SOME PROPERTIES OF THE METHOD OF STEEPEST ASCENT

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CHAPTER I

INTRODUCTION

A fairly common objective in industry is to find that level of the ingredients and operating charcteristics which maximizes or minimizes some characteristic of the end product. For example, a lens maker might be interested in minimizing the coefficient of expansion of the finished lens. He might feel that the decisive factors were the concentration of a particular ingredient , the rate at which the molten glass was allowed to cool, and the length of time the glass was retained in a liquid state before pouring.

Frequently, it is not practical to operate at the particular factor levels which optimizes the end product characteristic of interest. It may be that the cost or time involved is prohibitive. The practical limits on the factors involved define the factor space or the experimental region.

Let the controlled continuous variables, $x_1, x_2, \ldots, x_p$, be the independent factors and let η be the true measure of the characteristic of the end product. η is called the response and is dependent on the variables $x_1, x_2, \ldots, x_p$. Then the statistical model may be written as

$$y = \eta + e \qquad (1.1)$$

where y is the observed response and e is a measure of the failure of the mathematical model to conform to the real world. It will be assumed that $e \sim (0, \sigma^2)$.

In many situations where time and expense are prime considerations, it is imperative to adopt a strategy for approaching an optimal or stationary point in the experimental region using as few experiments as possible. One proposed strategy is the method of steepest ascent put forward as a statistical technique by G. E. P. Box and K. B. Wilson (1)[1] in 1951 . Further descriptions of this technique are given by O. L. Davies (2) and W. C. Cochran and G. M. Cox (3) .

Box and Wilson (1) have shown that the maximum gain in response in proceeding a distance r from a point 0 to a point P in a k-demensional space is achieved approximately by varying the factors in proportion to their first order partial derivatives at 0. The direction thus determined is called the direction of steepest ascent.

In practice, the controlled variables are coded and the direction of steepest ascent estimated in terms of the coded variables. This is done by using the method of least squares to fit a plane to the response surface and using the coefficients of the fitted plane as estimates of the partial derivatives at 0 . It will be shown in Chapter II that these estimates are unbiased. The steepest ascent path is uncoded and further experiments are performed along this path until it is felt that a maximum has been attained. Another set of experiments

[1] Note: ( ) refers to Selected Bibliography.

is run using this point as the design center and the foregoing procedure is repeated. The process is iterated until the experimenter feels that the process is being run in the proximity of a stationary point.

In chapter II some theorems regarding the estimation of the coefficients of the fitted plane will be presented. The content of a number of these theorems is no doubt known to experimenters but do not seem to have been formalized. Also an examination will be made of the relationship between variance, bias, mean square error, and spread of the points in the design. A design size is suggested so as to minimize the mean square error.

In chapter III a number of theorems regarding the path of steepest ascent will be presented. An interesting property of invariance of the steepest ascent line will be examined and a number of theorems involving the gradient line will also be given. Since the gradient to the factor space contours does not involve error, the study obviously suffers to the extent that the mathematical model fails to represent the experimental situation. In spite of this drawback, it is felt that some of the results will provide the experimenter with additional insight.

When the direction of steepest ascent in the coded variables is transformed to the uncoded variables, it is found that, in general, the resulting direction is no longer normal to the contours. This lack of invariance under a change of scale was noted by Box and Wilson (1) and more recently by O. Kempthorne (4). Chapter IV deals with the effect of the choice of units used in the coding and will examine in some detail the lack of invariance under a change of scale.

CHAPTER II

ESTIMATION OF FIRST ORDER PARTIAL DERIVATIVES AND DESIGN SIZE

Certain terms occur frequently in the ensuing discussion and it is necessary to establish their meaning at the outset.

Definition of Basic Terms

Definition 2.1. The space in which the controlled variables are allowed to vary will be called the factor space.

A point in the factor space will be denoted by $x = (x_1, x_2, \ldots, x_p)$. It will be assumed throughout that the experimenter can attain the point x without error.

Definition 2.2. The true response at a point x will be denoted by $\eta(x_1, x_2, \ldots, x_p)$ or more commonly by η.

The symbol η will always be taken as a polynomial in the variables $x_1, x_2, \ldots, x_p$. For example, the true response might be assumed to be quadratic, in which case η would have the form,

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{22} x_2^2 . \qquad (2.1)$$

Definition 2.3. The observed response at the point x will simply be called the "response" and will be denoted by y.

The response y is a measurable quantity the magnitude of which depends on the particular value of x. For example, a bacteriologist might be concerned with the effect of temperature and humidity on the bacteria count in a culture In this case the factors are temperature and humidity while the response is the number of bacteria expressed in appropriate units.

Definition 2.4. The random error, denoted by e, is the difference between the true response and the observed response.

The random errors will be assumed to be independent of each other, to have a mean of 0, and a variance of σ^2.

In conformance with definitions 2.2, 2.3, and 2.4, y, η, and e are related by the equation

$$y = \eta + e . \qquad (2.2)$$

When it is necessary to distinguish between responses at different points or to fix attention at a particular point in the factor space, the subscript i will be used. In this event, (2.2) is written as

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_{11} x_{1i}^2 + \beta_{12} x_{1i} x_{2i} + \beta_{22} x_{2i}^2 + e_i . \qquad (2.3)$$

In matrix notation this may be written as

$$y = (1,\ x_1,\ x_2,\ x_1^2,\ x_1x_2,\ x_2^2) \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_{11} \\ \beta_{12} \\ \beta_{22} \end{pmatrix} + e \qquad (2.4)$$

or more compactly by

$$y = X\beta + e . \qquad (2\ 5)$$

Many times it is desirable to consider concurrently a number of points in the factor space together with the associated responses and random errors. For this purpose the vector concept is well suited. N responses corresponding to N points in the factor space together with the N random errors may be summarized by the matrix equation

$$\begin{pmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_N \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{p1} \\ 1 & x_{12} & \cdots & x_{p2} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 1 & x_{1N} & \cdots & x_{pN} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \cdot \\ \cdot \\ \cdot \\ \beta_{pN} \end{pmatrix} + \begin{pmatrix} e_1 \\ e_2 \\ \cdot \\ \cdot \\ \cdot \\ e_N \end{pmatrix} \qquad (2.6)$$

or more compactly by

$$Y = X\beta + E . \qquad (2.7)$$

The matrix X as displayed in (2.6) shows at a glance the configuration of the points in the factor space. When the dimension of the matrix X is not apparent from the context it will be indicated.

