by the size of the experimental error, the complexity of the response surface, and the possibility of conducting experiments sequentially. In sequential experiments, each set of experiments is designed using the knowledge gained from the previous sets.

A sure way of finding optimum conditions would be to explore the whole experimental region by carrying out experiments on a grid of points throughout R. In such a case, the experiments are sequential, with a rather small experimental error. However, if the response surface is quite complicated, adequate approximation is possible only if the grid has a certain minimum density. The number of points on such a grid is usually too large to make the exploration of the entire region R practical [3, p.2].

Small experimental error allows small changes to be determined quite accurately. The experimenter can therefore choose to explore a small <u>sub-region</u> of the whole region R with only a few experiments. Sequential experiments will enable him to use the results obtained in one sub-region to move to a second in which a higher response exists. By a successive application of such a procedure, it is possible to reach a maximum or at least a near-stationary point of high response. There is a danger of missing a higher ultimate maximum but the risk is not very serious. The "one factor at a time" method, in which the level of one factor is varied while the levels of the others remain fixed, would be the obvious procedure but a more efficient one will be given.

For one variable x_1 the observed yield y can be plotted against x_1 and, if a smooth response curve results, the value of x_1 corresponding to the highest yield will provide an estimate of the maximum x_1.

On the other hand, the method of least squares could be used to fit a polynomial like equation (2) to the experimental points. To locate the position of the true maximum within a certain range, the fitted expression would be differentiated and the derivative equated to zero. If terms up to the third degree were included and b_0, b_1, b_{11}, and b_{111} were the least squares estimates of β_0, β_1, β_{11} and

β_{111}, the fitted equation would be

$$Y = b_0 + b_1 x_1 + b_{11} x_1^2 + b_{111} x_1^3. \tag{7}$$

Here, Y designates the value calculated from the fitted equation, as distinguished from η the true value, and from y the observed value, of the response. Differentiating both sides and equating the derivative to zero gives

$$dY/dx_1 = b_1 + 2b_{11} x_1 + 3b_{111} x_1^2 = 0. \tag{8}$$

The solution of this quadratic equation provides the value of x_1 corresponding to the maximum on the fitted curve.

The grid method may be used for k factors, provided the response surface is not too complicated. A yield surface is plotted through points of a grid in the experimental region at which trials have been performed. An estimate of the optimum combination is provided by the set of levels for the factors corresponding to the highest point on this surface. The method of differentiating a fitted surface is easily extended to k dimensions.

In practice there are two distinct phases involved in the procedure of determining optimum conditions. The procedure involved in each phase will be described first by considering two factors, x_1 and x_2, and will then be generalized.

2. Method of Steepest Ascent for Approaching a Stationary Point.

The steepest ascent technique is used in problems in which the starting conditions are remote from the optimum conditions and the experimental error is small. With only a few steps of the procedure it is possible to move rapidly through the factor space to a near-stationary region. This region will not contain a minimum, nor will it necessarily contain a true maximum. However, once such a region is located, only a few experiments are required to determine its nature.

When the initial conditions are remote from those at the maximum, such as those at the point P in Figure 2, it is possible to represent the surface in a local region by a sloping plane. By performing a suitable set of trials in a sub-region of P, the direction numbers b_1, b_2 relevant to the plane can be estimated and the steepest direction up the plane determined. This is the direction at right angles to the contour lines, and it will indicate how the factors must be varied to get a maximum increase in response. The experimenter then proceeds to another point in this determined direction, redetermines the direction numbers at it, and repeats the process to reach points of higher and higher response.

After the experimenter has moved quite high up the response surface, he will find that the direction numbers b_1, b_2 change more gradually and the surface slopes are small compared with the errors of estimation. He will have located a <u>near-stationary region</u>. The above method fails for a surface which has more than one peak. The existence of more than one peak would indicate a fundamental change in the mechanism of the reaction.

From a mathematical viewpoint, it is first assumed that within the region considered, the derivatives of the response function are continuous. It is required to proceed from a point P in a k-dimensional space to a point T at a distance r from P, at which the response gain is a maximum. P is conveniently chosen as the origin with response $\varphi(P) = \varphi(0)$. At T, $\varphi(T) = \varphi(x_1, x_2, \ldots, x_k)$. Since PT = r,

$$r^2 = \sum x_t^2 , \qquad (9)$$

and it is required to have $\varphi(T) - \varphi(P)$ a maximum subject to condition (9). The Lagrange multiplier μ is used [3, p.2] to construct the function

$$\psi = \varphi(T) - \varphi(P) - \tfrac{1}{2}\mu \sum x_t^2 \qquad (10)$$

The maximum is the point where $\partial\psi/\partial x_t$ are all zero, that is where the k equations

$$\mu x_t = \varphi_{x_t}(T), \quad t = 1,2,\ldots, k \qquad (11)$$

are satisfied. From equations (9) and (11),

$$\mu = \pm \left\{ \sum \left[\varphi_{x_t}(T) \right]^2 \right\}^{\frac{1}{2}} / r \qquad (12)$$

From the equations, one sees that the co-ordinates at T must be proportional to the first order derivatives of the response function at T if T is to be the point, distant r from P, at which the gain is greatest.

It is next assumed that φ can be represented about the origin by its Taylor's series in which terms of degree greater than d are ignored. Then, the equation

$$\varphi_t(T) = \left[D_t \sum_{s=0}^{d-1} \left\{(D_1x_1 + D_2x_2 + . \quad . + D_kx_k)^s / s!\right\}\right] \varphi(P) \qquad (13)$$

expresses the derivatives at T in terms of those at P [3, p.3]. Here, D_t denotes differentiation with respect to x_t and the expression within the square brackets is expanded and allowed to operate on φ. By substituting equation (13) into equation (11) and choosing μ so that solutions of equation (11) give a maximum, it is possible to obtain an expression for the co-ordinates of T in terms of the derivatives at P. Particularly, if second and higher degree terms are ignored, one gets k equations

$$\mu x_t = \varphi_t(P) \ , \quad t = 1,2,.., k, \qquad (14)$$

Which indicate the "steepest ascent" from P. Hence, if the first-order derivatives at P can be determined, by varying the factors in proportion to them it is possible to move in a direction at right angles to the contour hyperplanes to a better response at T.

The second degree approximation would be used in a wider sub-region with more experimental points if the experimental error were larger. The locus of T would be provided by solving the k linear equations

$$\mu x_t = \varphi_t + x_1\varphi_{1t} + x_2\varphi_{2t} + \cdots + x_k\varphi_{kt} \tag{15}$$

for a suitable set of values of μ, with the values of the derivatives taken at P = 0. If the derivatives could be determined without experimental error, formula (14) could be applied successively until a stationary point was reached. However, because of experimental error, the more the derivatives are reduced the more difficult it is to determine them with sufficient accuracy in a next set of experiments in order to proceed further. This is why the steepest ascent technique is used to locate a near-stationary region only. Having reached such a region, the experimenter will conduct detailed experiments to determine as accurately as possible the nature of the response surface there.

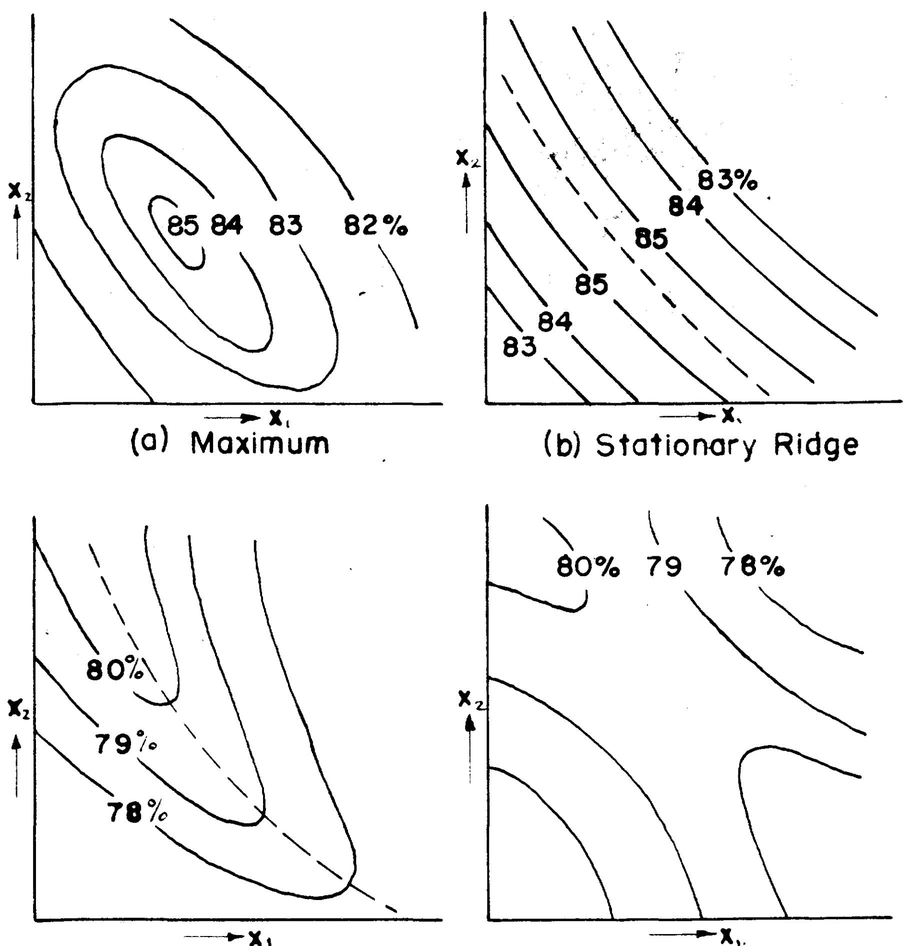
While carrying out a second group of observations, the experimenter should be at liberty to alter the units for the variables, especially if certain factors showed very small effects. The danger here is the possibility of confusing the small effects with the experimental error. Such a situation will arise if the average level for the factor is near a conditional maximum, if the unit is disproportionately chosen, or if the system does not depend on the factor level. A larger unit in the next set of experiments would indicate the reason for the above situation. The level associated with the value zero is referred to as the <u>base level</u>; the change in level of a variable from value

0 to value 1 is known as a unit.

It could happen that the expected increase does not occur when the experiment is performed in the direction calculated. It would be necessary to augment the group of observations already made, and perhaps even new levels would have to be chosen to allow for the estimation of all first and second order effects.

3. The Method of Local Exploration or Exploitation of a Near-Stationary Point.

A near-stationary region is no guarantee that the experimenter is near a maximum like that in Figure 4(a). It is quite possible for the surface to contain a ridge or a minimax. Surface ridges are of great practical importance. In the case of such a ridge, several factor combinations will give the same optimum response of cost or yield, and the experimenter may discover that some of these combinations provide an additional feature of the product, such as texture or quality. Such an additional feature is known as an auxiliary response. In a near-stationary region the experimenter should be interested in the exact nature of the local surface. If a true maximum like that in Figure 4(a) exists, its position will have to be estimated; if a ridge occurs, as in Figures 4(b) and 4(c), its direction and slope must be determined; for a minimax like Figure 4(d), the direction to take to reach a higher response will be required. Usually, for a small near-stationary region, a set of trials is performed, so arranged that an equation of the second degree provides a good fit to the response surface.



Types of surface in a near-stationary region shown by yield contours

Fig. 4

A (k+1)-dimensional paraboloid in the variables Y, $x_1, x_2, \ldots, x_k$ is a good approximation of the response surface in the neighborhood of the design [3,p.23].

$$Y = f_0 + f_1x_1 + f_2x_2 + \ldots + \tfrac{1}{2}f_{11}x_1^2 + \tfrac{1}{2}f_{22}x_2^2 + \ldots + f_{12}x_1x_2 + \ldots \quad (16)$$

Associated with such a surface are k-dimensional contours

$$Y_c = f_0 + f_1x_1 + f_2x_2 + \ldots + \tfrac{1}{2}f_{11}x_1^2 + \tfrac{1}{2}f_{22}x_2^2 + \ldots + f_{12}x_1x_2 + \ldots \quad (17)$$

on which the response is equal to Y_c.

If equation (16) is differentiated with respect to $x_1, x_2, \ldots, x_k$ in turn and the k linear simultaneous equations thus obtained solved, the co-ordinates of the stationary point S on the fitted surface are obtained. They are denoted by $x_1^0, x_2^0, \ldots, x_k^0$. When they are substituted in (16), one gets the predicted response at S.

