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CRITERIA FOR THE OPTIMAL DESIGN
OF EXPERIMENTAL TESTS

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16. Abstract

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SUMMARY

This report unifies in a concise manner some of the basic concepts that have been developed for the problem of finding optimal approximating functions which relate a set of controlled variables to a measurable response. The techniques outlined in this report have the potential for reducing the amount of testing required in experimental investigations. Specifically, two low-order polynomial models are considered as approximations to unknown functional relationships. For each model, optimal means of designing experimental tests are presented which, for a modest number of measurements, yield prediction equations that minimize the error of an estimated response anywhere inside a selected region of experimentation. Moreover, examples are provided for both models to illustrate their use. Finally, an analysis of a second-order prediction equation is given to illustrate ways of determining maximum or minimum responses inside the experimentation region.

INTRODUCTION

The purpose of this report is to unify some existing results of response-surface techniques that are available for the optimal design of experimental tests and to make them easily accessible to researchers in various disciplines. In experimental testing, it is vital that the test procedure be carefully planned to acquire only those measurements that are necessary to optimize the end result. Response-surface methods provide optimal means of selecting points to observe a dependent variable and to determine an approximating equation for an unknown functional form relating the dependent variable and a set of controlled variables. Specifically, consider the approximation of the unknown relation

$$y = f\left(u_1, u_2, \dots, u_k\right) \tag{1}$$

with some low-order polynomial inside a desired region defined by the controlled variables $u_1, u_2, \dots, u_k$. Moreover, consider an experiment in which the response y is to be measured at several selected values of the controlled variables for the purpose of

making the approximating polynomial form explicit. A basic question which is essentially the focal point of this report now arises: With respect to the controlled variables, where should the response be measured so that the resulting prediction equation minimizes the error between an estimated and an observed response anywhere inside the selected region? In other words, an optimal design is defined as one which yields a prediction model that minimizes the error of an estimated response. In the discussion of an answer to the question, consideration is given to a survey of response-surface methods as applied to design-optimization criteria for two polynomial models which have found wide industrial application (refs. 1 and 2). It is appropriate at this time to note that the term "response surface" has risen out of the geometric identification of the problem in that, for $k \geqq 2$ controlled variables, the solution can be characterized by surfaces of constant response.

Usually it is mathematically advantageous to restrict the range of each controlled variable. Thus, consider the transformation of the natural variables $u_1, u_2, \ldots, u_k$ to a new set of normalized variables $x_1, x_2, \ldots, x_k$. The implementation of this variable change is done according to the following scheme: Assume that, for each natural variable u_i, high and low values are selected such that they serve as boundaries to the selected region. Let $\bar{u}_i$ denote the average of these two values and s_i the absolute difference between $\bar{u}_i$ and either the high or low value of the ith natural variable. The change from u_i to x_i is then defined by the relation

$$x_i = \frac{u_i - \bar{u}_i}{s_i} \qquad (i = 1, 2, \ldots, k) \qquad (2)$$

As a result, the high and low values of u_i correspond, respectively, to +1 and -1 for x_i. Moreover, one unit of the normalized variable is equivalent to s_i units of the natural variable. Therefore, subsequent discussion is held in terms of the former with the inverse change to the latter readily available from equation (2).

Consideration is now given to a brief discussion of the form of two low-order polynomials which often serve as good approximations to the unknown function f. One is a linear function of the controlled variables whose form is the relation

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \epsilon \qquad (3)$$

where β_i (i = 0, 1, . . ., k) denotes the unknown coefficients and ϵ is the random error in the response y. This first-order model is often useful in studying a given response inside a narrow region of the controlled variables where little, if any, curvature in f is suspected. However, if the desired region is such that the response is not likely to be a linear function of the controlled variables, then the approximating function should be at least a second-order model given by

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$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{j=2}^{k} \sum_{i=1}^{j-1} \beta_{ij} x_i x_j + \epsilon \tag{4}$$

The term $\sum_{i=1}^{k} \beta_{ii} x_i^2$ represents a pure quadratic contribution while the term

$\sum_{j=2}^{k} \sum_{i=1}^{j-1} \beta_{ij} x_i x_j$ incorporates any cross-product effect. As an example, for $k = 2$, equation (4) reduces to

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \epsilon$$

Since a second-order model contains more unknown coefficients than one of first order, more measurements of the response are needed to estimate the unknown coefficients.

Finally, given a set of measurements of the response, it is possible to write either one of these models in the matrix form

$$\underline{y} = X\underline{\beta} + \underline{\epsilon} \tag{5}$$

where $\underline{y}$ is a column vector of n responses, X is an $n \times m$ (where $m = k + 1$) matrix of normalized-variable values, $\underline{\beta}$ is a column vector of m unknown parameters, and $\underline{\epsilon}$ is the $n \times 1$ vector of random errors. The vector ϵ represents the change in the response which cannot be accounted for explicitly. This, of course, includes changes due to model inaccuracy as well as measurement error.

SYMBOLS

B	symmetric matrix of quadratic parameters
k	number of controlled variables
M	orthogonal matrix
m_{ij}	fourth mixed moment in matrix $X'X$
n	number of response measurements
p_i	fourth pure moment in matrix $X'X$
$\underline{s}$	coordinate point of normalized variables

$\underline{s}_0$ solution to equation $\frac{dy}{d\underline{s}} = 0$

$u_1, u_2, \ldots, u_k$ controlled variables

$\underline{w}$ vectors of principal axes

X matrix of normalized variables

$x_1, x_2, \ldots, x_k$ normalized variables

$\underline{y}$ vector of measurements

α rotatability parameter

$\underline{\beta}$ vector of parameters

$\underline{\gamma}$ vector of linear parameters

$\underline{\epsilon}$ vector of random errors

$\lambda_1, \lambda_2, \ldots, \lambda_k$ eigenvalues of B

σ^2 common variance of random errors

Notation:

$\hat{}$ an estimate

$'$ (Prime)   transpose of matrix

$\_$ (Underlining)   vector

OPTIMAL FIRST-ORDER RESPONSE-SURFACE DESIGNS

Suppose that the unknown relation given by equation (1) is to be approximated by a first-order polynomial in which the jth response is depicted by the expression

$$y_j = \beta_0 + \sum_{i=1}^{k} \beta_i x_{ij} + \epsilon_j \qquad (j = 1, 2, \ldots, n; \quad n > k) \qquad (6)$$

In matrix form, this set of n linear equations in m unknown coefficients is written as

$$\underline{y} = X\underline{\beta} + \underline{\epsilon}$$

where

$$\underline{y} = \begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \qquad X = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{k1} \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ 1 & x_{1j} & x_{2j} & \cdots & x_{kj} \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ 1 & x_{1n} & x_{2n} & \cdots & x_{kn} \end{bmatrix} \qquad \underline{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \cdot \\ \cdot \\ \beta_k \end{bmatrix} \qquad \underline{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \cdot \\ \cdot \\ \epsilon_n \end{bmatrix}$$

The jth row of X represents the conditions of the controlled variables under which the jth measurement of the response is made.

By using the principle of least squares (refs. 1 and 3), estimates of the components of $\underline{\beta}$ are readily computed by the result

$$\hat{\underline{\beta}} = (X'X)^{-1}X'\underline{y}$$

where $\hat{\underline{\beta}}$ is the vector of estimates. Moreover, the variance-covariance matrix of $\hat{\underline{\beta}}$ is given by the relation

$$\text{var}\left(\hat{\underline{\beta}}\right) = \sigma^2(X'X)^{-1}$$

where σ^2 is the unknown common variance of the error vector $\underline{\epsilon}$ and represents the unaccountable change in the response y. Usually σ^2 is estimated by the unbiased estimate

$$\hat{\sigma}^2 = \frac{\underline{y}'\underline{y} - \hat{\underline{\beta}}'X\underline{y}}{n - m}$$

The (i,i) element of $\sigma^2(X'X)^{-1}$ coincides with the variance of $\hat{\beta}_i$, while the (i,j) element corresponds to the covariance between $\hat{\beta}_i$ and $\hat{\beta}_j$ for $i \neq j$. Moreover, since by definition the variance is a measure of dispersion, then $\text{var}\left(\hat{\underline{\beta}}\right)$ is indicative of the precision with which each coefficient in equation (6) is being estimated.

Consider now the prediction of a response at an arbitrary point, inside the desired region, whose coordinates in terms of the normalized variables are given by $\left(v_1, v_2, \ldots, v_k\right)$. The estimated value of $\hat{y}$ is computed from the relation

$$\hat{y} = \underline{v}'\hat{\underline{\beta}}$$

where

$$\underline{v}' = \begin{bmatrix} 1 & v_1 & v_2 & \cdots & v_k \end{bmatrix}$$

By using matrix manipulation, the variance of the predicted value $\hat{y}$ is given by

$$\text{var}(\hat{y}) = \underline{v}'(X'X)^{-1}\underline{v}\sigma^2 = \underline{v}'\ \text{var}\left(\hat{\underline{\beta}}\right)\underline{v} \tag{7}$$

Therefore, the conditions that minimize the residual variance of an estimated response $\hat{y}$ are the same as those that maximize the precision of $\hat{y}$, where precision is defined as the reciprocal of variance. From equation (7), it is clear that the only quantity subject to control is the design matrix X whose elements are the values of the controlled variables for which the response is to be measured. Hence, the problem of minimizing the variance of $\hat{y}$ is reduced to finding that design matrix X for which the elements of $\text{var}\left(\hat{\underline{\beta}}\right)$ are minimized. For this purpose, the following theorem is given: If the design matrix X is selected such that each column of X is mutually orthogonal to every other column in X, then the first-order approximation to the response surface is optimal in the sense that the residual variance of a predicted response is minimized. In other words, the optimal-design matrix X yields a diagonal matrix $X'X$ of the form

$$X'X = \begin{bmatrix} n & 0 & \cdots & 0 \\ 0 & n & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & & n \end{bmatrix} \tag{8}$$

where n is the number of measurements (ref. 4). The proof of this theorem is provided in the appendix.

The inverse of a diagonal matrix such as equation (8) is

$$(X'X)^{-1} = \begin{bmatrix} 1/n & 0 & \cdots & 0 \\ 0 & 1/n & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & & 1/n \end{bmatrix} \tag{9}$$

Thus, for a first-order model, the optimal-design configuration results in an expression for the error of a predicted response $\hat{y}$ given by

$$\text{var}(\hat{y}) = \begin{bmatrix} 1 & v_1 & v_2 & \cdots & v_k \end{bmatrix} \begin{bmatrix} \sigma^2/n & 0 & \cdots & 0 \\ 0 & \sigma^2/n & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & & \sigma^2/n \end{bmatrix} \begin{bmatrix} 1 \\ v_1 \\ \cdot \\ \cdot \\ \cdot \\ v_k \end{bmatrix} \tag{10}$$

Simplification of equation (10) yields the relation

$$\text{var}(\hat{y}) = \frac{\sigma^2}{n}\left(1 + \sum_{i=1}^{k} v_i^2\right) = \frac{\sigma^2}{n}\left(1 + r^2\right) \tag{11}$$

Equation (11) implies that the optimal first-order design yields an error, for a predicted

response $\hat{y}$, which is a function of $r = \sqrt{\sum_{i=1}^{k} v_i^2}$, the distance between the center of the

defined region and the point of interest $\left(v_1, v_2, \ldots, v_k\right)$.

One class of design configuration that is most useful for fitting first-order models and satisfies the optimality criterion is the 2^k factorial design. The factorial arrangement is accomplished by using as design points all possible combinations of the high and low values of the k controlled variables. This, of course, results in a total of $n = 2^k$ measurements of the response. Therefore, the 2^k factorial class of orthogonal designs is not only optimal in fitting first-order response-surface models but also provides considerable savings in time and expense as a result of the relatively small number of measurements needed for a moderate value of k.