Definition 2.5. The matrix X as displayed in (2.6) will be known as the design matrix for the assumed model.

Estimation of the First Order Partials

The method of steepest ascent calls for experimentation in a direction which is determined by the estimates of the first order partial derivatives of η evaluated at the origin. From a geometrical standpoint, this is equivalent to fitting a hyperplane to the response surface over some small initial region in the factor space and proceeding in a direction determined by the coefficients of the fitted plane. This strategy has an intuitive appeal for the type of responses likely to be encountered in practice.

In the case of quadratic type responses, the type about which this thesis is chiefly concerned, the design matrix may be chosen so that the first order partials are estimated readily without bias.

Definition 2.6. The response predicted at a point x by means of a hyperplane fitted from a design by the method of least squares will be denoted by $\hat{y}$.

The response predicted by means of a plane at a point $x = (x_1, x_2)$ is

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 \quad . \tag{2.8}$$

The question of what type of design to use in order to estimate the partial derivatives is an important one. It is especially desirable to have estimates which are unbiased and the ensuing discussion sheds light upon why factorial designs are a common choice for this purpose.

The X and β matrices of (2.7) may be partitioned into their constant, linear, and quadratic parts. Y may be written

$$Y = X_0 B_0 + X_1 B_1 + X_2 B_2 + E \qquad (2.9)$$

where

$$B_0 = 1, \quad B_1 = \begin{vmatrix} \beta_1 \\ \beta_2 \end{vmatrix}, \quad B_2 = \begin{vmatrix} \beta_{11} \\ \beta_{12} \\ \beta_{22} \end{vmatrix},$$

$$X_0 = \begin{vmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{vmatrix} \qquad X_1 = \begin{pmatrix} x_{11} & x_{21} \\ x_{12} & x_{22} \\ \cdot & \\ \cdot & \\ \cdot & \\ x_{1N} & x_{2N} \end{pmatrix} \text{and } X_2 = \begin{pmatrix} x_{11}^2 & x_{11}x_{21} & x_{21}^2 \\ x_{12}^2 & x_{12}x_{22} & x_{22}^2 \\ \cdot & & \\ \cdot & & \\ \cdot & & \\ x_{1N}^2 & x_{1N}x_{2N} & x_{2N}^2 \end{pmatrix}.$$

In matrix notation, the fitted plane is

$$\hat{y} = \hat{B}_0 + X_1 \hat{B}_1 \qquad (2.10)$$

where

$$\hat{B}_1 = (X_1' X_1)^{-1} X_1' Y . \qquad (2.11)$$

Now

$$E(\hat{B}_1) = (X_1'X_1)^{-1} X_1'(X_0B_0 + X_1B_1 + X_2B_2 + E) \qquad (2.12)$$

or

$$E(\hat{B}_1) = (X_1'X_1)^{-1} X_1'X_0B_0 + B_1 + (X_1'X_1)^{-1} X_1'X_2B_2 . \qquad (2.13)$$

Hence if $X_1' X_0 = \phi$ and $X_1'X_2 = \phi$, then $E(\hat{B}_1) = B_1$ and $\hat{B}_1$

will be an unbiased estimate of B_1. Factorial designs enjoy the property that $X_1'X_0 = \phi$ and $X_1'X_2 = \phi$ if the variables are properly coded. Also it is well known from least squares theory that the variance-covariance matrix of $\hat{B}_1$ is the same whether the quadratic terms are present or not.

Definition 2.7. A factorial design whose points form a 2-dimensional factor space will be called a rectangular grid, a square grid, or a unit grid according as the factor points form a rectangle, a square, or a unit square. If the length of the side of the square grid is $2h$, the grid will be said to be of size h.

Theorem 2.1. Let $y = \eta + e$ where

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{22} x_2^2 \qquad (2.14)$$

and let

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 \qquad (2.15)$$

be fitted from a rectangular grid whose center is at (0, 0).
Then if $e = 0$,

$$\left.\frac{\partial \eta}{\partial x_i}\right|_{(0,\,0)} = \hat{\beta}_i \,. \qquad i = 1, 2$$

Proof: Let the design matrix be

$$X = \begin{vmatrix} 1 & -h & -k \\ 1 & -h & k \\ 1 & h & -k \\ 1 & h & k \end{vmatrix} . \qquad (2.16)$$

Then by least squares,

$$\begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \text{diag.}\left(\frac{1}{4}, \frac{1}{4h^2}, \frac{1}{4k^2}\right) \begin{pmatrix} 1 & 1 & 1 & 1 \\ -h & -h & h & h \\ -k & k & -k & k \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} \qquad (2.17)$$

so that

$$\hat{\beta}_1 = \frac{1}{4h^2} \cdot h\,(4h\,\beta_1) = \beta_1$$

and

$$\hat{\beta}_2 = \frac{1}{4k^2} \cdot k\,(4k\,\beta_2) = \beta_2 . \qquad (2.18)$$

Now

$$\frac{\partial \eta}{\partial x_1} = \beta_1 + 2\beta_{11}x_1 + \beta_{12}x_2$$

and

$$\frac{\partial \eta}{\partial x_2} = \beta_2 + \beta_{12}x_1 + 2\beta_{22}x_2 \qquad (2.19)$$

which at (0, 0) reduce to

$$\frac{\partial \eta}{\partial x_1} = \beta_1 \quad \text{and} \quad \frac{\partial \eta}{\partial x_2} = \beta_2 . \qquad (2.20)$$

The question naturally arises as to whether the coefficients of the plane fitted without error are equal to the first order partials at an arbitrary point other than (0, 0). That the answer is in the affirmative is the content of theorem 2.2.