The nature of the system is made evident when the conicoid is reduced to <u>canonical form</u>. The origin is shifted to the stationary point S, which is the centre of the curves representing the contour surface, and the co-ordinate axes are rotated to correspond to the axes of the conicoids. Equation (17) then assumes the form

$$Y_c - Y_0 = \lambda_1 X_1^2 + \lambda_2 X_2^2 + \ldots + \lambda_k X_k^2 \, . \quad (18)$$

From the expression it is evident that, if λ_1 is negative, for example, there is a loss of response as one moves away from S. Large values of the λ's correspond to rapid changes while small values indicate slow changes.

Let us suppose that in a particular example the λ's, the directions of X_1, X_2, ... , X_k, and the location of a stationary point have all been determined. If all the λ's were negative, the fitted surface would have a true maximum at S, and the contour surfaces would be ellipsoids. If at least one λ were positive, there would be a col with elliptic hyperboloids for contour surfaces, and the positive λ's would indicate how the experimenter should move to a higher response. If at least one λ approached zero, the curves would be attenuated along the corresponding axis. Here, the contour surfaces would approach elliptic or hyperbolic cylinders, or the response would possess a ridge. The directions of the line, space, or plane, in which the response is nearly a constant could be determined. In practice, this is very important; the experimenter is able to set up alternate conditions for equal responses and thus work in some auxiliary response into the process. An analysis of the surface would indicate what further experiments may be needed.

It could happen that the stationary point of the fitted function is quite remote from the sub-region of the design near which it was expected. No accurate information about the true surface can be obtained here, but the fitted contour surface can provide useful information. It is possible for a slowly rising ridge leading to higher responses to exist in such a neighborhood. An axis (say X_1) of the fitted conic will be in the direction of this ridge and will have a small corresponding λ_1. The equations of the fitted contour surfaces may be referred to a local origin on X_1, whence they will be of the form

$$Yc - Yo = B_1X_1 + \lambda_1X_1^2 + \ldots + \lambda_kX_k^2, \quad (19)$$

Yo indicating the response at the origin. Here, the contour ridges would be paraboloids with axes along X_1, and B_1 measuring the slope of the ridge. The experimenter would have to explore the axis X_1 with further experiments.

C. Experimental and Composite Designs.

The concept of an experimental design was given in the introduction to this dissertation. A combination of levels of the factors corresponds to a point in the factor space, and the whole pattern of such points from which the surface is derived is called the experimental design. The four vertices of a square correspond to the 2^2 factorial design, the five vertices of a pentagon to the pentagonal design, and the eight vertices of a cube to the 2^3 factorial design. It is convenient to think of each of these figures as centered about the origin.

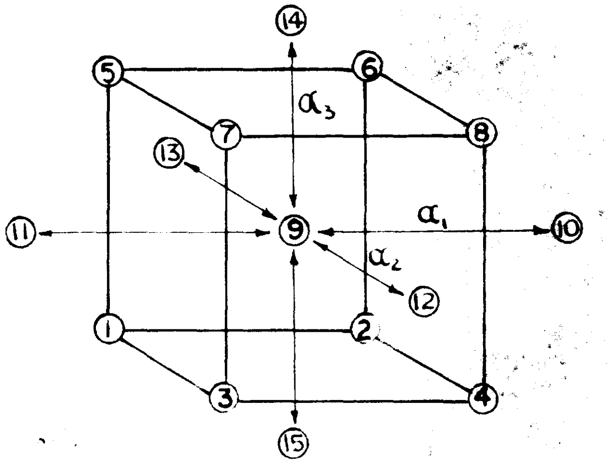
If L constants of a response surface equation are to be determined, the number N of experimental points should normally exceed the number L and certainly cannot be less than L [1,p.32]. If N were equal to L, the N values $Y_1, Y_2, \ldots, Y_N$ predicted by the fitted equation would agree with the observed values $y_1, y_2, \ldots, y_N$, and no conclusion could be drawn about the fit; if N were greater than L, the N values predicted by the equation would differ from the N observed values. The expression

$$S = \sum_{i=1}^{N} (y_i - Y_i)^2 \qquad (20)$$

is the residual sum of squares, and divided by N-L, the residual number of degrees of freedom, provides an estimate of the experimental error variance σ^2. The above holds provided that the real surface can be represented by a function of the form assumed. It may be necessary to take higher order effects into consideration.

Instances may arise which necessitate the estimate of all effects up to the second order. If the number of trials is not to exceed by much the number of constants to be estimated, resort must be made to composite designs, built from complete two-level factorial or fractional factorial designs. For example, consider three factors. First of all, a two-level design, in this case the 2^3 factorial, is chosen to provide estimates of all first order effects and all interaction effects of the second order. By adding seven further points, one at the centre and the other six in pairs along the co-ordinate axes at $\pm\alpha_1, \pm\alpha_2, \pm\alpha_3$

respectively, estimates of the quadratic effects may be obtained. The resulting arrangement of experimental points is shown in Figure 5.



A three-factor composite design.
Fig. 5

The design matrix is given in Table I. The points of the three-factor composite design have been numbered to correspond to the factor levels in Table I. For k factors, (2k+1) supplementary points would be added to the appropriate complete two-level factorial.

Composite designs allow the experimental work to proceed naturally in stages. If the first-order effects are

Table I

A THREE-FACTOR COMPOSITE DESIGN

Trial	Factor level x_1	x_2	x_3
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1
9	0	0	0
10	α_1	0	0
11	$-\alpha_1$	0	0
12	0	α_2	0
13	0	$-\alpha_2$	0
14	0	0	α_3
15	0	0	$-\alpha_3$

found to be quite large and the second-order interaction effects small, the experimenter will use the steepest ascent method to proceed to a new base. However, if the relative magnitude of the above effects is such that it is necessary to determine all second-order effects, then extra points will be added to form a composite design.

Taking for elements the levels of the k variables used in the N trials of an experiment an Nxk design matrix D is next defined. The elements x_{1u}, x_{2u},..., x_{ku} of the u^{th} row of D are the co-ordinates of a point in the k-dimensional factor space, and the N points thus defined make up the experimental design. Observations of the responses obtained at these points are denoted by a column vector Y, and the corresponding vector of expected values is $\eta = E(Y)$. If equation (5) is assumed to contain L terms, it may be written

$$\eta = \sum_{i=1}^{L} \beta_i X_i \; . \qquad (21)$$

The X_i are products and powers of the co-ordinates of the experimental points and are called the independent variables. Next, consider the NXL matrix of independent variables, whose elements are the N values of the L functions of the co-ordinates. If this matrix is denoted by X, equation (21) becomes

$$\eta = X\beta, \qquad (22)$$

where β is the LX1 vector of unknown constants. The method of least squares is used to fit the surface. It is assumed that the observational errors have constant variance σ^2, are uncorrelated, and also that X has rank L. Then [3, p.5],

(i) Unbiased estimates of the elements of the vector β, linear in the observations, with smallest variance are provided by the LX1 vector of estimates $B = TY$ where the <u>transforming matrix</u> T is $(X'X)^{-1}X'$.

(ii) The LXL matrix of variances and covariances of these estimates is $C^{-1}\sigma^2$ where $C = X'X$ is the matrix of sums of squares and products of the independent variables. C^{-1} is called the <u>precision matrix</u>.

(iii) An unbiased estimate of $(N-L)\sigma^2$ is provided by the residual sum of squares

$$(N-L)s^2 = (Y-XB)'(Y-XB) = Y'Y - B'CB = Y'Y - Y'XB.$$

Once a design for determining derivatives up to a given order is decided upon, the matrices T and C^{-1} are calculated and tabulated once for all. The same design may then be used whenever desired by making observations at levels proportional to the elements of D. The sums of products of the observations with the columns of the matrix T' provide estimates b_0, b_1, etc. of the β's. Their variances and covariances are given by the elements of C^{-1} multiplied by σ^2.

An <u>orthogonal design</u> can be obtained by taking $\alpha_1 = \alpha_2 = \ldots = \alpha_k = \alpha$ and suitably choosing α. In an orthogonal design, the sums of products of all pairs of independent variables are zero. That is, the sum of products of any two columns of the matrix X is zero. Table II shows how orthogonal composite designs are built up when the number of factors (k) is equal to 2, 3, and 4.

Table II

ORTHOGONAL COMPOSITE DESIGNS

Number of factors (k)	2	3	4
Basic two-level design	2^2	2^3	2^4
Number of extra points (2k+1)	5	7	9
Distance of axial points from centre (α)	1.000	1.215	1.414

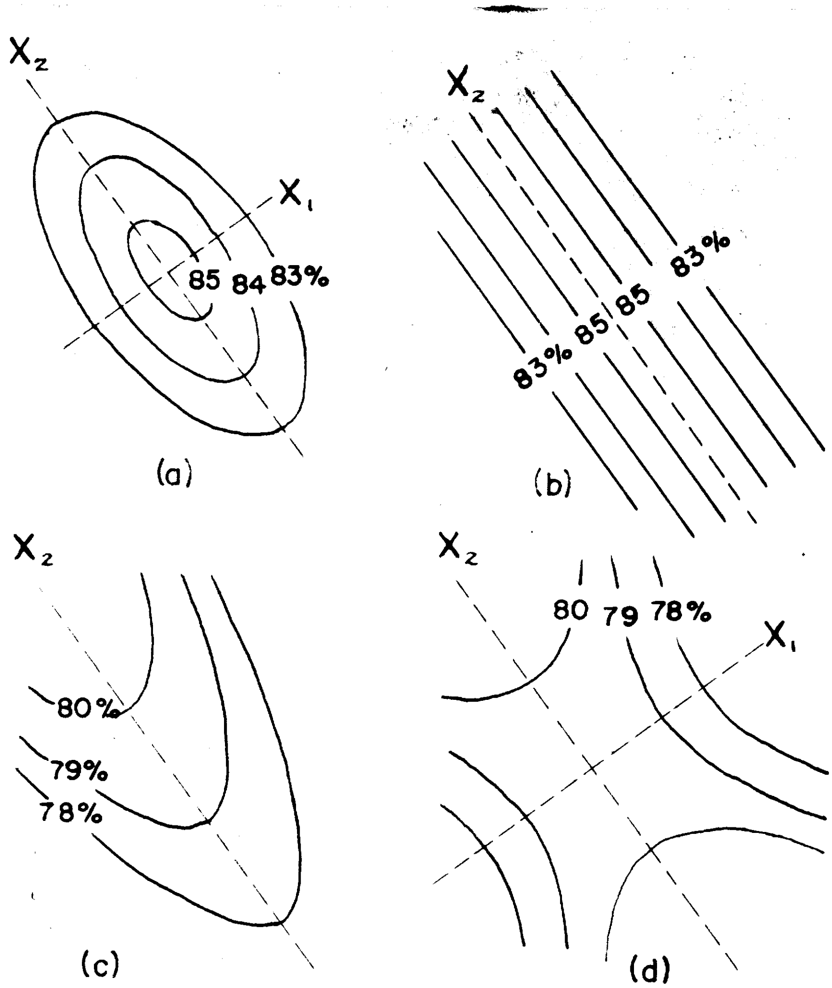
It must be mentioned that the matrix theory approach to experimental designs has one great advantage. It is applicable to both orthogonal and non-orthogonal composite designs. An alternate method applicable to orthogonal designs only is given in [6, p.519], along with the additional procedure to be used for a non-orthogonal design. The alternate method, however, is not as inclusive as the matrix approach.

D. Contours of Surfaces Generated by a Second Degree Equation in Two and in Three Dimensions.

A geometrical illustration of the fitted surface is possible with as many as three factors or variables. The canonical form of the response surface for a second degree equation in two dimensions is

$$Y-Y_s = \lambda_1 X_1^2 + \lambda_2 X_2^2, \qquad (23)$$

where Ys is the yield at the stationary point S. Figure 6 shows contour systems of such second degree equations in two variables. The coefficients λ_1 and λ_2 measure the increase or decrease in the yield in the direction of the corresponding axes. If both are negative, a true maximum exists at S; if both are positive, there is a true minimum at S. As can be ascertained from Figure 6, contour systems may represent a maximum, a minimax, a stationary ridge, or a rising ridge.