The following hypothetical example is presented to illustrate the procedures for an optimal first-order design. Consider the problem of studying the yield of a process as a function of agitation speed S, concentration C, and temperature T. It is believed that a first-order model such as equation (6) is sufficient to describe the yield inside a region bound by agitation speeds of 200 to 400 rpm, concentrations of 2 to 4 percent, and temperatures of 30° to 50° C. In accordance with the previous discussion, these natural variables are transformed to their normalized counterparts by the equations

$$x_1 = \frac{S - 300}{100}$$

$$x_2 = C - 3$$

and

$$x_3 = \frac{T - 40}{10}$$

Since there are $k = 3$ controlled variables, a total of $2^3 = 8$ measurements of the process yield is needed.

The design matrix X and the vector of measurements $\underline{y}$ are given as

$$
\begin{array}{cccc}
x_0 & x_1 & x_2 & x_3
\end{array}
$$

$$
X = \begin{bmatrix}
1 & -1 & -1 & -1 \\
1 & -1 & -1 & 1 \\
1 & -1 & 1 & -1 \\
1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 \\
1 & 1 & -1 & 1 \\
1 & 1 & 1 & -1 \\
1 & 1 & 1 & 1
\end{bmatrix}
\qquad
\underline{y} = \begin{bmatrix}
40 \\
54 \\
38 \\
56 \\
52 \\
62 \\
49 \\
59
\end{bmatrix}
$$

where the headings x_0, x_1, and so forth, indicate the column of values for the corresponding controlled variable. Since the dot product of any two distinct columns of X equals 0, $X'X$ is a diagonal matrix of the form

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

Moreover, by matrix multiplication,

$$
X'\underline{y} = \begin{bmatrix}
410 \\
34 \\
-6 \\
52
\end{bmatrix}
$$

As a result, the coefficients of the first-order model are computed to be $\hat{\beta}_0 = 51.25$, $\hat{\beta}_1 = 4.25$, $\hat{\beta}_2 = -0.75$, and $\hat{\beta}_3 = 6.50$. Therefore, the prediction equation in terms of the normalized variables is

$$
\hat{y} = 51.25 + 4.25x_1 - 0.75x_2 + 6.50x_3
$$

This provides an approximating function to use whenever the prediction of yield is needed at any arbitrary point interior to the region of experimentation. If, for example, $S = 250$ rpm $\left(x_1 = -\frac{1}{2}\right)$, $C = 3.5$ percent $\left(x_2 = \frac{1}{2}\right)$, and $T = 40^\circ$ C $\left(x_3 = 0\right)$, the predicted yield is $\hat{y} = 48.75$ percent. To compute the variance of this estimate $\hat{y}$, an estimate of σ^2 is computed. It turns out to be $\hat{\sigma}^2 = 6.625$ and equation (11) is used to compute the variance of the predicted yield

$$\text{var}(\hat{y}) = \frac{6.625}{8}\left(1 + \frac{1}{4} + \frac{1}{4}\right) = 1.24$$

Finally, by using the relations between normalized and natural variables, the approximating equation in terms of the latter reduces to

$$\hat{y} = 14.75 + 0.0425S - 0.75C + 0.65T$$

OPTIMAL SECOND-ORDER RESPONSE-SURFACE DESIGNS

Consideration is now given to a discussion of certain useful designs with attractive properties for fitting second-order models. It is assumed that a significant degree of curvature is suspected in the unknown function $y = f\left(u_1, u_2, \ldots, u_k\right)$ so as to warrant the use of a second-order polynomial in which the jth response is represented by

$$y_j = \beta_0 + \sum_{i=1}^{k} \beta_i x_{ij} + \sum_{i=1}^{k} \beta_{ii} x_{ij}^2 + \sum_{h=2}^{k} \sum_{i=1}^{h-1} \beta_{ih} x_{ij} x_{hj} + \epsilon_j \qquad (j = 1, 2, \ldots, n) \quad (12)$$

As in the previous case, equation (12) in matrix notation becomes

$$\underline{y} = X\underline{\beta} + \underline{\epsilon}$$

where now

$$X = \begin{bmatrix} 1 & x_{11}, \cdots, x_{k1} & x_{11}^2, \cdots, x_{k1}^2 & x_{11}x_{21}, \cdots, x_{k-1,1}x_{k1} \\ 1 & x_{12}, \cdots, x_{k2} & x_{12}^2, \cdots, x_{k2}^2 & x_{12}x_{22}, \cdots, x_{k-1,2}x_{k2} \\ \vdots & & & \\ 1 & x_{1n}, \cdots, x_{kn} & x_{1n}^2, \cdots, x_{kn}^2 & x_{1n}x_{2n}, \cdots, x_{k-1,n}x_{kn} \end{bmatrix} \qquad (13)$$

and

$$\underline{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \\ \beta_{11} \\ \vdots \\ \beta_{kk} \\ \beta_{12} \\ \vdots \\ \beta_{k-1,k} \end{bmatrix}$$

There are exactly $(k + 2)(k + 1)/2$ unknown coefficients in $\underline{\beta}$ and, thus, the dimensions of X are $n \times (k + 2)(k + 1)/2$, where n is the total number of measurements.

Since curvature is suspected, the response y should be measured for at least three distinct values of each controlled variable in order to estimate the quadratic effect. Based on the usefulness of the 2^k factorial design in the first-order model, it is logical to assume that a 3^k factorial design would be appropriate in fitting the quadratic model. However, for moderately large values of k, the measurements required for the experiment become prohibitively numerous. As a result, Box and Wilson (ref. 5) develop what they call a class of composite plans which require relatively few measurements and achieve certain optimal properties.