Theorem 2.2. Let y and $\hat{y}$ be as in (2.14) and (2.15) respectively and let $\hat{y}$ be fitted from a rectangular grid with center at (x_1^0, x_2^0). Then if $e = 0$,

$$\frac{\partial \eta}{\partial x_i}\bigg|_{(x_1^0,\, x_2^0)} = \hat{\beta}_i . \qquad i = 1, 2 .$$

Proof: Let the design matrix be

$$X = \begin{pmatrix} 1 & x_1^0-h & x_2^0-k \\ 1 & x_1^0-h & x_2^0+k \\ 1 & x_1^0+h & x_2^0-k \\ 1 & x_1^0+h & x_2^0+k \end{pmatrix} . \qquad (2.21)$$

Translate the center of the design to the origin by means of the translation

$$x_1' = x_1 - x_1^0$$
$$x_2' = x_2 - x_2^0 . \qquad (2.22)$$

Solving for x_1 and x_2 in (2.22) and substituting in (2.14), there results

$$\eta = \beta_0' + \beta_1'x_1' + \beta_2'x_2' + \beta_{11}'x_1'^2 + \beta_{12}'x_1'x_2' + \beta_{22}'x_2'^2 \qquad (2.23)$$

where

$$\beta_1' = \beta_1 + 2\beta_{11}x_1^0 + \beta_{12}x_2^0$$

and

$$\beta_2' = \beta_2 + \beta_{12}x_1^0 + 2\beta_{22}x_2^0 . \qquad (2.24)$$

The design (2.21) becomes the design (2.16) and hence, by theorem 2.1,

$$\hat{\beta}_1' = \beta_1' \text{ and } \hat{\beta}_2' = \beta_2' . \qquad (2.25)$$

If the partial derivatives (2.19), be evaluated at the point (x_1^0, x_2^0), the result is the right side of (2.24).

In the presence of error, the coefficients of the fitted plane are not equal to the first order partial derivatives evaluated at the center of the design. However, that the first order partial derivatives are estimated without bias by the linear fitted coefficients will be shown in theorems 2.3 and 2.4 .

<u>Theorem 2.3 .</u> Let $\hat{y}$ be fitted by a rectangular grid whose center is at (0, 0) . Then

$$E(\hat{\beta}_i) = \left.\frac{\partial \eta}{\partial x_i}\right|_{(0,\,0)} . \qquad i = 1, 2$$

Proof: From theorem 2.1, it is known that

$$\left.\frac{\partial \eta}{\partial x_i}\right|_{(0,\,0)} = \beta_i . \qquad i = 1, 2$$

It remains to show that $E(\hat{\beta}_i) = \beta_i$ but this is the content of equation (2.13) .

That the first order partial derivatives are estimated without bias at an arbitrary point is the content of theorem 2.4.

Theorem 2.4. Let y be fitted by means of a rectangular grid whose center is at the point (x_1^0, x_2^0). Then

$$E(\hat{\beta}_i) = \left. \frac{\partial \eta}{\partial x_i} \right|_{(x_1^0,\, x_2^0)} . \qquad i = 1, 2$$

Proof: The proof is accomplished by a translation to the origin as in theorem 2.2 followed by the application of theorem 2.3.

Frequently in what is to follow the response will be considered without error and the linear coefficients of the fitted plane will be used on that basis. Although in practice there will always be error, theorems 2.2 and 2.4 are comforting in that the linear coefficients are estimated without bias when error is taken into account.

Definition 2.8. The line through the center of the design in a direction determined by the fitted plane in the presence of error will be called the steepest ascent line.

For example, for two variables x_1 and x_2, the fitted plane has the form

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2$$

and the steepest ascent line through the origin is

$$x_2 = \frac{\hat{\beta}_2}{\hat{\beta}_1} x_1 . \qquad (2.26)$$

<u>Definition 2.9.</u> The line through a point in a direction determined by the first order partial derivatives at that point will be called the gradient line.

The gradient line through the origin for a quadratic surface is

$$x_2 = \frac{\beta_2}{\beta_1} x_1 . \qquad (2.27)$$

Responses at the Points of a Square Grid

Consider the response

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

$$= \beta_0 + (x_1, x_2)\begin{pmatrix}\beta_1 \\ \beta_2\end{pmatrix} + (x_1, x_2)\begin{pmatrix}\beta_{11} & \beta_{12/2} \\ \beta_{12/2} & \beta_{22}\end{pmatrix}\begin{pmatrix}x_1 \\ x_2\end{pmatrix} + e$$

$$= B_0 + ZB_1 + ZB_2Z' + e \qquad (2.28)$$

where $Z = (x_1, x_2)$, $B_0 = \beta_0$, $B_1 = \begin{pmatrix}\beta_1 \\ \beta_2\end{pmatrix}$

and $B_2 = \begin{pmatrix}\beta_{11} & \beta_{12/2} \\ \beta_{12/2} & \beta_{22}\end{pmatrix}$.

In this notation the predicted response of equation (2.8),

$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2$, becomes $\hat{y} = \hat{B}_0 + Z\hat{B}_1$. (2.29)

Now let $B_2 = I_2$ and suppose that the responses y_1, y_2, y_3, and y_4 are measured without error at the grid points $(-h, -h)$, $(-h, h)$, $(h, -h)$ and (h, h). Then at any of these grid points the response as given in (2. 28) may be written as

$$y = B_0 + ZB_1 + 2h^2 . \qquad (2.30)$$

According to least squares

$$\hat{\beta}_0 = 1/4(y_1 + y_2 + y_3 + y_4) = 1/4(4B_0 + 4ZI_2Z') = B_0 + 2h^2 . \qquad (2.31)$$

Also, since the responses are measured without error, $\hat{B}_1 = B_1$ so that equation (2. 29) becomes

$$\hat{y} = B_0 + 2h^2 + ZB_1 \qquad (2.32)$$

which is seen to be the same as y. If the center of the grid is not at the origin, a translation of the axes to the center of the grid results in new variables for which again $y = \hat{y}$ at the grid points. These results are summarized in theorem 2. 5 .