Contour systems generated by equations of second degree in two variables

Fig. 6

It must be remarked here that the relative magnitudes of λ_1 and λ_2 determine the degree of elongation of the contours. Mathematically, type 6(b) could be considered to represent a transition stage between 6(a) and 6(d). For a system such as type 6(c), it may be convenient to choose a point along the X_2-axis as origin, whence equation (23) takes on the form

$$Y - Ys = \lambda_1 X_1^2 + B_2 X_2, \qquad (24)$$

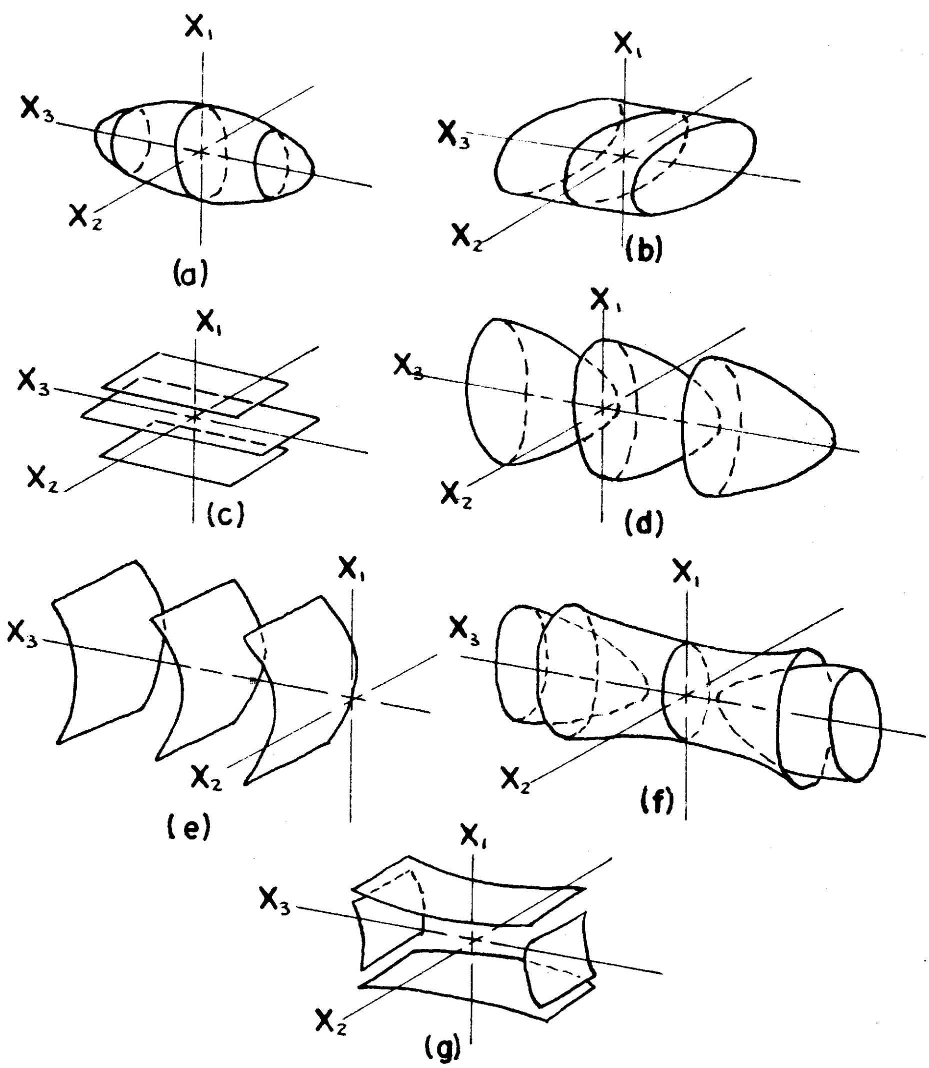
where B_2 measures the slope along the X_2-axis. It must be remembered, however, that the fitted equation supplies an adequate approximation to the response surface only in the immediate neighborhood of the design.

For a second degree equation in three dimensions the canonical form of the response surface is

$$Y - Ys = \lambda_1 X_1^2 + \lambda_2 X_2^2 + \lambda_3 X_3^2 \ . \qquad (25)$$

It is quite proper to think of the three-dimensional contour systems as being generated from those in two dimensions. Conversely, systems in two dimensions are cross-sections of those in three dimensions. Analogously, one may think of three-dimensional contours as being cross-sections of a four-dimensional <u>hypersurface</u>. Figure 7 shows some of the possible three-dimensional contour surfaces in a near-stationary region.

The table below gives the values of the λ coefficients in equation (25) as positive, negative, or zero for the seven types of contour surfaces depicted in Figure 7.



Some possible three-dimensional contour surfaces in a near-stationary region.

Fig. 7

Table III

COEFFICIENT VALUES FOR THREE-DIMENSIONAL CONTOURS

	Values of Coefficients		
Type	λ_1	λ_2	λ_3
(a)	+,-	+,-	+,-
(b)	-	-	0
(c)	-	0	0
(d)	-	-	0
(e)	-	0	0
(f)	-	-	+
(g)	-	0	+

E. <u>Canonical Analysis of the Fitted Second Degree Equation.</u>

The fitted second degree equation of a response surface in three dimensions is of the form

$$Y = b_0+b_1x_1+b_2x_2+b_3x_3+b_{11}x_1^2+b_{22}x_2^2+b_{33}x_3^2$$

$$+b_{12}x_1x_2+b_{13}x_1x_3+b_{23}x_2x_3. \qquad (26)$$

In the canonical analysis of such an equation, the experimenter is interested in determining the position of S and the value of Y_s, the values of λ_1, λ_2, and λ_3, and the directions of the axes X_1, X_2, and X_3.

Since the response is stationary at the point S, $\partial Y/\partial x_1$, $\partial Y/\partial x_2$, and $\partial Y/\partial x_3$ are all zero. Equation (26) is differentiated with respect to each of the variables x_1, x_2, and x_3 and the results equated to zero to yield the set of equations

$$\begin{aligned} 2b_{11}x_1 + b_{12}x_2 + b_{13}x_3 &= -b_1 \\ b_{12}x_1 + 2b_{22}x_2 + b_{23}x_3 &= -b_2 \\ b_{13}x_1 + b_{23}x_2 + 2b_{33}x_3 &= -b_3 \end{aligned} \qquad (27)$$

The solution of these simultaneous equations in three unknowns gives the co-ordinates of the stationary point S, namely (x_1^0, x_2^0, x_3^0). When these are substituted in equation (26), the yield Y_s is obtained.

Equation (26) must next be reduced to the canonical form given in equation (25). The characteristic equation

$$f(\lambda) = \begin{vmatrix} b_{11}-\lambda & \frac{1}{2}b_{12} & \frac{1}{2}b_{13} \\ \frac{1}{2}b_{12} & b_{22}-\lambda & \frac{1}{2}b_{23} \\ \frac{1}{2}b_{13} & \frac{1}{2}b_{23} & b_{33}-\lambda \end{vmatrix} = 0 \qquad (28)$$

is solved to determine the coefficients $\lambda_1, \lambda_2, \lambda_3$. The three values of λ which when substituted in (28) cause the determinant to vanish are the values $\lambda_1, \lambda_2, \lambda_3$. When multiplied out, the determinant becomes a cubic equation in λ of the form

$$f(\lambda) = \lambda^3 + \alpha\lambda^2 + \beta\lambda + \gamma = 0. \qquad (29)$$

The values of the constants α, β, γ are calculated from the known values b_{11}, b_{12}, etc. The method of divided differences (see Appendix 11A of [6, p.563]) may be used to approximate to the values of λ_1, λ_2, and λ_3.

To determine the direction of the new axes an orthogonal matrix M for which

$$X = M(x - x^{o}) \qquad (30)$$

is required. If M_t is the vector corresponding to the t^{th} row of M, then

$$M_t \left(\tfrac{1}{2}F - I\lambda_t\right) = 0 \;, \qquad (31)$$

where F is the matrix $\{f_{st}\}$ of second order derivatives [3, p.30]. If λ_1 is substituted in equation (31) the set of homogeneous equations

$$\begin{aligned} \theta M_{11} + \kappa M_{12} + \pi M_{13} &= 0 \\ \kappa M_{11} + \rho M_{12} + \tau M_{13} &= 0 \\ \pi M_{11} + \tau M_{12} + \omega M_{13} &= 0 \end{aligned} \qquad (32)$$

is obtained. The solutions are proportional to the elements of the first row of M. If M_{11} is put equal to 1, the set may be solved to give $M_{11} = 1$, $M_{12} = \zeta$, $M_{13} = \xi$. Since M is orthogonal, the sum of squares of the elements in any row or column is unity. Thus, if the elements M_{11}, M_{12}, M_{13} are divided by the square root of their sums, the first row of M is obtained. Similarly, by substituting λ_2 and λ_3 in equation (32) the remaining elements of M are obtained. It is then possible to express the X's in terms of the x's. A more detailed description of determining M may be found in [6, p.547].

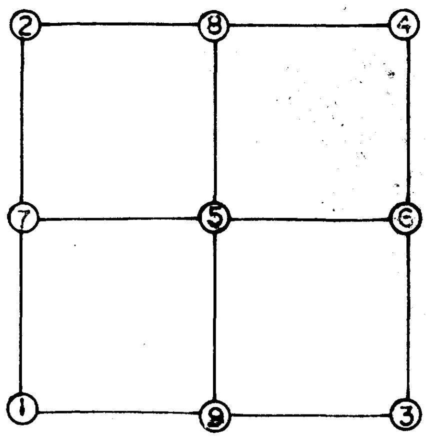
The above analysis can very easily be applied to a second degree equation in two dimensions, and can be easily extended to a second degree equation in k dimensions. It should be mentioned that an important property of an orthogonal transformation is that the matrix of the reciprocal transformation by means of which the x's may be expressed in terms of the X's is the transpose of the matrix of the original transformation.

CHAPTER III

SOME EXAMPLES OF DESIGNS AND CORRESPONDING SURFACES MET IN PRACTICE

A. A 2^2 Composite Design Yielding Ellipses for Contours of the Fitted Surface.

The first example to be dealt with is one in which only two factors x_1 and x_2 are the subject of study. The effects of first and second order are determined by using a 2^2 composite design, shown in Figure 8. It may also be referred to as a 3^2 factorial design.



A two-factor composite design
Fig. 8

The matrices arising in this problem are as follows:

$$D = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{cc} x_1 & x_2 \end{array} \\ \begin{bmatrix} -1 & -1 \\ -1 & 1 \\ 1 & -1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & -1 \end{bmatrix} \end{array} \qquad X = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{cccccc} x_0 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array} \\ \begin{bmatrix} 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & -1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

Here, it is remarked that x_0 is the variable corresponding to β_0 and is always unity.

$$X' = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & 0 & 1 & -1 & 0 & 0 \\ -1 & 1 & -1 & 1 & 0 & 0 & 0 & 1 & -1 \\ 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad X'X = \begin{bmatrix} 9 & 0 & 0 & 6 & 6 & 0 \\ 0 & 6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 \\ 6 & 0 & 0 & 6 & 4 & 0 \\ 6 & 0 & 0 & 4 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix}$$

$$C^{-1} = (X'X)^{-1} = \begin{array}{c} \\ b_0 \\ b_1 \\ b_2 \\ b_{11} \\ b_{22} \\ b_{12} \end{array} \begin{array}{c} \begin{array}{cccccc} b_0 & b_1 & b_2 & b_{11} & b_{22} & b_{12} \end{array} \\ \begin{bmatrix} 5/9 & 0 & 0 & -1/3 & -1/3 & 0 \\ 0 & 1/6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/6 & 0 & 0 & 0 \\ -1/3 & 0 & 0 & 1/2 & 0 & 0 \\ -1/3 & 0 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 \end{bmatrix} \end{array}$$

$$T' = X(X'X)^{-1} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{array} \begin{array}{c} \begin{array}{cccccc} b_0 & b_1 & b_2 & b_{11} & b_{22} & b_{12} \end{array} \\ \begin{bmatrix} -1/9 & -1/6 & -1/6 & 1/6 & 1/6 & 1/4 \\ -1/9 & -1/6 & 1/6 & 1/6 & 1/6 & -1/4 \\ -1/9 & 1/6 & -1/6 & 1/6 & 1/6 & -1/4 \\ -1/9 & 1/6 & 1/6 & 1/6 & 1/6 & 1/4 \\ 5/9 & 0 & 0 & -1/3 & -1/3 & 0 \\ 2/9 & 1/6 & 0 & 1/6 & -1/3 & 0 \\ 2/9 & -1/6 & 0 & 1/6 & -1/3 & 0 \\ 2/9 & 0 & 1/6 & -1/3 & 1/6 & 0 \\ 2/9 & 0 & -1/6 & -1/3 & 1/6 & 0 \end{bmatrix} \end{array} \qquad Y = \begin{array}{c} \% \\ \begin{bmatrix} 76.7 \\ 81.3 \\ 85.1 \\ 80.8 \\ 86.5 \\ 84.1 \\ 80.2 \\ 85.2 \\ 84.2 \end{bmatrix} \end{array}$$

Method I described in [7, p.303] was used to invert the matrix X'X.