The most frequently used composite plan is the so-called central-composite design which is basically a 2^k factorial design augmented by $2k + 1$ additional points to allow for the estimation of the $(k + 2)(k + 1)/2$ parameters in equation (12). In terms of the normalized variables, the additional $2k + 1$ points in a central-composite design are as follows:

x_1	x_2	$\cdots$	x_k
0	0	$\ldots$	0
$-\alpha$	0	$\ldots$	0
α	0	$\ldots$	0
0	$-\alpha$	$\ldots$	0
0	α	$\ldots$	0
$\cdot$	$\cdot$		$\cdot$
$\cdot$	$\cdot$		$\cdot$
$\cdot$	$\cdot$		$\cdot$
0	0	$\ldots$	$-\alpha$
0	0	$\ldots$	α

This design provides five distinct values of each controlled variable for measuring the response y if $|\alpha| \neq 1$; namely, ± 1, $\pm \alpha$, and 0 where $(0,0,...,0)$ corresponds to the center of the experimentation region. Therefore, in a central-composite design, 2^k measurements are taken according to a 2^k factorial arrangement, one measurement is taken at the center, and the remaining $2k$ measurements are taken at a distance α from the center of the design region. The following sketch provides a geometric representation of the experimentation region for a central-composite plan with three controlled variables:

x_2

$(0,\alpha,0)$

$(-1,1,-1)$ $(1,1,-1)$

$(0,0,-\alpha)$

$(-1,1,1)$ $(1,1,1)$

$(-\alpha,0,0)$ $(0,0,0)$ $(\alpha,0,0)$ x_1

$(-1,-1,-1)$ $(1,-1,-1)$

$(0,0,\alpha)$

x_3 $(-1,-1,1)$ $(1,-1,1)$

$(0,-\alpha,0)$
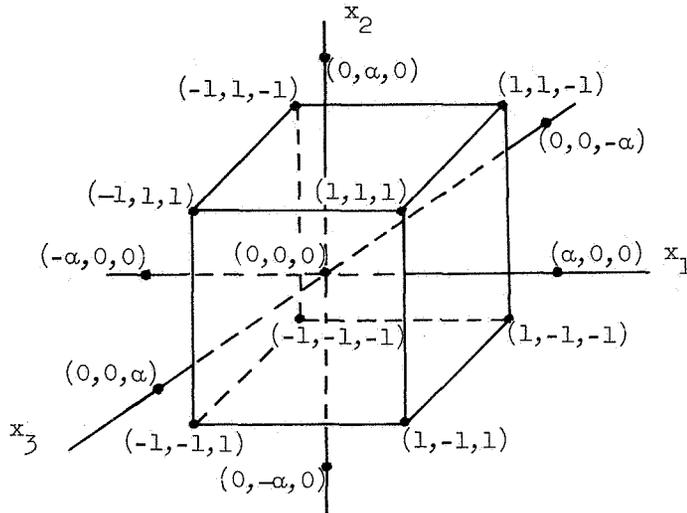
Depending on the choice of α, the central-composite design is nearly optimal in minimizing the error between a predicted and an observed response at any arbitrary point inside a defined region for a second-order model. One optimality criterion is a property called rotatability. A design is said to be rotatable if the variance of a predicted response is unaltered when the design is rotated through an arbitrary angle about the center of the experimentation region. To illustrate the effect of rotatability, consider a central-composite design with two controlled variables and $\alpha = 1$. The design matrix X according to equation (13) is given by

$$
X = \begin{array}{cccccc}
x_0 & x_1 & x_2 & x_1^2 & x_2^2 & x_1 x_2 \\
\end{array}
\left[\begin{array}{cccccc}
1 & -1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & 1 & 1 & -1 \\
1 & 1 & -1 & 1 & 1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 \\
1 & -1 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 1 & 0 & 0 \\
1 & 0 & -1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 \\
\end{array}\right]
\tag{14}
$$

Thus,

$$
X'X = \left[\begin{array}{cccccc}
9 & 0 & 0 & 6 & 6 & 0 \\
0 & 6 & 0 & 0 & 0 & 0 \\
0 & 0 & 6 & 0 & 0 & 0 \\
6 & 0 & 0 & 6 & 4 & 0 \\
6 & 0 & 0 & 4 & 6 & 0 \\
0 & 0 & 0 & 0 & 0 & 4 \\
\end{array}\right]
$$

and

$$(X'X)^{-1} = \begin{bmatrix} 5/9 & 0 & 0 & -1/3 & -1/3 & 0 \\ 0 & 1/6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/6 & 0 & 0 & 0 \\ -1/3 & 0 & 0 & 1/2 & 0 & 0 \\ -1/3 & 0 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 \end{bmatrix}$$

Assume the measurements are taken according to this design matrix, and the approximating equation is thus determined.

Consider now the prediction of a response at a point with coordinates (a_1, a_2). The estimated value is given by

$$\hat{y} = \underline{a}'\hat{\underline{\beta}}$$

where

$$\underline{a}' = \begin{bmatrix} 1 & a_1 & a_2 & a_1^2 & a_2^2 & a_1 a_2 \end{bmatrix}$$

and $\hat{\underline{\beta}}$ is the vector of estimates corresponding to equation (12). As before, the variance of $\hat{y}$ is given by the relation

$$\text{var}(\hat{y}) = \underline{a}'(X'X)^{-1}\underline{a}\sigma^2 \tag{15}$$

After appropriate substitution into and simplification of equation (15),

$$\text{var}(\hat{y}) = \sigma^2\left(\frac{5}{9} - \frac{1}{2}a_1^2 - \frac{1}{2}a_2^2 + \frac{1}{2}a_1^4 + \frac{1}{2}a_2^4 + \frac{1}{4}a_1^2 a_2^2\right) \tag{16}$$

which is a function of location within the region of experimentation. Specifically, consider the variance of a predicted response at two points which are equidistant from the center of the desired region and whose coordinates are given by (0.7,0.7) and by $\left(\sqrt{0.98},0\right)$. Substituting into equation (16) and simplifying yield

$$\text{var}(\hat{y})_{(.7,.7)} = 0.3656\sigma^2$$

while

$$\text{var}(\hat{y})_{\left(\sqrt{.98},0\right)} = 0.5457\sigma^2$$

Thus, even though these two points are equidistant from the center, the error in the predicted response of the former is obviously smaller than in that of the latter. Hence, a design which is not rotatable discriminates against direction. This occurrence is indeed

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a disadvantage since it is likely that any two points which are equidistant from the experimental center are equally important. It is apparent that an optimal (orthogonal) first-order design previously discussed, is also rotatable.