<u>Theorem 2. 5 .</u> Let y be measured without error and be given by (2. 28) wherein $B_2 = I_2$. Then the least squares plane passes through the responses at the points of a square grid.

Suppose now that the matrix B_2 is allowed to be of the form

$$B_2 = \begin{pmatrix} b_{11} & 0 \\ 0 & b_{22} \end{pmatrix}$$ so that the circular contours considered in theorem 2. 5 become elliptical.

Theorem 2.6. Let y be measured without error and be given by (2.28) wherein $B_2 = \text{diag.}(b_{11}, b_{22})$. Then the least squares plane passes through the responses at the points of a square grid.

Proof: The responses at the grid points are given by

$$y = B_0 + ZB_1 + h^2 b_{11} + h^2 b_{22}. \qquad (2.33)$$

Now

$$\hat{B}_0 = 1/4(y_1 + y_2 + y_3 + y_4) = 1/4(4B_0 + 4ZB_2Z')$$

$$= 1/4[4B_0 + 4(h^2 b_{11} + h^2 b_{22})] = B_0 + h^2 b_{11} + h^2 b_{22}. \qquad (2.34)$$

Since $\hat{B}_1 = B_1$,

$$\hat{y} = B_0 + h^2 b_{11} + h^2 b_{22} + ZB_1 \qquad (2.35)$$

so that on the grid points, $y = \hat{y}$.

It can be readily verified that $y \neq \hat{y}$ when the matrix B_2 has off-diagonal elements. Theorems 2.5 and 2.6 can both be generalized but since 2.5 is a special case of 2.6 it will suffice to generalize the latter.

Theorem 2.7. Let y be measured without error and be of the form $y = \eta + e$ where $\eta = B_0 + ZB_1 + ZB_2Z'$ (2.36) and where the dimensions of B_0, Z, B_1, and B_2 are respectively 1×1, $1 \times p$, $p \times 1$ and $p \times p$. Let $B_2 = \text{diag.}(b_{11}, b_{22}, \ldots, b_{pp})$.

Then the least squares hyperplane, $\hat{y} = \hat{B}_0 + Z\hat{B}_1$, passes through the responses at the points of a p-dimensional square grid.

Proof: The responses at the grid points are given by

$$y = B_0 + ZB_1 + h^2(b_{11} + b_{22} + \ldots + b_{pp}) . \qquad (2.37)$$

Now

$$\hat{\beta}_0 = 1/N(y_1 + y_2 + \ldots + y_N) = 1/N(NB_0 + NZB_2Z')$$

$$= B_0 + h^2(b_{11} + b_{22} + \ldots + b_{pp}) \qquad (2.38)$$

where $N = 2^p$.

Since $\hat{B}_1 = B_1$,

$$\hat{y} = B_0 + h^2(b_{11} + b_{22} + \ldots + b_{pp}) + ZB_1 = y .$$

This relationship between the least squares plane fitted from the grid points and the responses at these points is surprising. It is remarkable that the responses at the grid points should lie in a plane. Apparently the grid points in the factor space are members of a set of points for which the response is the same as the predicted response. What is the locus of these points in the factor space? Evidently the answer may be found by setting $y = \hat{y}$. In order to visualize the geometry, consider the two dimensional case of theorem 2.6 with b_{11} and b_{22} replaced by β_{11} and β_{22}. Then $\{x_1, x_2 \mid y = \hat{y}\}$ satisfies the equation

$$\beta_{11}x_1^2 + \beta_{22}x_2^2 = h^2(\beta_{11} + \beta_{22}) \qquad (2.39)$$

which may be written as

$$\frac{x_1^2}{\frac{h^2(\beta_{11}+\beta_{22})}{\beta_{11}}} + \frac{x_2^2}{\frac{h^2(\beta_{11}+\beta_{22})}{\beta_{22}}} = 1 . \qquad (2.40)$$

Suppose that the contours are elliptical and that y attains a maximum value at some point in the factor space so that β_{11} and β_{22} are both negative. Then $\{x_1, x_2 \mid y > \hat{y}\}$ lies within the ellipse given in (2. 40) while $\{x_1, x_2 \mid y < \hat{y}\}$ lies outside the ellipse given in (2. 40).

If in (2. 40), $\beta_{11} = \beta_{22}$, (2. 40) may be written as

$$x_1^2 + x_2^2 = 2h^2 \qquad (2.41)$$

which is a circle of radius $\sqrt{2}\,h$. Suppose that an experiment is performed at a non-grid point on this circle. If the observed response, y, and the predicted response, $\hat{y}$, are nearly the same at this point, it indicates that β_{11} and β_{22} are approximately of the same magnitude. If in addition, the experimenter has reason to believe that $\beta_{12} = 0$, then circular contours are indicated.

Choice of Design Size

Suppose that the β's of the fitted plane are estimated by means of a square grid of size h whose center is at (0, 0). Then

$$X = \begin{pmatrix} 1 & -h & -h \\ 1 & -h & h \\ 1 & h & -h \\ 1 & h & h \end{pmatrix} \qquad (2.42)$$

and

$$(X'X)^{-1} = \text{diag.}\left(\frac{1}{4}, \frac{1}{4h^2}, \frac{1}{4h^2}\right)$$

so that var. $\hat{\beta}_1$ = var. $\hat{\beta}_2 = \dfrac{\sigma^2}{4h^2}$.