Estimates b_0, b_1, etc. of the β's are obtained next. These are supplied by the sums of products of the observations with the columns of the matrix T'. For example,

$$b_0 = (-1/9)(76.7) + (-1/9)(81.3) + (-1/9)(85.1) + (-1/9)(80.8) + (5/9)(86.5) + 2/9(84.1) + 2/9(80.2) + 2/9(85.2) + 2/9(84.2) = 86.21 \pm 0.33\sigma.$$

Similarly,

$$b_1 = 1.97 \pm 0.41\sigma \quad b_2 = 0.23 \pm 0.41\sigma \quad b_{11} = -3.93 \pm 0.41\sigma$$
$$b_{22} = -1.38 \pm 0.41\sigma \quad b_{12} = -2.22 \pm 0.50\sigma$$

An estimate of the response surface equation is

$$Y = 86.21 + 1.97x_1 + 0.23x_2 - 3.93x_1^2 - 1.38x_2^2 - 2.22x_1x_2. \quad (33)$$

Differentiating equation (33) with respect to the variables x_1 and x_2 and equating to zero gives the set of equations

$$\begin{aligned} 7.86x_1 + 2.22x_2 &= 1.97 \\ 2.22x_1 + 2.76x_2 &= 0.23 \,, \end{aligned} \tag{34}$$

which, upon solution, gives $x_1^0 = 0.29$ and $x_2^0 = -0.14$ as co-ordinates of the point S. Substituting these values in equation (33) gives

$$Y_s = 86.50 \,.$$

The characteristic equation is

$$\begin{vmatrix} -3.93 - \lambda & -1.11 \\ -1.11 & -1.38 - \lambda \end{vmatrix} = 0 \tag{35}$$

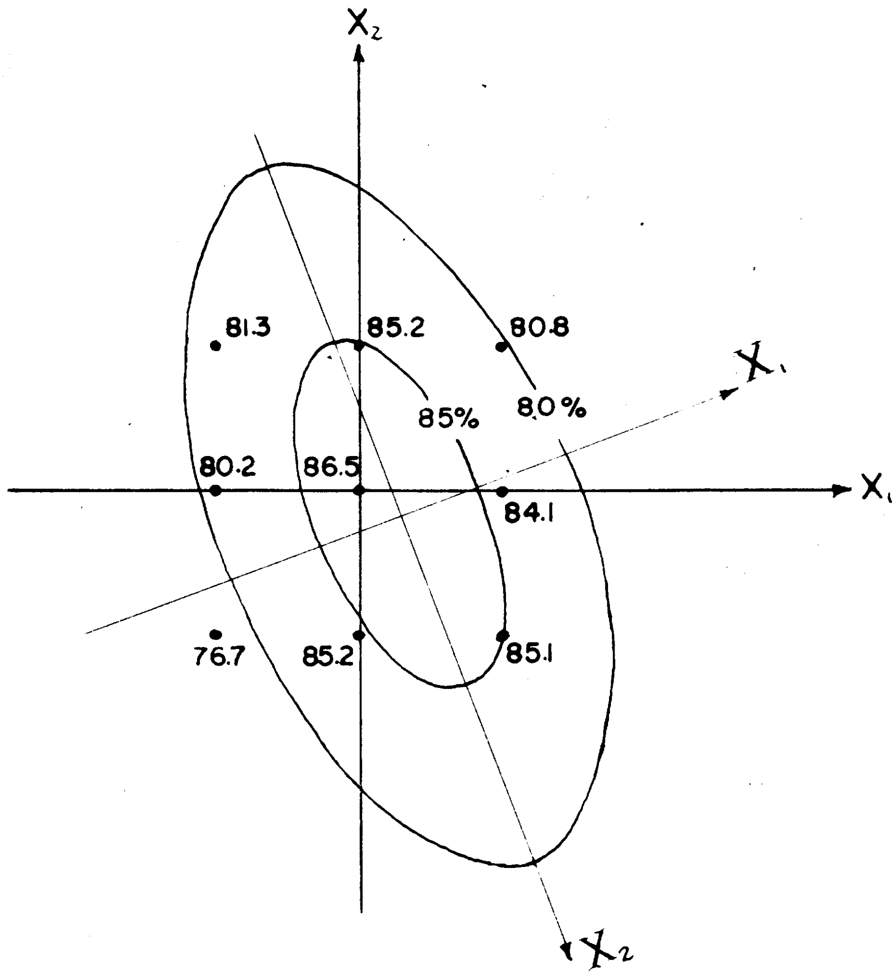
i.e., $\lambda^2 + 5.31\lambda + 4.19 = 0$,

from which $\lambda_1 = -4.35$, $\lambda_2 = -0.96$.

The canonical form may now be written as

$$Y - 86.50 = -4.35X_1^2 - 0.96X_2^2 \,, \tag{36}$$

which indicates elliptical contours with S a true maximum. The 80% and 85% contours are shown in Figure 9.



Contours of fitted surface and observed yields at experimental points
Fig. 9

The transformation matrix M is derived next. M_{11} and M_{12} are solutions of the equations

$$\begin{aligned} 0.42M_{11} - 1.11M_{12} &= 0 \\ -1.11M_{11} + 2.97M_{12} &= 0 , \end{aligned} \qquad (37)$$

while M_{21} and M_{22} are solutions of the equations

$$-2.97M_{21} - 1.11M_{22} = 0$$
$$-1.11M_{21} - 0.42M_{22} = 0 \; . \qquad (38)$$

The solutions yield the matrix

$$M = \begin{bmatrix} 0.936 & 0.352 \\ 0.352 & -0.936 \end{bmatrix} . \qquad (39)$$

The transformation to X co-ordinates is given by

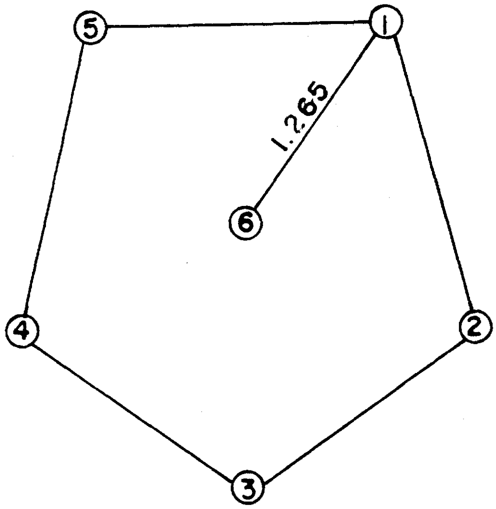
$$X_1 = 0.936(x_1 - 0.29) + 0.352(x_2 + 0.14)$$
$$X_2 = 0.352(x_1 - 0.29) - 0.936(x_2 + 0.14), \qquad (40)$$

while the reciprocal transformation to x co-ordinates is given by

$$x_1 - 0.29 = 0.936X_1 + 0.352X_2$$
$$x_2 + 0.14 = 0.352X_1 - 0.936X_2. \qquad (41)$$

B. <u>A Pentagonal Design Showing a Rising Ridge.</u>

The pentagonal design used here is an arrangement of five points in the shape of a regular pentagon with a point in the centre, chosen so that the uppermost side is horizontal and the distance from the centre to each vertex is 1.265.



'A pentagonal design

Fig. 10

Two factors x_1 and x_2 are also the subject of study in this problem. The following are the matrices in the problem:

$$D = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{array}{c} \begin{array}{cc} x_1 & x_2 \end{array} \\ \begin{bmatrix} 0.744 & 1.023 \\ 1.203 & -0.391 \\ 0.000 & -1.265 \\ -1.203 & -0.391 \\ -0.744 & 1.023 \\ 0.000 & 0.000 \end{bmatrix} \end{array} \qquad Y = \begin{array}{c} \% \\ \begin{bmatrix} 73.6 \\ 50.4 \\ 49.4 \\ 61.3 \\ 75.7 \\ 65.6 \end{bmatrix} \end{array}$$

$X =$

	x_0	x_1	x_2	x_1^2	x_2^2	x_1x_2
1	1.000	0.744	1.023	0.554	1.047	0.761
2	1.000	1.203	-0.391	1.447	0.153	-0.470
3	1.000	0.000	-1.265	0.000	1.600	0.000
4	1.000	-1.203	-0.391	1.447	0.153	0.470
5	1.000	-0.744	1.023	0.554	1.047	-0.761
6	1.000	0.000	0.000	0.000	0.000	0.000

$X' =$

1.000	1.000	1.000	1.000	1.000	1.000
0.744	1.203	0.000	-1.203	-0.744	0.000
1.023	-0.391	-1.265	-0.391	1.023	0.000
0.554	1.447	0.000	1.447	0.554	0.000
1.047	0.153	1.600	0.153	1.047	0.000
0.761	-0.470	0.000	0.470	-0.761	0.000

$X'X =$

6.0	0.0	0.0	4.0	4.0	0.0
0.0	4.0	0.0	0.0	0.0	0.0
0.0	0.0	4.0	0.0	0.0	0.0
4.0	0.0	0.0	4.8	1.6	0.0
4.0	0.0	0.0	1.6	4.8	0.0
0.0	0.0	0.0	0.0	0.0	1.6

$$C^{-1} = (X'X)^{-1} = \begin{array}{c} \\ b_0 \\ b_1 \\ b_2 \\ b_{11} \\ b_{22} \\ b_{12} \end{array} \begin{array}{cccccc} b_0 & b_1 & b_2 & b_{11} & b_{22} & b_{12} \end{array} \left[\begin{array}{cccccc} 1 & 0 & 0 & -0.625 & -0.625 & 0 \\ 0 & 0.25 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.25 & 0 & 0 & 0 \\ -0.625 & 0 & 0 & 0.625 & 0.3125 & 0 \\ -0.625 & 0 & 0 & 0.3125 & 0.625 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.625 \end{array}\right]$$

$$T' = X(X'X)^{-1} = \begin{array}{cccccc} b_0 & b_1 & b_2 & b_{11} & b_{22} & b_{12} \end{array} \left[\begin{array}{cccccc} 0 & 0.186 & 0.255 & 0.048 & 0.202 & 0.476 \\ 0 & 0.301 & -0.098 & 0.327 & -0.077 & -0.294 \\ 0 & 0.000 & -0.314 & -0.125 & 0.375 & 0.000 \\ 0 & -0.301 & -0.098 & 0.327 & -0.077 & 0.294 \\ 0 & -0.186 & 0.255 & 0.048 & 0.202 & -0.476 \\ 1 & 0.000 & 0.000 & -0.625 & -0.625 & 0.000 \end{array}\right]$$

The estimates of b_0, b_1, etc. of the β's are as follows:

$b_0 = 65.60 \pm 0.50\sigma$ $b_1 = -3.671 \pm 0.50\sigma$ $b_2 = 11.613 \pm 0.50\sigma$

$b_{11} = -3.482 \pm 0.56\sigma$ $b_{22} = -0.918 \pm 0.56\sigma$

$b_{12} = 2.205 \pm 0.79\sigma$.

An estimate of the response surface equation is

$$Y = 65.60 - 3.671x_1 + 11.613x_2 - 3.482x_1^2 - 0.918x_2^2 + 2.205x_1x_2 . \quad (42)$$

The co-ordinates of S and the predicted yield at this point are

$x_1^0 = 2.381$, $x_2^0 = 9{,}184$, $Y_s = 114.56\%$.

The characteristic equation

$$\begin{vmatrix} -3.482 - \lambda & 1.102 \\ 1.102 & -0.918 - \lambda \end{vmatrix} = 0 , \qquad (43)$$

i.e., $\lambda^2 + 4.400\lambda + 1.981 = 0$,

gives $\lambda_1 = -3.890$ and $\lambda_2 = -0.510$.