To obtain the conditions for rotatability in a second-order design, it better serves the purpose of this paper if most of the theory is omitted and emphasis is placed on only essential features. (For detailed information, see refs. 2 and 5 to 7.) In the present paper, it is necessary to define the following quantities in terms of the normalized variables $x_1, x_2, \ldots, x_k$:

$$
\left.
\begin{aligned}
p_i &= \frac{1}{n} \sum_{h=1}^{n} x_{ih}^{4} \\[2em]
m_{ij} &= \frac{1}{n} \sum_{h=1}^{n} x_{ih}^{2} x_{jh}^{2}
\end{aligned}
\right\}
\qquad (i,j = 1, 2, \ldots, n; \quad i \neq j) \qquad (17)
$$

Notice that all of these quantities are elements of the matrix $X'X$. Moreover, p_i is the fourth pure moment while m_{ij} if the fourth mixed moment. In terms of p_i and m_{ij}, the conditions for rotatability in a second-order response surface are as follows:

(1) All odd moments through order four equal 0

(2) The ratio of the fourth pure moment to the fourth mixed moment equals 3 $\Big($that is, $\dfrac{p_i}{m_{ij}} = 3\Big)$ for all $i,j = 1, 2, \ldots, k; \quad i \neq j$

Condition (1) requires that moments such as $\frac{1}{n} \sum_{h=1}^{n} x_{ih}, \ \frac{1}{n} \sum_{h=1}^{n} x_{ih} x_{jh}, \ \frac{1}{n} \sum_{h=1}^{n} x_{ih}^{2} x_{jh},$ $\frac{1}{n} \sum_{h=1}^{n} x_{ih}^{3}, \ \frac{1}{n} \sum_{h=1}^{n} x_{ih}^{3} x_{jh},$ and so forth, which are elements of the matrix $X'X$, all equal 0 for all i and j when $i \neq j$.

Consider imposing rotatability on a central-composite design. By the nature of this design, it is easy to verify that condition (1) is satisfied. Thus, in a central-composite design, rotatability is equivalent to determining the value α which satisfies the requirement that

$$
\frac{p_i}{m_{ij}} = 3
$$

By using the matrix X given in equation (14) as an example, it can be generalized that

$$\sum_{h=1}^{n} x_{ih}^{4} = 2^{k} + 2\alpha^{4}$$

and that

$$\sum_{h=1}^{n} x_{ih}^{2} x_{jh}^{2} = 2^{k}$$

for any central-composite design. Therefore, the value of α for which

$$\frac{2^{k} + 2\alpha^{4}}{2^{k}} = 3$$

is

$$\alpha = 2^{k/4} \tag{18}$$

This value assures rotatability in a central-composite design for a given k.

To illustrate a rotatable second-order central-composite design, consider the case of $k = 2$ controlled variables. By using equation (18), it is readily determined that $\alpha = \sqrt{2}$ for $k = 2$. Thus, the geometric representation of the desired region is the octagon of the following sketch:
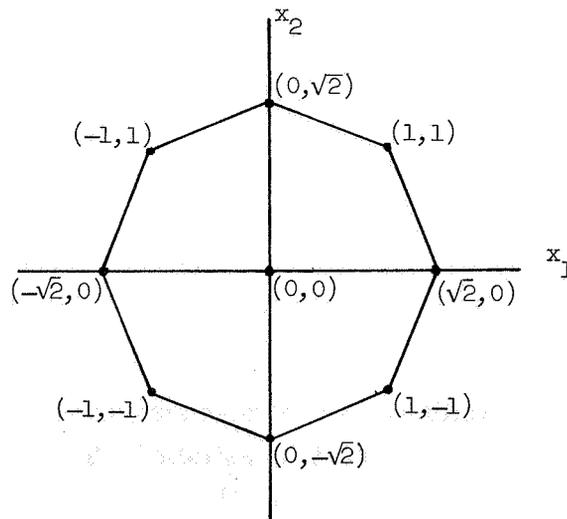
The design points are at the center and at the eight vertices of the octagon. Therefore, the design matrix X follows from this configuration and is given by

$$X = \begin{array}{cccccc}
x_0 & x_1 & x_2 & x_1^2 & x_2^2 & x_1 x_2 \\
\end{array}$$

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

It can be verified that all odd moments through order four equal 0, $p_i = \frac{12}{9}$, $m_{ij} = \frac{4}{9}$, and rotatability is thus attained. Perhaps it is important to remark here that to convert normalized units equal to $\pm\sqrt{2}$ or 0 to corresponding natural units, equation (2) can be used to solve for the natural variable.

In addition to rotatability, another equally important property is now considered for a second-order central-composite design. Recall that, by the definition of rotatability, the variance of a predicted response at any arbitrary point interior to the experimentation region is a function of the distance r from the point to the center of the region. Since the variance increases as the distance from the center increases, Box and Hunter (ref. 6) develop criteria so that the error of a predicted response at $r = 1$ is the same as the error at the design center. Such a consideration is based on the notion that the prediction of a response anywhere inside the region for which $r < 1$ is of uniform importance and, therefore, the error should be the same. This attractive property of uniform error can be achieved through a judicious choice of the value for the fourth mixed moment m_{ij} without loss of rotatability. Specifically, the value of m_{ij} which gives rise to a uniform error for predicting a response anywhere inside a region bounded by $r = 1$ is made possible by measuring the response more than once at the center of the design. For rotatable second-order designs, these values of m_{ij} are given for up to and including six controlled variables as follows:

k	m_{ij}
2	0.3187
3	.4093
4	.5106
5	.6120
6	.7056

For a central-composite design, there remains to derive an expression which, for a given k, relates the uniform-error value of m_{ij} to the corresponding number of measurements of the response needed at the center of the design. Let the total number of measurements be

$$n = 2^k + 2k + n_c$$

where n_c indicates the number of measurements at the center. Since m_{ij} is the dot product of the squares of the ith and jth columns of X divided by n, then for a central-composite design

$$m_{ij} = \frac{2^k}{2^k + 2k + n_c} \tag{19}$$

In solving equation (19) for n_c, the relation reduces to

$$n_c = \frac{2^k}{m_{ij}} - \left(2^k + 2k\right) \tag{20}$$

where the value of m_{ij} has already been defined for $k \leqq 6$ controlled variables. Since n_c must be an integer, values obtained by equation (20) have to be rounded off to the nearest whole number and, thus, absolutely uniform variance cannot be achieved. The necessary parameters for a second-order rotatable central-composite design with nearly uniform variance are given, for up to six controlled variables, as

k	Value of α for rotatability	No. of measurements at center for uniform error	Total no. of measurements
2	1.414	5	13
3	1.682	6	20
4	2.000	7	31
5	2.378	10	52
6	2.828	15	91