It would seem advisable to take h as large as possible so as to reduce the variance. However, enlargement of the design, while reducing the variance, generally increases the bias. The failure of the estimator $\hat{y}$ is due to the unavoidable variability of the data and to the inadequacy of the assumed model in representing the true model. A measure which takes into account both of these factors is the mean-square-error, hereafter referred to as m. s. e.

By definition,

$$\text{m.s.e.}\ (\hat{\beta}_1) = E(\hat{\beta}_1 - \beta_1)^2 . \qquad (2.43)$$

This may be written so as to display the relationship between m.s.e., variance and bias as

$$E(\hat{\beta}_1 - \beta_1)^2 = E[\hat{\beta}_1 - E(\hat{\beta}_1)]^2 + [E(\hat{\beta}_1) - \beta_1]^2 \qquad (2.44)$$

where the first term on the right is the var $\hat{\beta}_1$ and the second term is the (bias in $\hat{\beta}_1$)^2 .

The following discussion attempts to give an indication of the grid size required in order to minimize the m.s.e .

Suppose that the experimenter has chosen the model

$$y = \eta + e \tag{2.45}$$

where

$$\eta = \beta_0 + b_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{22} x_2^2 \tag{2.46}$$

but in reality,

$$y = \eta_1 + e \tag{2.47}$$

where

$$\eta_1 = \eta + \beta_{111} x_1^3 . \tag{2.48}$$

Now

$$\begin{pmatrix} \hat\beta_0 \\ \hat\beta_1 \\ \hat\beta_2 \end{pmatrix} = \text{diag.}\left(\frac{1}{4}, \frac{1}{4h^2}, \frac{1}{4h^2} \right) \begin{pmatrix} 1 & 1 & 1 & 1 \\ -h & -h & h & h \\ -h & h & -h & h \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} \tag{2.49}$$

so that

$$E(\hat\beta_1) = \frac{1}{4h}(4h\beta_1 + 4h^3\beta_{111} - e_1 - e_2 + e_3 + e_4) = \beta_1 + h^2\beta_{111} . \tag{2.50}$$

Hence ,

$$(\text{bias in } \hat\beta_1)^2 = [E(\hat\beta_1) - \beta_1]^2 = (\beta_1 + h^2\beta_{111} - \beta_1)^2 = h^4\beta_{111}^2 . \tag{2.51}$$

Substituting the var $\hat\beta_1$ and the (bias in $\hat\beta_1$)^2 into (2.44) there results,

$$\text{m.s.e.}(\hat\beta_1) = \frac{\sigma^2}{4h^2} + h^4\beta_{111}^2 . \tag{2.52}$$

Now β_{111} is generally unknown but may be expressed as

$$\beta_{111} = c\,\sigma^2 \qquad (2.53)$$

and on substitution in (2.52) there results

$$\text{m.s.e.}\,(\hat{\beta}_1) = \frac{\sigma^2}{4h^2} + h^4 c^2 \sigma^4 . \qquad (2.54)$$

Differentiating (2.54) with respect to h and solving for the h which minimizes m.s.e. ($\hat{\beta}_1$) ,

$$\frac{d\ \text{m.s.e.}}{dh}\,(\hat{\beta}_1) = -\frac{2\sigma^2}{4h^3} + 4h^3 c^2 \sigma^4 = 0 \qquad (2.55)$$

and

$$h = \frac{\sqrt{2}}{2\,(c\sigma)^{1/3}} . \qquad (2.56)$$

If (2.56) is differentiated with respect to h the result is

$$\frac{d^2\ \text{m.s.e.}\,(\hat{\beta}_1)}{dh^2} = \frac{3\sigma^2}{2}\,h^{-4} + 12\,h^2 c^2 \sigma^4 . \qquad (2.57)$$

Since all of the exponents are even, (2.57) is positive which insures that the h of (2.56) minimizes the m.s.e. ($\hat{\beta}_1$) .

Now suppose that instead of (2.47), the actual response has the form

$$y = \eta_2 + e \qquad (2.58)$$

where

$$\eta_2 = \eta + \beta_{222} x_2^3 . \qquad (2.59)$$

In this case, it is readily verified that $E(\hat{\beta}_1) = \beta_1$ so that $(\text{bias in } \hat{\beta}_1) = 0$.

The use of similar calculations produces Table I. Table I is a summary of the values of h required to minimize the associated mean square errors in the presence of all possible combinations of cubic terms. These combinations are listed in the far left column. In this column the number 1 stands for $\beta_{111} x_1^3$, 2 for $\beta_{222} x_2^3$, 3 for $\beta_{112} x_1^2 x_2$ and 4 for $\beta_{122} x_1 x_2^2$. With this coding the mixture $\beta_{111} x_1^3 + \beta_{112} x_1^2 x_2 + \beta_{122} x_1 x_2^2$ is written simply as 1, 3, 4 .

TABLE I

DESIGN SIZE NECESSARY TO MINIMIZE M. S. E. $\hat{\beta}_1$

Cubic Terms	M. S. E. $\hat{\beta}_1$	(Bias in $\hat{\beta}_1)^2$	h to min M.S.E.
1	$\sigma^2/4h^2 + h^4\beta_{111}^2$	$h^4\beta_{111}^2$	$\sqrt{2}/2(c\sigma)^{1/3}$
2	$\sigma^2/4h^2$	0	h large
3	$\sigma^2/4h^2$	0	h large
4	$\sigma^2/4h^2 + \beta_{122}^2 h^4$	$h^4\beta_{122}^2$	$\frac{\sqrt{2}}{2(c\sigma)^{1/3}}$
1, 2	$\sigma^2/4h^2 + h^4\beta_{111}^2$	$h^4\beta_{111}^2$	$\frac{\sqrt{2}}{2(c\sigma)^{1/3}}$
1, 3	$\sigma^2/4h^2 + h^4\beta_{111}^2$	$h^4\beta_{111}^2$	$\frac{\sqrt{2}}{2(c\sigma)^{1/3}}$
1, 4	$\sigma^2/4h^2 + h^4(\beta_{111}+\beta_{122})^2$	$h^4(\beta_{111}+\beta_{122})^2$	$\frac{2^{1/6}}{2(c\sigma)^{1/3}}$
2, 3	$\sigma^2/4h^2$	0	h large
2, 4	$\sigma^2/4h^2 + \beta_{122}^2 h^4$	$h^4\beta_{112}^2$	$\frac{\sqrt{2}}{2(c\sigma)^{1/3}}$
3, 4	$\sigma^2/4h^2 + \beta_{122}^2 h^4$	$h^4\beta_{112}$	$\frac{\sqrt{2}}{2(c\sigma)^{1/3}}$
1, 2, 3	$\sigma^2/4h^2 + h^4\beta_{111}^2$	$h^4\beta_{111}^2$	$\frac{\sqrt{2}}{2(c\sigma)^{1/3}}$
1, 2, 4	Like 1, 4		
1, 3, 4	Like 1, 4		
2, 3, 4	Like 4		
1, 2, 3, 4	Like 1, 4		