The canonical form of equation (42) is

$$Y - 114.56 = -3.890X_1^2 - 0.510X_2^2 . \qquad (44)$$

From the sets of equations

$$\begin{aligned} 0.408\, M_{11} + 1.102\, M_{12} &= 0 \\ 1.102\, M_{11} + 2.972\, M_{12} &= 0 \end{aligned} \qquad (45)$$

and

$$\begin{aligned} -2.972\, M_{21} + 1.102\, M_{22} &= 0 \\ 1.102\, M_{21} - 0.408\, M_{22} &= 0 , \end{aligned} \qquad (46)$$

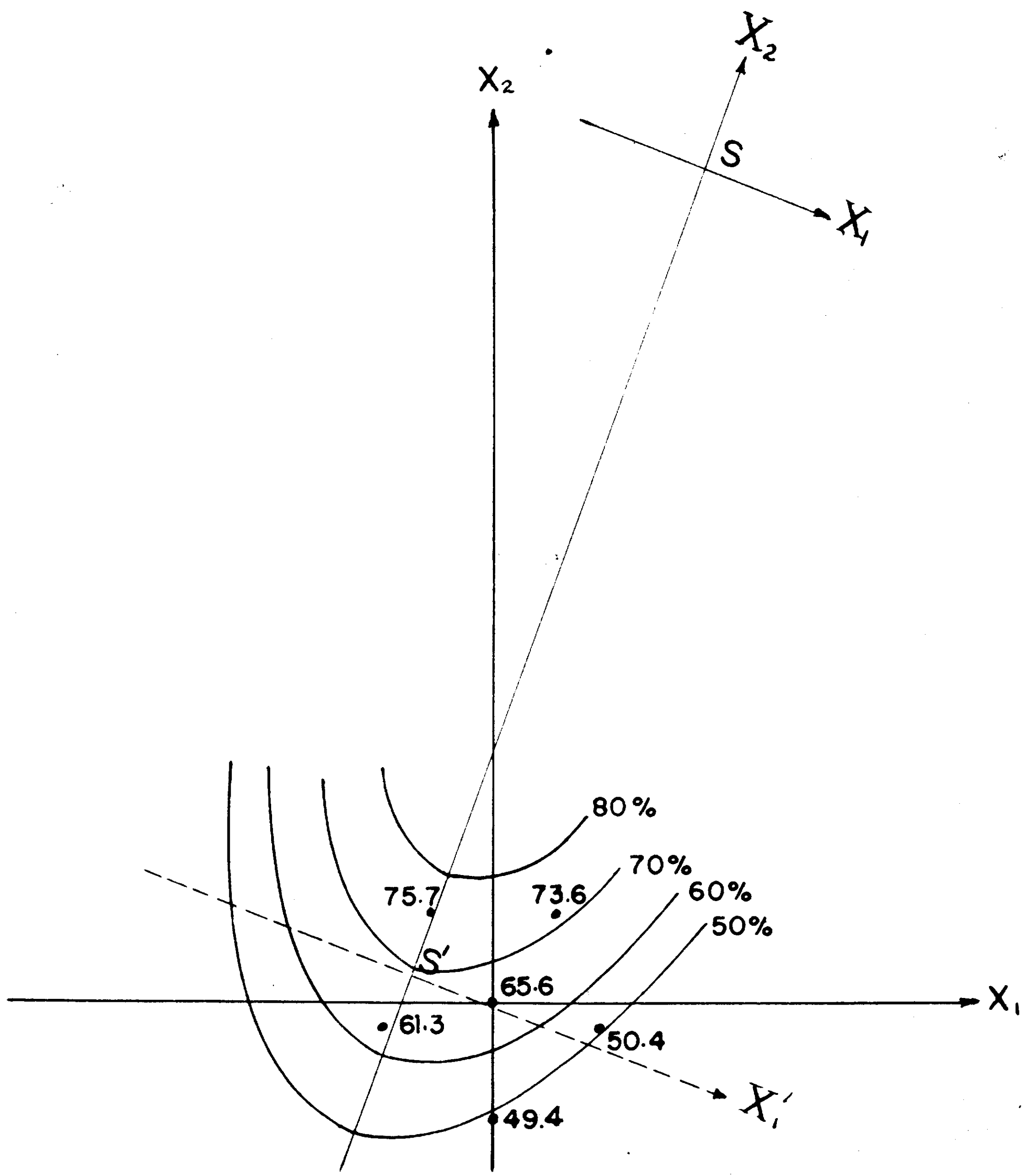
the matrix $M = \begin{bmatrix} 0.938 & -0.347 \\ 0.347 & 0.938 \end{bmatrix}$ (47)

is obtained.

An analysis of the canonical form (44) is now in order. The canonical form indicates that the fitted contour surfaces are ellipses elongated along the X_2 axis and the stationary point S is a maximum. From the co-ordinates of the centre, it is noted that S is remote from the centre of the design at O. No conclusions about the nature of the surface in the neighborhood of S can be drawn, since it is quite unlikely that the fitted equation would have any relevance at such a remote point. Also, the predicted yield of nearly 115% is obviously an impossible value. However, the part of

the fitted equation near the design should provide a satisfactory approximation to the local surface, and it is this portion of the design in which one should be interested.
It is observed that the transformation to X co-ordinates is given by

$$X_1 = 0.938(x_1 - 2.381) - 0.347(x_2 - 9.184)$$
$$X_2 = 0.347(x_1 - 2.381) + 0.938(x_2 - 9.184). \qquad (48)$$



Canonical reduction in the neighborhood of a rising ridge in two variables Fig. 11

Considering the problem in terms of the co-ordinates X_1 and X_2 instead of x_1 and x_2, and substituting $x_1 = 0$, $x_2 = 0$ in equation (48), the centre O of the design is found to be at

$$X_1 = 0.954 \qquad X_2 = -9.442 \; .$$

It is seen that 0.954 and -9.442 are the shortest distances from the X_2 and X_1 axes respectively, and the X_2-axis passes close to O. Since λ_2 is relatively small, the contours are drawn out along the X_2-axis. It is concluded that the design has been performed near a rising ridge, the direction of which is along the X_2-axis. The canonical form (44) is referred to a local origin on this nearby ridge, which is conveniently taken to be at

$$X_1 = 0, \quad X_2 = -9.442$$

the nearest point to O on the ridge. It is denoted by S'. Writing

$$X_1' = X_1, \quad X_2' = X_2 + 9.442$$

and substituting in equation (45), the equation, with origin at S', is

$$Y - 69.09 = -3.890X_1'^2 - 0.510X_2'^2 + 9.631X_2', \qquad (49)$$

where 9.631 measures the slope up the ridge. The ridge is rising steeply, and it would be necessary to explore the axis of this ridge in the direction of increasing yield. It is to be noted that the nature of the system, illustrated in Figure 11, can be fully appreciated without resort to geometrical illustration. This is very important in the general multi-variable case. Canonical reduction can be undertaken however many variables exist and will often make it possible to understand the nature of complex systems.

C. A 2^3 Composite Design Yielding Ellipsoids for Contours of the Fitted Hypersurface.

This third example concerns the improvement of a process in which two solids A and B are fused at high temperature to give a third substance C. The object is to reduce the manufacturing cost of C. The amount B was kept constant throughout the experiment and the three factors were studied at levels assumed to be as chosen on the basis of previous experimental work, as indicated in Table IV. The response

Table IV

FACTOR LEVELS FOR THE 2^3 FACTORIAL EXPERIMENT

Factor	Factor level -1	Factor level 1	Base level	Unit
Temperature ^{0}C (T)	245	255	250	5.0
Fusion time-hours (t)	22	28	25	3.0
Molar ratio A/B (M)	4	5	4.5	0.5

recorded as cost is an arbitrary relative estimate of the cost of manufacturing a unit quantity of the product at each of the conditions tried. It is possible to express the standardized variables x_1, x_2, x_3 in terms of the natural variables as follows:

$$x_1 = (T-250)/5 \quad x_2 = (C-25)/3 \quad x_3 = (M-4.5)/0.5 \quad (50)$$

It was first assumed that quadratic and higher order effects were negligible, as were also interaction effects of third order or greater. Using a 2^3 factorial design the matrices D, X, X', X'X, C^{-1}, T^1 and Y were set up as usual and the following estimates obtained:

$b_0 = 12.265 \pm 0.35\sigma$ $b_1 = 0.875 \pm 0.35\sigma$

$b_2 = 3.375 \pm 0.35\sigma$ $b_3 = 3.500 \pm 0.35\sigma$

$b_{12} = -3.875 \pm 0.35\sigma$ $b_{13} = -1.625 \pm 0.35\sigma$

$b_{23} - 1.875 \pm 0.35\sigma$

It is to be observed that, from the relative size of the interaction terms, the steepest descent process (since a minimum is being sought) is unlikely to be very effective; the design had to be augmented to determine all effects of second order. A 2^3 composite design was incorporated for the purpose, and seven more experiments were run for a total of 15 experimental points and corresponding results. The matrices, with the results obtained, now follow.

$$D = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \end{array} \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ 2 & 0 & 0 \\ -2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 2 \\ 0 & 0 & -2 \end{bmatrix} \end{array} \qquad Y = \begin{bmatrix} 3 \\ 15 \\ 13 \\ 11 \\ 7 \\ 12 \\ 24 \\ 16 \\ 5 \\ 20 \\ 17 \\ 21 \\ 8 \\ 17 \\ 8 \end{bmatrix}$$

$X =$

	x_0	x_1	x_2	x_3	x_1^2	x_2^2	x_3^2	x_1x_2	x_1x_3	x_2x_3
1	1	-1	-1	-1	1	1	1	1	1	1
2	1	1	-1	-1	1	1	1	-1	-1	1
3	1	-1	1	-1	1	1	1	-1	1	-1
4	1	1	1	-1	1	1	1	1	-1	-1
5	1	-1	-1	1	1	1	1	1	-1	-1
6	1	1	-1	1	1	1	1	-1	-1	1
7	1	-1	1	1	1	1	1	-1	-1	1
8	1	1	1	1	1	1	1	1	1	1
9	1	0	0	0	0	0	0	0	0	0
10	1	2	0	0	4	0	0	0	0	0
11	1	-2	0	0	4	0	0	0	0	0
12	1	0	2	0	0	4	0	0	0	0
13	1	0	-2	0	0	4	0	0	0	0
14	1	0	0	2	0	0	4	0	0	0
15	1	0	0	-2	0	0	4	0	0	0

$$X' = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 0 & 2 & -2 & 0 & 0 & 0 & 0 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 0 & 0 & 0 & 2 & -2 & 0 & 0 \\
-1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 2 & -2 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 4 & 4 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 4 & 4 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 4 & 4 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

$$
X'X = \begin{bmatrix}
15 & 0 & 0 & 0 & 16 & 16 & 16 & 0 & 0 & 0 \\
0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 \\
16 & 0 & 0 & 0 & 40 & 8 & 8 & 0 & 0 & 0 \\
16 & 0 & 0 & 0 & 8 & 40 & 8 & 0 & 0 & 0 \\
16 & 0 & 0 & 0 & 8 & 8 & 40 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8
\end{bmatrix}
$$

The estimates of b_0, b_1, etc. of the β's are as follows:

$b_0 = 5.000 \pm 0.33\sigma$ $\quad$ $b_1 = 0.813 \pm 0.25\sigma$

$b_2 = 3.313 \pm 0.25\sigma$ $\quad$ $b_3 = 2.188 \pm 0.25\sigma$

$b_{11} = 3.931 \pm 0.11\sigma$ $\quad$ $b_{22} = 2.931 \pm 0.11\sigma$

$b_{33} = 2.431 \pm 0.11\sigma$ $\quad$ $b_{12} = -3.875 \pm 0.35\sigma$

$b_{13} = -1.625 \pm 0.35\sigma$ $\quad$ $b_{23} = 1.875 \pm 0.35\sigma$

$$
C^{-1} = (X'X)^{-1} =
\begin{array}{c|cccccccccc}
 & b_0 & b_1 & b_2 & b_3 & b_{11} & b_{22} & b_{33} & b_{12} & b_{13} & b_{23} \\
\hline
b_0 & \frac{7}{9} & 0 & 0 & 0 & -\frac{2}{9} & -\frac{2}{9} & -\frac{2}{9} & 0 & 0 & 0 \\
b_1 & 0 & \frac{1}{16} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
b_2 & 0 & 0 & \frac{1}{16} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
b_3 & 0 & 0 & 0 & \frac{1}{16} & 0 & 0 & 0 & 0 & 0 & 0 \\
b_{11} & -\frac{2}{9} & 0 & 0 & 0 & \frac{13}{144} & \frac{17}{288} & \frac{17}{288} & 0 & 0 & 0 \\
b_{22} & -\frac{2}{9} & 0 & 0 & 0 & \frac{17}{288} & \frac{13}{144} & \frac{17}{288} & 0 & 0 & 0 \\
b_{33} & -\frac{2}{9} & 0 & 0 & 0 & \frac{17}{288} & \frac{17}{288} & \frac{13}{144} & 0 & 0 & 0 \\
b_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} & 0 & 0 \\
b_{13} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} & 0 \\
b_{23} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8}
\end{array}
$$