ANALYSIS OF SECOND-ORDER PREDICTION EQUATIONS

Although the primary task of this report is the discussion of optimal-design concepts for the determination of a prediction equation, the task is not complete without at least a brief discussion of the analysis of such an equation, especially with respect to locating local maxima or minima. Once the prediction equation of a second-order response surface is available, it is usually desirable to determine the coordinates of the controlled variables at which the response is maximum (or minimum). In locating this point, let the predicted response $\hat{y}$ at any point $\underline{s}' = \begin{bmatrix} s_1 & s_2 & \ldots & s_k \end{bmatrix}$ be written in terms of the normalized variables as

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$$\hat{y} = \hat{\beta}_0 + \underline{s}'\hat{\underline{\gamma}} + \underline{s}'B\underline{s} \tag{21}$$

where

$$\hat{\underline{\gamma}}' = \begin{bmatrix} \hat{\beta}_1 & \hat{\beta}_2 & \cdots & \hat{\beta}_k \end{bmatrix}$$

and

$$B = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \cdots & \hat{\beta}_{1k}/2 \\ \hat{\beta}_{12}/2 & \hat{\beta}_{22} & \cdots & \hat{\beta}_{2k}/2 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \hat{\beta}_{1k}/2 & \cdots & \cdots & \hat{\beta}_{kk} \end{bmatrix} \tag{22}$$

Let $\underline{s}_0$ be the coordinates of the point at which the response is maximum (or minimum) within the experimentation region. The vector $\underline{s}_0$ is found by solving the equation

$$\frac{d\hat{y}}{d\underline{s}} = 0$$

Thus, by differentiating equation (21) and by virtue of the symmetry in B,

$$\frac{d\hat{y}}{d\underline{s}} = \hat{\underline{\gamma}} + 2B\underline{s}$$

which, upon simplification, reduces to the needed relation

$$\underline{s}_0 = -\frac{1}{2} B^{-1}\hat{\underline{\gamma}} \tag{23}$$

The predicted response $\hat{y}_0$ corresponding to $\underline{s}_0$ is determined, by substituting equation (23) into equation (21) and simplifying, as

$$\hat{y}_0 = \hat{\beta}_0 - \frac{1}{2}\hat{\underline{\gamma}}'B^{-1}\hat{\underline{\gamma}} + \frac{1}{4}\hat{\underline{\gamma}}'B^{-1}\hat{\underline{\gamma}}$$

$$= \hat{\beta}_0 + \frac{1}{2}\left(-\frac{1}{2}\hat{\underline{\gamma}}'B^{-1}\hat{\underline{\gamma}}\right)$$

$$= \hat{\beta}_0 + \frac{1}{2}\underline{s}_0'\hat{\underline{\gamma}} \tag{24}$$

Therefore, if in fact there exists a point within the experimentation region which yields maximum (or minimum) response, the coordinates of such a point are given by equation (23) while the maximum (or minimum) response is given by equation (24). The reader is cautioned that the existence of either a maximum or a minimum at $\underline{s}_0$ is not guaran-

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teed because of the possibility that $\underline{s}_0$ may be a saddle point. Thus, it is imperative to determine the nature of the response $\hat{y}_0$ at the point $\underline{s}_0$. In pursuit of this goal, consider rewriting equation (21) by translating it from the current origin (design center) to the point $\underline{s}_0$. This involves defining a new vector $\underline{t} = \underline{s} - \underline{s}_0$. As a result, equation (21) becomes

$$\hat{y} = \hat{\beta}_0 + \underline{t}'\hat{\underline{\gamma}} + \underline{s}_0'\hat{\underline{\gamma}} + \left(\underline{t}'B + \underline{s}_0'B\right)\left(\underline{t} + \underline{s}_0\right)$$

$$= \hat{\beta}_0 + \underline{s}_0'\hat{\underline{\gamma}} + \underline{s}_0'B\underline{s}_0 + \underline{t}'\hat{\underline{\gamma}} + \underline{t}'B\underline{s}_0 + \underline{s}_0'B\underline{t} + \underline{t}'B\underline{t}$$

$$= \hat{\beta}_0 + \underline{s}_0'\hat{\underline{\gamma}} + \underline{s}_0'B\underline{s}_0 + \underline{t}'\left(\hat{\underline{\gamma}} + 2B\underline{s}_0\right) + \underline{t}'B\underline{t}$$

However, $\hat{\beta}_0 + \underline{s}_0'\hat{\underline{\gamma}} + \underline{s}_0'B\underline{s}_0$ is the predicted response at the point $\underline{s}_0$, and $\hat{\underline{\gamma}} + 2B\underline{s}_0 = 0$. Therefore, the translation of equation (21) from the design center to the point $\underline{s}_0$ results in the relation

$$\hat{y} = \hat{y}_0 + \underline{t}'B\underline{t} \tag{25}$$

Since B, as defined by equation (22), is a real symmetric matrix, the principal-axis theorem is invoked to rotate equation (25) to a new set of variables $w_1, w_2, \ldots, w_k$ and thus reduce it to its canonical form, from which the nature of the response at $\underline{s}_0$ is immediately apparent. The rotation is accomplished by an orthogonal transformation of the form

$$\underline{t} = M\underline{w} \tag{26}$$

where $\underline{w}' = \begin{bmatrix} w_1 & w_2 & \ldots & w_k \end{bmatrix}$ and M is the orthogonal matrix of the transformation. Substituting equation (26) into equation (25) yields