CHAPTER III

PROPERTIES OF THE METHOD OF STEEPEST ASCENT

In accordance with the method of steepest ascent, an initial set of experiments are performed in order to determine the steepest ascent path. Additional experiments are performed at points along the path until it is felt that further appreciable gain cannot be realized. No use is made of information available at these points other than to decide whether or not additional experimentation should be carried on along the path.

Now it would seem that an acceptable strategy would be to run the first additional point somewhere on the steepest ascent line and use this point together with the original design points to calculate a new path of steepest ascent. This process could be repeated, altering the path on the basis of information obtained at each additional point. The rather surprising fact for certain designs is that, if additional points are taken on the path and used together with the original points to calculate a new path, the new path turns out to be the same as the original one. This result will be proved after the introduction of formulae which simplify the calculation of the path based on additional points.

An Invariance Property of the Steepest Ascent Path

Suppose that N_1 initial observations are taken at points in the factor space where the response is given by $y = \eta + e$ where η is quadratic in the p variables, $x_1, x_2, \ldots, x_p$. In matrix notation the N_1 responses at the N_1 design points can be written

$$Y_1 = X_1 \beta + E_1 \qquad (3.1)$$

where X_1 is the $N_1 \times q$ design matrix, q is the number of parameters in the model, β is a $q \times 1$ vector of unknown parameters, E_1 is an $N_1 \times 1$ vector of random errors, and Y_1 is the $N_1 \times 1$ vector of responses. Let

$$\hat{y} = X \hat{\beta} \qquad (3.2)$$

be the least squares prediction of y based on the initial design X_1.

Now suppose that N_2 additional observations are taken. Denote the associated $N_2 \times q$ design matrix by X_2 and the response vector by Y_2. Let X and Y be the design matrix and response vector associated with the $N_1 + N_2 = N$ observations and let $\hat{\alpha}$ be the least-squares estimate of $\hat{\beta}$ where $\hat{\alpha}$ is based upon all of the N observations. Further let

$$(X_1' X_1) = S_1$$

$$(X_2' X_2) = S_2$$

$$(X' X) = S. \qquad (3.3)$$

Then

$$S^{-1} = \left((X_1', X_2') \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \right)^{-1} = (X_1'X_1 + X_2'X_2)^{-1} = (S_1 + S_2)^{-1}$$

$$= \left((I + S_2 S_1^{-1}) S_1 \right)^{-1} = S_1^{-1}(I + S_2 S_1^{-1})^{-1} = S_1^{-1}(I + X_2' X_2 S_1^{-1})^{-1}. \tag{3.4}$$

Now by using the relationship

$$(I + AB)^{-1} = I - A(I + BA)^{-1} B \tag{3.5}$$

in (3.4) and associating X_2' with A and $X_2 S_1^{-1}$ with B, there results

$$S^{-1} = S_1^{-1} - S_1^{-1} X_2' (I + X_2 S_1^{-1} X_2')^{-1} X_2 S_1^{-1} . \tag{3.6}$$

Now let

$$J = X_2 S_1^{-1}$$

$$R = X_2 S_1^{-1} X'_2$$

$$G = (I + R)^{-1}$$

$$Q = Y_2 - X_2 \hat{\beta} . \tag{3.7}$$

Then (3.6) may be written

$$S^{-1} = S_1^{-1} - J'GJ . \tag{3.8}$$

Now

$$\hat{\alpha} = S^{-1} X' Y = (S_1^{-1} - J'GJ)(X_1', X_2') \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}$$

$$= (S_1^{-1} - J'GJ)(X_1'Y_1 + X_2'Y_2)$$

$$= S_1^{-1}X_1'Y_1 + S_1^{-1}X_2'Y_2 - J'GJX_1'Y_1 - J'GJX_2'Y_2 . \qquad (3.9)$$

The second term of (3.9) may be written

$$S_1^{-1}X_2'Y_2 = J'Y_2 = J'GG^{-1}Y_2 = J'G(I + JX_2')Y_2 = J'GY_2 + J'GJX_2'Y_2 . \qquad (3.10)$$

Substituting (3.10) in (3.9) there results

$$\hat{\alpha} = \hat{\beta} + J'GY_2 - J'GX_2\hat{\beta} = \hat{\beta} + J'G(Y_2 - X_2\hat{\beta}) = \hat{\beta} + J'GQ. \qquad (3.11)$$

The advantage in using (3.8) and (3.11) is that in finding S^{-1} and $\hat{\alpha}$, the dimension of the matrix (I + R) which must be inverted is $N_2 \times N_2$. These expressions can be used profitably whenever N_2 is less than q.

The method for finding $\hat{\alpha}$ and S^{-1} based on new observations with a minimum of calculation was set forth by R. L. Plackett (5) and the expressions for $\hat{\alpha}$ and S but not their derivation, are to be found in (1) .