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

	b_0	b_1	b_2	b_3	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
1	$\frac{1}{9}$	$\frac{-1}{16}$	$\frac{-1}{16}$	$\frac{-1}{16}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
2	$\frac{1}{9}$	$\frac{1}{16}$	$\frac{-1}{16}$	$\frac{-1}{16}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$
3	$\frac{1}{9}$	$\frac{-1}{16}$	$\frac{1}{16}$	$\frac{-1}{16}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$-\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$
4	$\frac{1}{9}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{-1}{16}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$
5	$\frac{1}{9}$	$\frac{-1}{16}$	$\frac{-1}{16}$	$\frac{1}{16}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$
6	$\frac{1}{9}$	$\frac{1}{16}$	$\frac{-1}{16}$	$\frac{1}{16}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$-\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$
7	$\frac{1}{9}$	$\frac{-1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$
8	$\frac{1}{9}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{-1}{72}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
9	$\frac{7}{9}$	0	0	0	$-\frac{1}{9}$	$-\frac{1}{9}$	$-\frac{1}{9}$	0	0	0
10	$-\frac{1}{9}$	$\frac{1}{8}$	0	0	$\frac{5}{36}$	$\frac{1}{72}$	$\frac{1}{72}$	0	0	0
11	$-\frac{1}{9}$	$-\frac{1}{8}$	0	0	$\frac{5}{36}$	$\frac{1}{72}$	$\frac{1}{72}$	0	0	0
12	$-\frac{1}{9}$	0	$\frac{1}{8}$	0	$\frac{1}{72}$	$\frac{5}{36}$	$\frac{1}{72}$	0	0	0
13	$-\frac{1}{9}$	0	$-\frac{1}{8}$	0	$\frac{1}{72}$	$\frac{5}{36}$	$\frac{1}{72}$	0	0	0
14	$-\frac{1}{9}$	0	0	$\frac{1}{8}$	$\frac{1}{72}$	$\frac{1}{72}$	$\frac{5}{36}$	0	0	0
15	$-\frac{1}{9}$	0	0	$-\frac{1}{8}$	$\frac{1}{72}$	$\frac{1}{72}$	$\frac{5}{36}$	0	0	0

An estimate of the response surface equation is

$$Y = 5.000 + 0.813x_1 + 3.313x_2 + 2.188x_3 + 3.931x_1^2 + 2.931x_2^2 + 2.431x_3^2 + 3.875x_1x_2 - 1.625x_1x_3 + 1.875x_2x_3. \qquad (51)$$

The equations yielding the co-ordinates of S are

$$
\begin{aligned}
7.862x_1 - 3.875x_2 - 1.625x_3 &= -0.813 \\
-3.875x_1 + 5.862x_2 + 1.875x_3 &= -3.313 \qquad (52) \\
-1.625x_1 + 1.875x_2 + 4.862x_3 &= -2.188 ,
\end{aligned}
$$

giving $x_1^0 = -0.5898$, $x_2^0 = -0.8533$, $x_3^0 = -0.3180$,

and $Y_s = 2.1342$.

The characteristic equation or discriminating cubic is

$$
\begin{vmatrix}
3.931-\lambda & -1.937 & -0.812 \\
-1.937 & 2.931-\lambda & 0.937 \\
-0.812 & 0.937 & 2.431-\lambda
\end{vmatrix} = 0 \qquad (53)
$$

i.e., $\lambda^3 - 9.303\lambda^2 + 22.953\lambda - 16.489 = 0$,

which gives $\lambda_1 = 1.3688$, $\lambda_2 = 2.0514$, $\lambda_3 = 5.8728$.

The canonical form may now be written as

$$Y - 2.1342 = 1.3688X_1^2 + 2.0514X_2^2 + 5.8728X_3^2, \qquad (54)$$

which indicates ellipsoidal contours with the centre a true minimum.

From the sets of equations

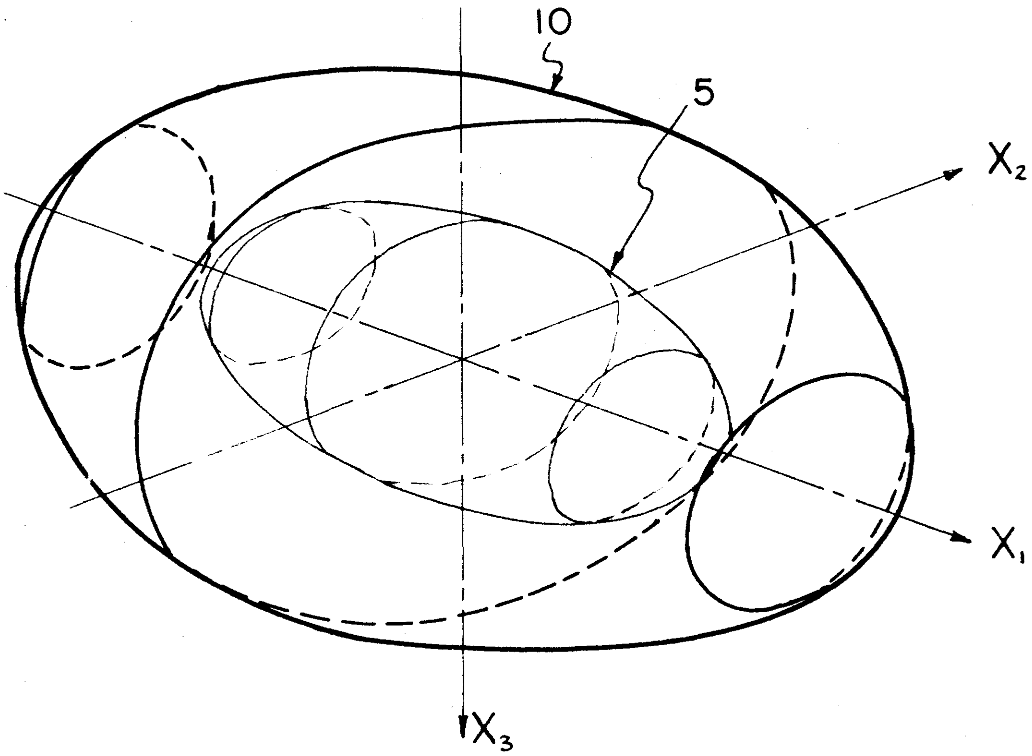
$$
\begin{aligned}
2.562M_{11} - 1.937M_{12} - 0.812M_{13} &= 0 \\
-1.937M_{11} + 1.562M_{12} + 0.937M_{13} &= 0 \qquad (55) \\
-0.812M_{11} + 0.937M_{12} + 1.062M_{13} &= 0,
\end{aligned}
$$

$$
\begin{aligned}
1.880M_{21} - 1.937M_{22} - 0.812M_{23} &= 0 \\
-1.937M_{21} + 0.880M_{22} + 0.937M_{23} &= 0 \qquad (56) \\
-0.812M_{21} + 0.937M_{22} + 0.380M_{23} &= 0,
\end{aligned}
$$

and
$$-1.942M_{31} - 1.937M_{32} - 0.812M_{33} = 0$$
$$-1.937M_{31} - 2.942M_{32} + 0.937M_{33} = 0 \qquad (57)$$
$$-0.812M_{31} + 0.937M_{32} - 3.442M_{33} = 0 ,$$

the matrix
$$M = \begin{bmatrix} 0.4856 & 0.8057 & -0.3395 \\ 0.4629 & 0.0768 & 0.8834 \\ 0.7347 & -0.5900 & -0.3336 \end{bmatrix} \qquad (58)$$

is obtained. The contour representation at levels 5 and 10 for the canonical form (54) is shown in Figure 12.

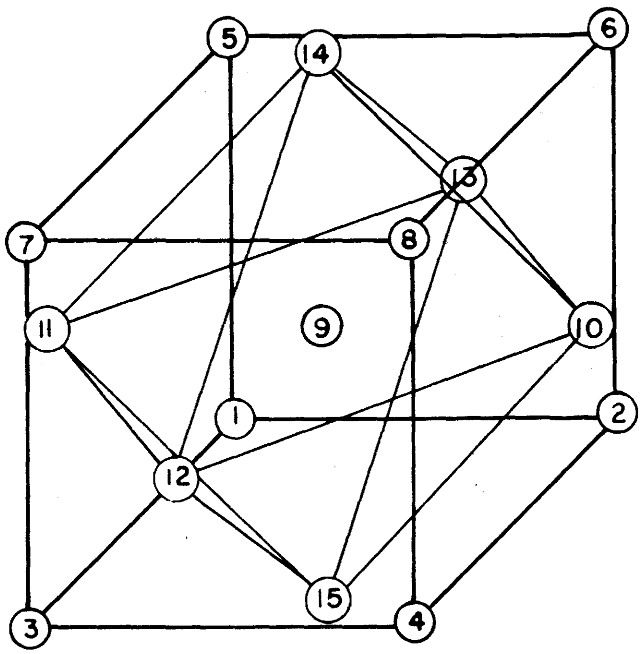


Canonical reduction in the neighborhood of a true minimum in three variables

Fig. 12

D. The Cubic-Octahedral Design Yielding an Approximate Stationary Plane Ridge in Three Variables.

The cubic-octahedral design is obtained by superimposing a 2^3 factorial design on an octahedral design, with the octahedron having its edge equal to 2, in such a way that the vertices of the octahedron fall on the axes of the cube. The design, with the points numbered to correspond to the design matrix D, is shown in Figure 13. This design may be



The cubic-octahedral design

Fig. 13

thought of as a 2^3 composite design with $\alpha = \sqrt{2}$, but this is not an indication of how the design was derived. It is more compact than the 2^3 composite design.

In this example it was assumed that two reactants, A and B, formed a mixture of C and D.

$$A + B \rightarrow C + D \qquad (59)$$

The final product included a mixture of C and D, and unchanged A and B. The object is to obtain the maximum yield of C. The factors varied are temperature (T), initial concentration of A(c), and time of reaction (t). The starting quantity of B was kept constant throughout. It was further assumed that prior experimental work led to the factor level selections given in Table V.

Table V

FACTOR LEVELS FOR THE CUBIC-OCTAHEDRAL EXPERIMENT

Factor	Factor level -1	Factor level +1	Base level	Unit
Temperature °C (T)	152	162	157	5
Concentration of A% (c)	30	35	32.5	2.5
Time of reaction-hours (t)	6	9	7.5	1.5

The variables x_1, x_2, x_3 are expressed in terms of the natural variables as follows:

$$x_1 = (T-157)/5 \quad x_2 = (C-32.5)/2.5 \quad x_3 = (t-7.5)/1.5 \qquad (60)$$

The cubic-octahedral design allows estimates of quadratic effects and interaction effects of the second order. A tabulation of the required matrices follows.

$$D = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \end{array} \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \left[\begin{array}{ccc} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ -\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & -\sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & -\sqrt{2} \end{array}\right] \end{array} \qquad Y = \begin{array}{c} \% \\ \left[\begin{array}{c} 49.9 \\ 64.3 \\ 60.3 \\ 62.4 \\ 58.8 \\ 64.4 \\ 64.3 \\ 57.7 \\ 62.7 \\ 62.4 \\ 56.9 \\ 63.5 \\ 61.0 \\ 62.9 \\ 59.9 \end{array}\right] \end{array}$$

$$
\begin{array}{cc}
 & \begin{array}{cccccccccc} x_0 & x_1 & x_2 & x_3 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3 \end{array} \\
X = & \left[\begin{array}{cccccccccc}
1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\
1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 \\
1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 \\
1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & \sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\
1 & -\sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & \sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\
1 & 0 & -\sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & \sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 \\
1 & 0 & 0 & -\sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0
\end{array}\right]
\end{array}
$$

$$
X' = \left[\begin{array}{ccccccccccccccc}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 0 & \sqrt{2} & -\sqrt{2} & 0 & 0 & 0 & 0 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 0 & 0 & 0 & \sqrt{2} & -\sqrt{2} & 0 & 0 \\
-1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & \sqrt{2} & -\sqrt{2} \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 2 & 2 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 2 & 2 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 2 & 2 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right]
$$

$$X'X = \begin{bmatrix} 15 & 0 & 0 & 0 & 12 & 12 & 12 & 0 & 0 & 0 \\ 0 & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12 & 0 & 0 & 0 & 0 & 0 & 0 \\ 12 & 0 & 0 & 0 & 16 & 8 & 8 & 0 & 0 & 0 \\ 12 & 0 & 0 & 0 & 8 & 16 & 8 & 0 & 0 & 0 \\ 12 & 0 & 0 & 0 & 8 & 8 & 16 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 \end{bmatrix}$$

$$C^{-1} = (X'X)^{-1} = \begin{array}{c} \\ b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_{11} \\ b_{22} \\ b_{33} \\ b_{12} \\ b_{13} \\ b_{23} \end{array} \begin{array}{cccccccccc} b_0 & b_1 & b_2 & b_3 & b_{11} & b_{22} & b_{33} & b_{12} & b_{13} & b_{23} \\ \frac{2}{3} & 0 & 0 & 0 & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{4} & 0 & 0 & 0 & \frac{3}{16} & \frac{1}{16} & \frac{1}{16} & 0 & 0 & 0 \\ -\frac{1}{4} & 0 & 0 & 0 & \frac{1}{16} & \frac{3}{16} & \frac{1}{16} & 0 & 0 & 0 \\ -\frac{1}{4} & 0 & 0 & 0 & \frac{1}{16} & \frac{1}{16} & \frac{3}{16} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} \end{array}$$