$$\hat{y} = \hat{y}_0 + \underline{w}'M'BM\underline{w} \tag{27}$$

However, since B is symmetric, then

$$M'BM = \begin{bmatrix} \lambda_1 & 0 & 0 & \ldots & 0 \\ 0 & \lambda_2 & 0 & \ldots & 0 \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ 0 & 0 & & & \lambda_k \end{bmatrix}$$

where $\lambda_1, \lambda_2, \ldots, \lambda_k$ are the eigenvalues of B. Hence,

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$$\underline{w}'M'BM\underline{w} = \begin{bmatrix} w_1 & w_2 & \cdots & w_k \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdots & \lambda_k \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \cdot \\ \cdot \\ \cdot \\ w_k \end{bmatrix}$$

$$= \lambda_1 w_1^2 + \lambda_2 w_2^2 + \ldots + \lambda_k w_k^2$$

and the relation given by equation (25) reduces to its canonical form given by

$$\hat{y} = \hat{y}_0 + \sum_{i=1}^{k} \lambda_i w_i^2 \tag{28}$$

Equation (28) was derived from equation (21) by translating the latter to $\underline{s}_0$ and then rotating it to the principal axes $w_1, w_2, \ldots, w_k$. As a result, the nature of the response at the point $\underline{s}_0$ is manifested by determining the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ of B.

Through an inspection of the canonical form given by equation (28), the interpretation of the response at $\underline{s}_0$ is as follows:

(1) The response $\hat{y}_0$ is maximum if all eigenvalues are negative

(2) The response $\hat{y}_0$ is minimum if all eigenvalues are positive

(3) The response $\hat{y}_0$ is neither maximum nor minimum if all of the eigenvalues
   are not of the same sign; this constitutes a saddle point at $\underline{s}_0$

If the response at $\underline{s}_0$ is maximum, a move in any direction away from $\underline{s}_0$ results in a decrease of the response. Conversely, if the response at $\underline{s}_0$ is minimum, a move away from $\underline{s}_0$ produces an increase in the response. In either case, the more pronounced change occurs along that axis whose corresponding eigenvalue has the greatest magnitude. When a saddle point is encountered, a move away from $\underline{s}_0$ along an axis w_i may result in an increase or a decrease of the response depending on whether the ith eigenvalue is positive or negative. Finally, it is necessary to remark that it is possible for the coordinates of the point $\underline{s}_0$ to fall outside the region under consideration. If such is the case, further experimentation in the direction of the point $\underline{s}_0$ is recommended depending, of course, on the experimenter's goals.

Again, it is beneficial to provide an example to illustrate the procedures for a second-order model. Consider the situation in which a researcher attempts to determine criteria for regenerative adsorbents appropriate for CO_2 control in manned spacecraft. Of specific interest is the ability to predict CO_2 adsorption rate across a gas film layer

as a function of velocity V, CO_2 partial pressure P, and plate temperature T. To determine a second-order prediction model, 20 measurements are taken according to a rotatable central-composite design where the response is the total grams of CO_2 adsorbed by the plate in a 10-minute period.

The relations between natural and normalized variables are

$$x_1 = \frac{V - 45.72}{22.86}$$

$$x_2 = \frac{P - 12.0}{5.3}$$

and

$$x_3 = \frac{T - 14}{8}$$

Moreover, the range of experimental investigation for each of the three controlled variables is given in both normalized and natural units as follows:

Normalized units	Velocity, m/min	CO_2 partial pressure, mm Hg	Plate temperature, °C
-1.682	7.32	3.1	0.54
-1.000	22.86	6.7	6
.000	45.72	12.0	12
+1.000	68.58	17.3	22
+1.682	84.13	20.9	27.46

The X and $X'X$ matrices, the vector of measurements $\underline{y}$, and the vector $X'\underline{y}$ for this example are given as follows:

$$
X = \begin{array}{c}
\begin{array}{cccccccccc}
x_0 & x_1 & x_2 & x_3 & x_1^{\,2} & x_2^{\,2} & x_3^{\,2} & x_1x_2 & x_1x_3 & x_2x_3
\end{array}\\
\left[\begin{array}{cccccccccc}
1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1\\
1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1\\
1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1\\
1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1\\
1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1\\
1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1\\
1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & 1\\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1\\
1 & -1.682 & 0 & 0 & 2.828 & 0 & 0 & 0 & 0 & 0\\
1 & 1.682 & 0 & 0 & 2.828 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & -1.682 & 0 & 0 & 2.828 & 0 & 0 & 0 & 0\\
1 & 0 & 1.682 & 0 & 0 & 2.828 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & -1.682 & 0 & 0 & 2.828 & 0 & 0 & 0\\
1 & 0 & 0 & 1.682 & 0 & 0 & 2.828 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right]
\end{array}
$$

$$X'X = \begin{bmatrix} 20 & 0 & 0 & 0 & 13.656 & 13.656 & 13.656 & 0 & 0 & 0 \\ 0 & 13.656 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 13.656 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 13.656 & 0 & 0 & 0 & 0 & 0 & 0 \\ 13.656 & 0 & 0 & 0 & 24 & 8 & 8 & 0 & 0 & 0 \\ 13.656 & 0 & 0 & 0 & 8 & 24 & 8 & 0 & 0 & 0 \\ 13.656 & 0 & 0 & 0 & 8 & 8 & 24 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 \end{bmatrix}$$

$$\underline{y} = \begin{bmatrix} 1.996 \\ 2.812 \\ 5.171 \\ 5.035 \\ 2.676 \\ 4.173 \\ 3.266 \\ 6.668 \\ 2.359 \\ 3.583 \\ 2.449 \\ 5.851 \\ 2.223 \\ 2.994 \\ 6.519 \\ 6.218 \\ 6.354 \\ 5.583 \\ 6.491 \\ 5.781 \end{bmatrix}$$

$$X'\underline{y} = \begin{bmatrix} 88.2020 \\ 7.6377 \\ 14.2052 \\ 3.0658 \\ 48.6010 \\ 55.2694 \\ 46.5507 \\ 0.9530 \\ 4.2190 \\ -2.3130 \end{bmatrix}$$