Theorem 3.1. Let a unit grid with center at the origin be used to determine the steepest ascent line $x_2 = \frac{\hat{\beta}_2}{\hat{\beta}_1} x_1$. If a second steepest ascent line, $x_2 = \frac{\hat{\alpha}_2}{\hat{\alpha}_1} x_1$ is determined by means of the initial grid and an additional point on the first line, the second line will be the same as the first line.

Proof: The grid design is given as

$$X_1 = \begin{pmatrix} 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} \qquad (3.12)$$

and the fifth point may be taken as

$$X_2 = (1, h\hat{\beta}_1, h\hat{\beta}_2) . \qquad (3.13)$$

Now by (3.11)

$$\hat{\alpha} = \hat{\beta} + J'GQ$$

and since in the present application $N_2 = 1$, both G and Q are scalars. Now

$$J' = S_1^{-1}X_2' = \frac{1}{4}I_3X_2' = \frac{1}{4}X_2' \qquad (3.14)$$

so that

$$\begin{pmatrix} \hat{\alpha}_0 \\ \hat{\alpha}_1 \\ \hat{\alpha}_2 \end{pmatrix} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 1 \\ h\hat{\beta}_1 \\ h\hat{\beta}_2 \end{pmatrix} GQ . \qquad (3.15)$$

It follows that

$$\hat{\alpha}_0 = \hat{\beta}_0 + \frac{1}{4}GQ = \hat{\beta}_0\left(1 + \frac{GQ}{4\beta_0}\right)$$

$$\hat{\alpha}_1 = \hat{\beta}_1 + \frac{1}{4}h\hat{\beta}_1 GQ = \hat{\beta}_1\left(1 + \frac{hGQ}{4}\right)$$

$$\hat{\alpha}_2 = \hat{\beta}_2 + \frac{1}{4} h \hat{\beta}_2 GQ = \hat{\beta}_2 (1 + \frac{hGQ}{4}) . \quad (3.16)$$

Hence

$$\frac{\hat{\alpha}_2}{\hat{\alpha}_1} = \frac{\hat{\beta}_2}{\hat{\beta}_1} \quad (3.17)$$

so that $x_2 = \frac{\hat{\beta}_2}{\hat{\beta}_1} x_1$ is the same line as $x_2 = \frac{\hat{\alpha}_2}{\hat{\alpha}_1} x_1$.

It is to be noted that the proportionality of the coefficients in the last proof did not extend to $\hat{\beta}_0$ and $\hat{\alpha}_0$. The factor h was not specified and it may be seen from (3.15) or (3.16) that if h is chosen so that

$$h \hat{\beta}_0 = 1 , \quad (3.18)$$

then (3.15) becomes

$$\hat{\alpha} = \hat{\beta} + \frac{1}{4} h GQ \hat{\beta} = (I + \frac{1}{4} h GQ)\hat{\beta} \quad (3.19)$$

from which it is apparent that the proportionality property does extend to $\hat{\alpha}_0$ and $\hat{\beta}_0$.

The magnitude of h determines the step size taken along the steepest ascent line. Apparently the choice of h as given by (3.18) has no particular merit other than simplifying the calculations.

<u>Definition 3.1.</u> If the second steepest ascent line is the same as the first, the steepest ascent line will be said to be invariant. Thus the mathematical expression of invariance is

$$\frac{\hat{\alpha}_j}{\hat{\alpha}_i} = \frac{\hat{\beta}_j}{\hat{\beta}_i}, \quad i, \ j = 1, 2, \ldots, p \qquad (3.20)$$

Theorem 3.1 proves the property of invariance for $p = 2$. It is natural to inquire if invariance holds in p-dimensional space in general. That it does for certain designs is affirmed in theorem 3.2.

Theorem 3.2. Let $\hat{\beta}$ be determined from the $2^p = N_1$ points of a p-dimensional unit grid design with center at the origin. Let $\hat{\alpha}$ be determined from these points and the additional point $X_2 = (1, h\hat{\beta}_1, \ldots, h\hat{\beta}_p)$. Then

$$\frac{\hat{\beta}_j}{\hat{\beta}_i} = \frac{\hat{\alpha}_j}{\hat{\alpha}_i}, \quad i, \ j = 1, 2, \ldots, p.$$

Proof:

$$(X_1'X_1)^{-1} = \frac{1}{N_1} I_{p+1} \quad \text{so that}$$

$$J' = \frac{1}{N_1} I_{p+1} \ X_2' = \frac{1}{N_1} \begin{pmatrix} 1 \\ h\hat{\beta}_1 \\ \cdot \\ \cdot \\ \cdot \\ h\hat{\beta}_p \end{pmatrix}.$$

Now by (3.11), $\hat{\alpha} = \hat{\beta} + J'GQ$ and since $N_2 = 1$, G and Q are scalars. Substituting in (3.11) there results

$$\begin{pmatrix} \hat{\alpha}_0 \\ \hat{\alpha}_1 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\alpha}_p \end{pmatrix} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\beta}_p \end{pmatrix} + \frac{GQ}{N_1} \begin{pmatrix} 1 \\ h\hat{\beta}_1 \\ \cdot \\ \cdot \\ \cdot \\ h\hat{\beta}_p \end{pmatrix} \qquad (3.21)$$

so that

$$\hat{\alpha}_i = \left(1 + \frac{GQh}{N_1}\right) \hat{\beta}_i \qquad i = 1, 2, \ldots, p.$$

from which (3. 20) follows.

The relationship between the design matrix, the additional points, and the invariance property is given in theorem 3. 3 . Consider the following conditions:

(a) $$\frac{\hat{\alpha}_j}{\hat{\alpha}_i} = \frac{\hat{\beta}_j}{\hat{\beta}_i} \qquad i, j = 1, 2, \ldots, p$$

(b) $$X_2 = (1, h\hat{\beta}_1, h\hat{\beta}_2, \ldots, h\hat{\beta}_p)$$

(c) $$(X_1'X_1)^{-1} = \begin{pmatrix} u & 0 \\ 0 & vI_p \end{pmatrix} .$$

Condition (a) is the mathematical statement of invariance. Condition (b) insures that X_2 is in the direction of steepest ascent while condition (c) deals with the form of the design matrix.