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

	b_0	b_1	b_2	b_3	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
1	$\frac{-1}{12}$	$\frac{-1}{12}$	$\frac{-1}{12}$	$\frac{-1}{12}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
2	$\frac{-1}{12}$	$\frac{1}{12}$	$\frac{-1}{12}$	$\frac{-1}{12}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{-1}{8}$	$\frac{-1}{8}$	$\frac{1}{8}$
3	$\frac{-1}{12}$	$\frac{-1}{12}$	$\frac{1}{12}$	$\frac{-1}{12}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$-\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$
4	$\frac{-1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{-1}{12}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$
5	$\frac{-1}{12}$	$\frac{-1}{12}$	$\frac{-1}{12}$	$\frac{1}{12}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$
6	$\frac{-1}{12}$	$\frac{1}{12}$	$\frac{-1}{12}$	$\frac{1}{12}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$-\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$
7	$\frac{-1}{12}$	$\frac{-1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$
8	$\frac{-1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
9	$\frac{2}{3}$	0	0	0	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	0	0	0
10	$\frac{1}{6}$	$\frac{1}{12}\sqrt{2}$	0	0	$\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	0	0	0
11	$\frac{1}{6}$	$\frac{-1}{12}\sqrt{2}$	0	0	$\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	0	0	0
12	$\frac{1}{6}$	0	$\frac{1}{12}\sqrt{2}$	0	$-\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$	0	0	0
13	$\frac{1}{6}$	0	$\frac{-1}{12}\sqrt{2}$	0	$-\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$	0	0	0
14	$\frac{1}{6}$	0	0	$\frac{1}{12}\sqrt{2}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$	0	0	0
15	$\frac{1}{6}$	0	0	$\frac{-1}{12}\sqrt{2}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$	0	0	0

The estimates of b_0, b_1, etc. of the β's are as follows:

$$b_0 = 62.725 \pm 0.30\sigma \qquad b_1 = 1.941 \pm 0.30\sigma$$

$$b_2 = 0.903 \pm 0.30\sigma \qquad b_3 = 1.046 \pm 0.30\sigma$$

$$b_{11} = -1.542 \pm 0.25\sigma \qquad b_{22} = -0.242 \pm 0.25\sigma$$

$$b_{33} = -0.668 \pm 0.25\sigma \qquad b_{12} = 3.062 \pm 0.30\sigma$$

$$b_{13} = -2.188 \pm 0.30\sigma \qquad b_{23} = -1.212 \pm 0.30\sigma$$

An estimate of the response surface equation is

$$Y = 62.725 + 1.941x_1 + 0.903x_2 + 1.046x_3 - 1.542x_1^2 - 0.242x_2^2 - 0.668x_3^2 - 3.062x_1x_2 - 2.188x_1x_3 - 1.212x_2x_3. \qquad (61)$$

Equations for the co-ordinates of S are

$$\begin{aligned} 3.084x_1 + 3.062x_2 + 2.188x_3 &= 1.941 \\ 3.062x_1 + 0.484x_2 + 1.212x_3 &= 0.903 \\ 2.188x_1 + 1.212x_2 + 1.336x_3 &= 1.046 , \end{aligned} \qquad (62)$$

giving $x_1^0 = 0.110$, $x_2^0 = 0.268$, $x_3^0 = 0.359$,

and $Y_s = 63.14$.

The discriminating cubic is

$$\begin{vmatrix} -1.542-\lambda & -1.531 & -1.094 \\ -1.531 & -0.242-\lambda & -0.606 \\ -1.094 & -0.606 & -0.668-\lambda \end{vmatrix} = 0 , \qquad (63)$$

i.e., $\lambda^3 + 2.452\lambda^2 - 2.343\lambda - 0.142 = 0$,

which has the roots $\lambda_1 = -3.176$, $\lambda_2 = -0.057$, $\lambda_3 = 0.781$.

The equation of the contour surfaces may now be written as

$$Y - 63.14 = -3.176X_1^2 - 0.057X_2^2 + 0.781X_3^2. \qquad (64)$$

The fitted contour surfaces are hyperboloids of one sheet; the sections by the planes $X_1 = 0$, $X_2 = 0$ are hyperbolas, and that by $X_3 = 0$ is an ellipse.

From the sets of equations

$$\begin{aligned} 1.634M_{11} - 1.531M_{12} - 1.094M_{13} &= 0 \\ -1.531M_{11} + 2.934M_{12} - 0.606M_{13} &= 0 \\ -1.094M_{11} - 0.606M_{12} + 2.508M_{13} &= 0 \,, \end{aligned} \tag{65}$$

$$\begin{aligned} -1.485M_{21} - 1.531M_{22} - 1.094M_{23} &= 0 \\ -1.531M_{21} - 0.195M_{22} - 0.606M_{23} &= 0 \\ -1.094M_{21} - 0.606M_{22} - 0.611M_{23} &= 0 \,, \end{aligned} \tag{66}$$

and

$$\begin{aligned} 2.323M_{31} + 1.531M_{32} + 1.094M_{33} &= 0 \\ 1.531M_{31} + 1.023M_{32} + 0.606M_{33} &= 0 \\ 1.094M_{31} + 0.606M_{32} + 1.449M_{33} &= 0 \,, \end{aligned} \tag{67}$$

the matrix $M = \begin{bmatrix} 0.666 & 0.429 & 0.394 \\ 0.308 & 0.341 & -0.888 \\ 0.579 & 0.809 & -0.097 \end{bmatrix}$ (68)

is obtained.

The transformation to the x co-ordinates is given by

$$\begin{aligned} X_1 &= 0.666(x_1 - 0.110) + 0.429(x_2 - 0.268) + 0.394(x_3 - 0.359) \\ X_2 &= 0.308(x_1 - 0.110) + 0.341(x_2 - 0.268) - 0.888(x_3 - 0.359) \\ X_3 &= 0.579(x_1 - 0.110) + 0.809(x_2 - 0.268) - 0.097(x_3 - 0.359) \,, \end{aligned} \tag{69}$$

while the reciprocal transformation is given by

$$\begin{aligned} x_1 - 0.110 &= 0.666X_1 + 0.308X_2 + 0.579X_3 \\ x_2 - 0.268 &= 0.429X_1 + 0.341X_2 + 0.809X_3 \\ x_3 - 0.359 &= 0.394X_1 - 0.888X_2 - 0.097X_3 \,. \end{aligned} \tag{70}$$

An interpretation of the results follows next. From equation (64), λ_2 and λ_3 are probably not significantly different from zero. Since λ_3 is positive, it would indicate that increases occur while moving away from S along the X_3 - axis. A series of experiments would have to be conducted as a check. It is assumed here that, after further experimentation, both λ_2 and λ_3 were shown to be negligibly small compared to λ_1, and that λ_1 retained its present value even after the addition of further information.

Approximately, therefore, the canonical form ofthe equation is

$$Y - 63.14 = -3.176X_1^2$$

or

$$X_1 = \pm\sqrt{\frac{Y - 63.14}{-3.176}} \tag{71}$$

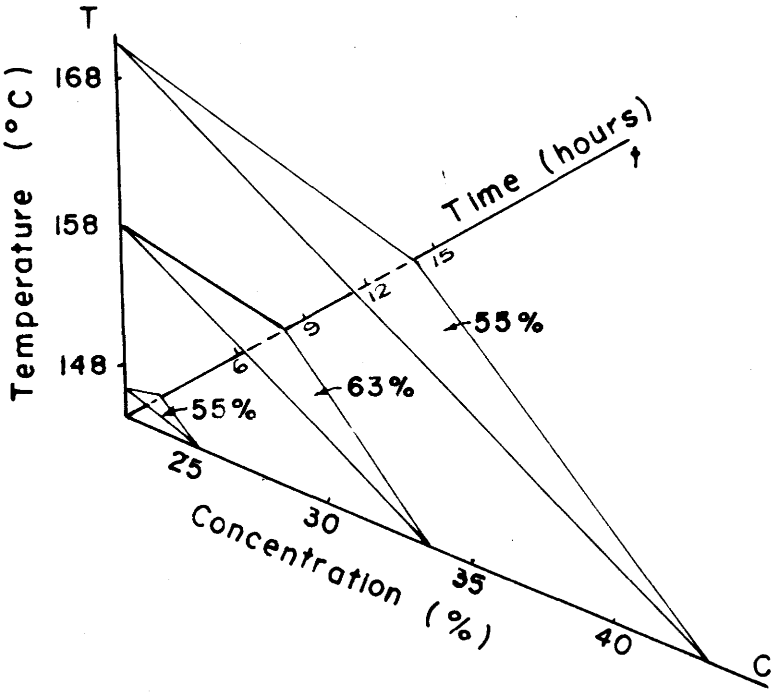
This equation defines pairs of parallel planes on which the yield is Y. For Y = 63.14, we have a plane $X_1 = 0$ on which the yield is maximal at approximately 63%. Its equation is

$$0.666(x_1 - 0.110) + 0.429(x_2 - 0.268) + 0.394(x_3 - 0.359) = 0. \tag{72}$$

By using equation (60), it may also be given in the original co-ordinates by

$$0.133T + 0.172c + 0.263t = 28.773. \tag{73}$$

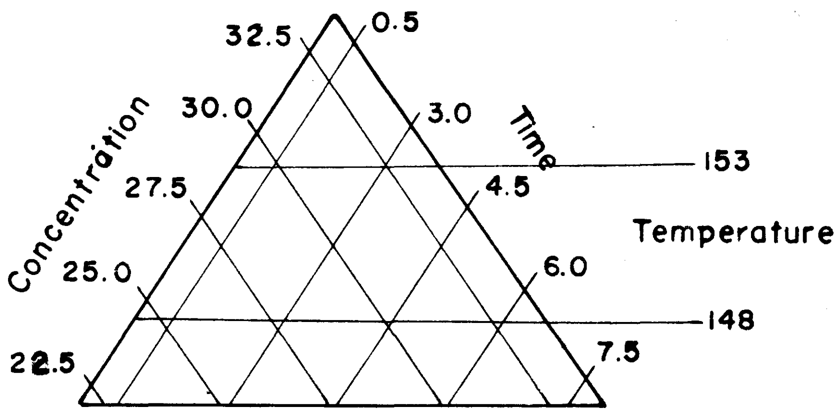
In Figure 14 are shown the maximal plane and the corresponding planes for Y = 55%. It must be remembered that only locally to the experimental design can the approximation in equation (73) be expected to apply.



Near-stationary plane (yield about 63%) with accompanying 55% contour planes

Fig. 14

Here, we have a situation in which a change in any one or two of the variables, temperature, concentration, or time, can be compensated for by a suitable change in the level of the other variables. An auxiliary characteristic may be worked into the experimental effort. The alternative sets of conditions giving about the same yield are shown quite conveniently in Figure 15. The diagram represents the plane of



Plane of maximum yield of C (approx. 63%)

Fig. 15

maximum yield, and the straight lines ruled across it are the lines of intersection of the planes T = 148°C., T = 153°C., c = 22.5%, c = 25.0%, etc.

From the above experimental points a great deal of information about the time, temperature, concentration system has been obtained. However, the conclusions are not exact and further experiments would be required to confirm whatever conclusions had been drawn. It could be that the surface on which the yield is nearly stationary has some slight curvature.

CHAPTER IV

SEVERAL ORIGINAL DESIGNS FOR THREE VARIABLES

The experimental designs included in this chapter have been formed from some regular and quasi-regular solids [5, p.52]. Each solid used was considered to have its edge equal to 2. The co-ordinates of its vertices, with the centre of the solid considered as the origin, made up the experimental design. Table VI includes all the data required for the formation of these designs. τ has the value of the real root of the equation $\tau^2 = \tau + 1$, i.e., $\tau = \frac{1+\sqrt{5}}{2}$.