Solving for the coefficients of the second-order model gives the prediction equation in terms of the normalized variables as

$$\hat{y} = 6.1283 + 0.5596x_1 + 1.0406x_2 + 0.2246x_3 - 0.9350x_1^2 - 0.5181x_2^2$$

$$- 1.0632x_3^2 + 0.1191x_1x_2 + 0.5274x_1x_3 - 0.2891x_2x_3$$

The prediction equation in terms of the natural variables reduces to

$$\hat{y} = -12.2808 + 0.13591V + 0.68956P + 0.44319T - 0.001789V^2 - 0.01844P^2$$

$$- 0.016613T^2 + 0.000983VP + 0.002884VT - 0.006818PT$$

By appealing to an analysis of the second-order prediction equation, the matrix B as defined by equation (22) is found to be

$$B = \begin{bmatrix} -0.9350 & 0.0595 & 0.2637 \\ 0.0595 & -0.5181 & -0.1445 \\ 0.2637 & -0.1445 & -1.0632 \end{bmatrix}$$

while the vector is

$$\underline{\gamma}' = \begin{bmatrix} 0.5596 & 1.0406 & 0.2246 \end{bmatrix}$$

Therefore, by using equation (23), the normalized coordinates of $\underline{s}_0$ are

$$\underline{s}_0 = \begin{bmatrix} 0.382 \\ 1.031 \\ 0.060 \end{bmatrix} \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix}$$

The coordinates are clearly inside the region of investigation. Moreover, the amount of CO_2 adsorbed at $\underline{s}_0$ is estimated to be $\hat{y}_0 = 6.7780$ grams. As the analysis is continued, the eigenvalues of B are found to be $\lambda_1 = -0.4820$, $\lambda_2 = -0.7347$, and $\lambda_3 = -1.3000$ and thus the canonical form of the prediction equation is

$$\hat{y} = 6.7780 - 0.4820w_1^2 - 0.7347w_2^2 - 1.300w_3^2 \tag{29}$$

Since all eigenvalues are negative, the amount of CO_2 adsorbed at $\underline{s}_0$ is maximum. In terms of natural units, therefore, maximum CO_2 adsorption occurs at a velocity of 54.45 m/min, a CO_2 partial pressure of 17.5 mm Hg, and a plate temperature of 14.48° C. From equation (29), it is apparent that the amount of CO_2 adsorbed, away from $\underline{s}_0$, is more sensitive to change in either w_2 or w_3 than in w_1.

CONCLUDING REMARKS

Before scientific and engineering measurements are made for determining empirical relationships between variables of interest, it is always advantageous to devote considerable effort to identifying such things as what is to be measured, where it should be measured, and how much is to be measured. The validity of the derived empirical model ultimately depends on such considerations. Therefore, by considering two low-order polynomial models, the essence of this report is to bring forth criteria necessary for well-planned experimental tests. In fact, the techniques described in this report are not only

essentially optimal in the sense of yielding prediction equations which minimize the error between a measured and a predicted response but are also economical in that they require a relatively small number of measurements.

Langley Research Center,
      National Aeronautics and Space Administration,
            Hampton, Va., October 26, 1972.

APPENDIX

PROOF OF THEOREM OF EQUATION (8)

The theorem of equation (8), which is to be proved, is stated as follows: If the design matrix X is selected such that each column of X is mutually orthogonal to every other column in X, then the first-order approximation to the response surface is optimal in the sense that the residual variance of a predicted response is minimized.

Consider the determinant of $X'X$. Let a_{hh} be the (h,h) element of $X'X$ and let A_{hh} be the cofactor of a_{hh} in $X'X$. Moreoever, let $A_{ij:hh}$ be the cofactor of a_{ij} in A_{hh} for $i,j \neq h$. Since X is a matrix of full rank $m < n$, the matrix $X'X$ is a positive definite symmetric matrix; thus, consider Cauchy's expansion (ref. 8) of $|X'X|$ given by

$$|X'X| = a_{hh}A_{hh} - \sum_{i=0}^{m}\sum_{j=0}^{m} a_{hi}a_{hj}A_{ij:hh}$$

$$= a_{hh}A_{hh} - Q \qquad (h = 0, 1, 2, \ldots, m; \quad i,j \neq h)$$

where $a_{hh}A_{hh}$ is a scalar and Q is a positive definite quadratic form in a_{hi} for $h \neq i$. Multiplying through by σ^2 and dividing by $|X'X|$ yields

$$\sigma^2 = \frac{\sigma^2(a_{hh}A_{hh})}{|X'X|} - \frac{\sigma^2 Q}{|X'X|} \tag{A1}$$

Since a_{hh} is the hth diagonal element of $X'X$, then a_{hh} is the sum of squares of the elements in the hth column of X. However, these elements are all either -1 or +1; thus, $a_{hh} = n$. Moreover, $\dfrac{A_{hh}}{|X'X|}$ is the hth diagonal element of $(X'X)^{-1}$. Then, by definition,

$$\text{var}\left(\hat{\beta}_h\right) = \frac{\sigma^2 A_{hh}}{|X'X|}$$

where $\hat{\beta}_h$ is the hth component of the estimate vector $\underline{\hat{\beta}}$. Substituting into equation (A1) yields

$$\sigma^2 = n\,\text{var}\left(\hat{\beta}_h\right) - \frac{\sigma^2 Q}{|X'X|}$$

or

$$\text{var}\left(\hat{\beta}_h\right) = \frac{\sigma^2}{n} + \frac{\sigma^2 Q}{n|X'X|} = \frac{\sigma^2}{n}\left(1 + \frac{Q}{|X'X|}\right)$$

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Since $X'X$ is positive definite, $|X'X| > 0$; moreover, since Q is positive definite, the term $\dfrac{Q}{|X'X|}$ can be no smaller than 0. In fact, it can equal 0 only when all the off-diagonal elements a_{hi} equal 0 for $h \neq i$. This implies that $X'X$ is a diagonal matrix which, in turn, implies that each column of X is mutually orthogonal with every other column in X. Therefore, $\text{var}(\hat{\beta})$ is minimized when $X'X$ is of the form given by equation (8).

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