A. The Tetrahedral Design

The matrices for the design are as follows:

$$D = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix} \end{array} \frac{1}{\sqrt{2}} \qquad X = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} x_0 & x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} 1 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 1 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 1 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \end{array}$$

$$X' = \begin{bmatrix} 1 & 1 & 1 & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \qquad X'X = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

TABLE VI

REGULAR AND QUASI-REGULAR SOLIDS

SOLID (edge 2)	Vertices	Edges	Faces	Co-ordinates of vertices	Distance from centre to vertex
TETRAHEDRON	4	6	4 equilateral triangles	$\frac{1}{\sqrt{2}}(1,1,1)$ $\frac{1}{\sqrt{2}}(1,-1,-1)$ $\frac{1}{\sqrt{2}}(-1,1,-1)$ $\frac{1}{\sqrt{2}}(-1,-1,1)$	1.225
CUBE	8	12	6 squares	$(\pm 1,\pm 1,\pm 1)$	1.732
OCTAHEDRON	6	12	8 equilateral triangles	$(\pm\sqrt{2},0,0)$ $(0,\pm\sqrt{2},0)$ $(0,0,\pm\sqrt{2})$	1.414
ICOSAHEDRON	12	30	20 equilateral triangles	$(\pm\tau,\pm 1,0)$ $(0,\pm\tau,\pm 1)$ $(\pm 1,0,\pm\tau)$	1.455
DODECAHEDRON	20	30	12 pentagons	$(\pm\tau^2,0,\pm 1)$ $(\pm 1,\pm\tau^2,0)$ $(0,\pm 1,\pm\tau^2)$ $(\pm 1,\pm 1,\pm 1)$	2.802
CUBOCTAHEDRON	12	24	6 squares 4 equilateral triangles	$(\pm\sqrt{2},\pm\sqrt{2},0)$ $(0,\pm\sqrt{2},\pm\sqrt{2})$ $(\pm\sqrt{2},0,\pm\sqrt{2})$	2.000
ICOSIDODE-CAHEDRON	30	60	12 pentagons 20 equilateral triangles	$(\pm 2\tau,0,0)$ $(0,\pm 2\tau,0)$ $(0,0,\pm 2\tau)$ $(\pm\tau^2,\pm 1,\pm\tau)$ $(\pm\tau,\pm\tau^2,\pm 1)$ $(\pm 1,\pm\tau,\pm\tau^2)$	3.236

$$C^{-1} = (X'X)^{-1} = \begin{array}{c} \\ b_0 \\ b_1 \\ b_2 \\ b_3 \end{array} \begin{array}{c} \begin{array}{cccc} b_0 & b_1 & b_2 & b_3 \end{array} \\ \begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} \end{array} \quad T' = X(X'X)^{-1} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} b_0 & b_1 & b_2 & b_3 \end{array} \\ \begin{bmatrix} 1 & \sqrt{2} & \sqrt{2} & \sqrt{2} \\ 1 & \sqrt{2} & -\sqrt{2} & -\sqrt{2} \\ 1 & -\sqrt{2} & \sqrt{2} & -\sqrt{2} \\ 1 & \sqrt{2} & -\sqrt{2} & \sqrt{2} \end{bmatrix} \end{array} \Bigg\} \frac{1}{4}$$

B. <u>The Octahedral Design</u>

The matrices for this design are as follows:

$$D = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} \sqrt{2} & 0 & 0 \\ -\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & -\sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & -\sqrt{2} \end{bmatrix} \end{array} \qquad X = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{array}{c} \begin{array}{cccc} x_0 & x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} 1 & \sqrt{2} & 0 & 0 \\ 1 & -\sqrt{2} & 0 & 0 \\ 1 & 0 & \sqrt{2} & 0 \\ 1 & 0 & -\sqrt{2} & 0 \\ 1 & 0 & 0 & \sqrt{2} \\ 1 & 0 & 0 & -\sqrt{2} \end{bmatrix} \end{array}$$

$$X' = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ \sqrt{2} & -\sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} & -\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{2} & -\sqrt{2} \end{bmatrix}$$

$$X'X = \begin{bmatrix} 6 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix} \qquad C^{-1} = (X'X)^{-1} = \begin{array}{c} \\ b_0 \\ b_1 \\ b_2 \\ b_3 \end{array} \begin{array}{c} \begin{array}{cccc} b_0 & b_1 & b_2 & b_3 \end{array} \\ \begin{bmatrix} \frac{1}{6} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{bmatrix} \end{array}$$

$$T' = X(X'X)^{-1} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{array}{c} \begin{array}{cccc} b_0 & b_1 & b_2 & b_3 \end{array} \\ \left[\begin{array}{cccc} 1/6 & \frac{1}{4}\sqrt{2} & 0 & 0 \\ 1/6 & -\frac{1}{4}\sqrt{2} & 0 & 0 \\ 1/6 & 0 & \frac{1}{4}\sqrt{2} & 0 \\ 1/6 & 0 & -\frac{1}{4}\sqrt{2} & 0 \\ 1/6 & 0 & 0 & \frac{1}{4}\sqrt{2} \\ 1/6 & 0 & 0 & -\frac{1}{4}\sqrt{2} \end{array}\right] \end{array}$$

C. <u>The Octa-tetrahedral Design</u>.

This composite design was derived by superimposing an octahedron on a tetrahedron, with the axes of the two solids coinciding, and including the origin.

Its matrices are as follows:

$$D = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \end{array} \overset{\begin{array}{ccc} x_1 & x_2 & x_3 \end{array}}{\left[\begin{array}{ccc} \sqrt{2} & 0 & 0 \\ -\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & -\sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & -\sqrt{2} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 \end{array}\right]} \quad X = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \end{array} \overset{\begin{array}{cccccccccc} x_0 & x_1 & x_2 & x_3 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3 \end{array}}{\left[\begin{array}{cccccccccc} 1 & \sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 1 & -\sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & -\sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & \sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & -\sqrt{2} & 0 & 0 & 2 & 0 & 0 & 0 \\ 1 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 1 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ 1 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ 1 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right]}$$

$$X' = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ \sqrt{2} & -\sqrt{2} & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \sqrt{2} & -\sqrt{2} & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{2} & -\sqrt{2} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 2 & 2 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 2 & 2 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 \end{bmatrix}$$

$$X'X = \begin{bmatrix} 11 & 0 & 0 & 0 & 6 & 6 & 6 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 9 & 1 & 1 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 1 & 9 & 1 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 1 & 1 & 9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$C^{-1} = (X'X)^{-1} = \begin{array}{c} \\ b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_{11} \\ b_{22} \\ b_{33} \\ b_{12} \\ b_{13} \\ b_{23} \end{array} \begin{array}{c} \begin{array}{cccccccccc} b_0 & b_1 & b_2 & b_3 & b_{11} & b_{22} & b_{33} & b_{12} & b_{13} & b_{23} \end{array} \\ \left[\begin{array}{cccccccccc} \frac{11}{13} & 0 & 0 & 0 & \frac{-6}{13} & \frac{-6}{13} & \frac{-6}{13} & 0 & 0 & 0 \\ 0 & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{-6}{13} & 0 & 0 & 0 & \frac{19}{52} & \frac{25}{104} & \frac{25}{104} & 0 & 0 & 0 \\ \frac{-6}{13} & 0 & 0 & 0 & \frac{25}{104} & \frac{19}{52} & \frac{25}{104} & 0 & 0 & 0 \\ \frac{-6}{13} & 0 & 0 & 0 & \frac{25}{104} & \frac{25}{104} & \frac{19}{52} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \end{array}$$

$$T' = X(X'X)^{-1} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \end{array} \begin{array}{c} \begin{array}{cccccccccc} b_0 & b_1 & b_2 & b_3 & b_{11} & b_{22} & b_{33} & b_{12} & b_{13} & b_{23} \end{array} \\ \left[\begin{array}{cccccccccc} \frac{-1}{13} & \frac{1}{6}\sqrt{2} & 0 & 0 & \frac{7}{26} & \frac{1}{52} & \frac{1}{52} & 0 & 0 & 0 \\ \frac{-1}{13} & -\frac{1}{6}\sqrt{2} & 0 & 0 & \frac{7}{26} & \frac{1}{52} & \frac{1}{52} & 0 & 0 & 0 \\ \frac{-1}{13} & 0 & \frac{1}{6}\sqrt{2} & 0 & \frac{1}{52} & \frac{7}{26} & \frac{1}{52} & 0 & 0 & 0 \\ \frac{-1}{13} & 0 & -\frac{1}{6}\sqrt{2} & 0 & \frac{1}{52} & \frac{7}{26} & \frac{1}{52} & 0 & 0 & 0 \\ \frac{-1}{13} & 0 & 0 & \frac{1}{6}\sqrt{2} & \frac{1}{52} & \frac{1}{52} & \frac{7}{26} & 0 & 0 & 0 \\ \frac{-1}{13} & 0 & 0 & -\frac{1}{6}\sqrt{2} & \frac{1}{52} & \frac{1}{52} & \frac{7}{26} & 0 & 0 & 0 \\ \frac{2}{13} & \frac{1}{12}\sqrt{2} & \frac{1}{12}\sqrt{2} & \frac{1}{12}\sqrt{2} & \frac{-1}{26} & \frac{-1}{26} & \frac{-1}{26} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{2}{13} & \frac{1}{12}\sqrt{2} & \frac{-1}{12}\sqrt{2} & \frac{-1}{12}\sqrt{2} & \frac{-1}{26} & \frac{-1}{26} & \frac{-1}{26} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{2}{13} & \frac{-1}{12}\sqrt{2} & \frac{1}{12}\sqrt{2} & \frac{-1}{12}\sqrt{2} & \frac{-1}{26} & \frac{-1}{26} & \frac{-1}{26} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{2}{13} & \frac{-1}{12}\sqrt{2} & \frac{-1}{12}\sqrt{2} & \frac{1}{12}\sqrt{2} & \frac{-1}{26} & \frac{-1}{26} & \frac{-1}{26} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{11}{13} & 0 & 0 & 0 & \frac{-6}{13} & \frac{-6}{13} & \frac{-6}{13} & 0 & 0 & 0 \end{array}\right] \end{array}$$

It must be mentioned that icosahedral, cuboctahedral, cubic-tetrahedral, and icosidodecahedral designs were set up but these yielded matrices X'X whose corresponding determinants were 0. Thus, it was impossible to invert these matrices to get the matrix C^{-1} for the respective designs.

Finally, table VII is included to show the number of constants (L) to be determined for response equations of varying degree [1, p.29].

Table VII

NUMBER OF CONSTANTS TO BE DETERMINED
FOR EQUATIONS OF VARYING DEGREE

Number of Factors	d - Degree of equation			
	1	2	3	4
2	3	6	10	15
3	4	10	20	35
4	5	15	35	70
5	6	21	56	126

CHAPTER V

CONCLUDING REMARKS

An account of certain descriptive and mathematical aspects of experimental designs, response surfaces, and optimum conditions, supplemented with examples of surfaces which arise in experimental research, has been presented in the preceding chapters. Unfortunately, a great number of assumptions had to be made, and hypothetical problems set up. The ideal situation would have been to work in conjunction with an experimenter, applying the above theory to his problem as the experimental work progressed. This would have been a more gratifying experience since the ultimate in experimental design work is achieved only by a joint effort of both the statistician and the experimenter.

It is also to be noted that only quantitative factors, such as time, temperature, concentration, etc. have been used in the experimental work to which the experimental designs have been applied. G. E. P. Box states in [1, p.58] that, when some of the factors are qualitative variables, with very special exceptions, there is no way of finding the optimum other than carrying out separate investigations for each qualitative 'factor' combination.

The analysis of results from the experiments using the designs has been aimed only at estimating desired effects.

However, the study of experimental design and response surfaces can be extended to the calculation of confidence intervals, and to tests of significance by means of the analysis of variance technique. Also, confidence regions may be set up for the stationary point on a fitted second-degree surface, as is demonstrated in [2, p.196]. The theory of aliases and biases, and of the inclusion of additional observations are also a part of the topic. It may happen that an estimate of a required effect also includes estimates of one or more other effects. These effects are then confounded and may be said to be aliases of one another. A bias is a persistent or systematic error. Wherever possible, a comparison between the empirical and theoretical results, as illustrated in [4, p.287] would be of added interest.

Finally, the respective roles of the statistician and the experimenter in experimental design work must be mentioned. G. E. P. Box states in [1, p.26]:

> "The statistician's role is not, and cannot be, to design experiments in any absolute sense. The statistician's function is to advise the experimenter on the best positioning of experimental points in a space which the experimenter must of necessity construct for him, and construct purely on the basis of the experimenter's expert background knowledge of the subject in which he is experimenting. Were this not so there would be little point in training chemists, biologists, physicists, etc., only statisticians."

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