<u>Theorem 3. 3 .</u> Any two of the above three conditions implies the third.

Proof: Let $\hat{\alpha}$, $\hat{\beta}$, S_1^{-1}, and X_2 be partitioned as indicated.

$$\hat{\alpha} = \begin{pmatrix} \hat{\alpha}_0 \\ \hline \hat{\alpha}_1 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\alpha}_p \end{pmatrix} = \begin{pmatrix} A_0 \\ A_1 \end{pmatrix}, \qquad \hat{\beta} = \begin{pmatrix} \hat{\beta}_0 \\ \hline \hat{\beta}_1 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\beta}_p \end{pmatrix} = \begin{pmatrix} B_0 \\ B_1 \end{pmatrix},$$

$$S_1^{-1} = \left(\begin{array}{c|ccccc} u & 0 & 0 & \cdots & 0 \\ \hline 0 & v & 0 & \cdots & 0 \\ 0 & 0 & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ 0 & 0 & \cdot & \cdots & v \end{array}\right) = \begin{bmatrix} u & 0 \\ 0 & vI_p \end{bmatrix}, \qquad (3.22)$$

and

$$X_2 = (1 \ \ h\hat{\beta}_1 \ \ldots \ h\hat{\beta}_p) = (X_{20}, X_{21}) = (1, h B_1') .$$

To prove that (b) and (c) imply (a), the equation $\hat{\alpha} = \hat{\beta} + J'GQ$ is written using the above partitions as

$$\begin{pmatrix} A_0 \\ A_1 \end{pmatrix} = \begin{pmatrix} B_0 \\ B_1 \end{pmatrix} + \begin{pmatrix} u & 0 \\ 0 & vI_p \end{pmatrix} \begin{pmatrix} 1 \\ hB_1 \end{pmatrix} GQ . \qquad (3.23)$$

On equating corresponding members and using the values indicated in (3.22), there results

$$A_0 = B_0 + u\,G\,Q \quad \text{and}$$

$$A_1 = B_1 + vI_p hB_1 GQ . \quad (3.24)$$

Now GQ is a scalar so that

$$A_1 = B_1(1 + vh\,GQ) \quad (3.25)$$

from which condition (a) follows.

To prove that (a) and (c) imply (b), by condition (a), A_1 may be written as kB_1. Hence

$$\begin{pmatrix} A_0 \\ kB_1 \end{pmatrix} = \begin{pmatrix} B_0 \\ B_1 \end{pmatrix} + \begin{pmatrix} u & 0 \\ 0 & vI_p \end{pmatrix} \begin{pmatrix} 1 \\ X_{21}' \end{pmatrix} GQ$$

so that

$$A_0 = B_0 + uGQ \quad (3.26)$$

$$kB_1 = B_1 + vI_p X_{21}' GQ . \quad (3.27)$$

It follows from (3.27) that

$$(k - 1)B_1 = GQ\,v\,X_{21}'. \text{ Hence } X_{21} = \frac{k-1}{vGQ} B_1'$$

which indicates that X_{21} is a scalar multiple of B_1' as in condition (b) .

In order to prove that (a) and (b) imply (c) , the symmetric matrix S_1^{-1} is partitioned as

$$S_1^{-1} = \left(\begin{array}{c|cccc} c_{00} & c_{01} & \cdot & \cdot & \cdot\ c_{0p} \\ \hline c_{10} & c_{11} & \cdot & \cdot & \cdot\ c_{1p} \\ \cdot & \cdot & & & \\ \cdot & \cdot & & & \\ \cdot & \cdot & & & \\ c_{p0} & c_{p1} & \cdot & \cdot & \cdot\ c_{pp} \end{array}\right) = \begin{pmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{pmatrix} .$$

Now

$$J = (1,\ hB_1{}') \begin{pmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{pmatrix}$$

so that

$$J' = \begin{pmatrix} c_{00} & c_{01} \\ c_{10} & c_{11} \end{pmatrix} \begin{pmatrix} 1 \\ hB_1 \end{pmatrix} = \begin{pmatrix} C_{00} + C_{01}hB_1 \\ C_{10} + C_{11}h\,B_1 \end{pmatrix}.$$

Hence

$$\begin{pmatrix} A_0 \\ A_1 \end{pmatrix} = \begin{pmatrix} B_0 \\ B_1 \end{pmatrix} + \begin{pmatrix} C_{00} + C_{01}h\,B_1 \\ C_{10} + C_{11}h\,B_1 \end{pmatrix} GQ. \qquad (3.28)$$

On equating corresponding elements of (3. 28) , there results

$$A_0 = B_0 + C_{00}GQ + C_{01}hB_1GQ \qquad (3.29)$$

and

$$A_1 = B_1 + C_{10}GQ + C_{11}hB_1GQ. \qquad (3.30)$$

Now by (a), A_1 may be written as kB_1 so that (3. 30) becomes

$$kB_1 = B_1 + C_{10}GQ + C_{11}hB_1GQ. \qquad (3.31)$$

Since (3. 31) holds for all B_1, $C_{10} = 0$ so that (3. 31) becomes

$$(kI_p - hGQC_{11})B_1 = B_1. \qquad (3.32)$$

It follows that

$$(kI_p - hGQC_{11}) = I_p \qquad (3.33)$$

so that

$$c_{11} = \frac{kI_p - I_p}{hGQ} = \frac{(k-1)I_p}{hGQ}.$$

Hence C_{11} is a diagonal matrix as in condition (c). Since $C_{10} = 0$, the expression for A_0 in (3.29) becomes

$$A_0 = B_0 + C_{00} G Q \tag{3.34}$$

so that

$$C_{00} = \frac{A_0 - B_0}{G Q} . \tag{3.35}$$

Note that if the invariance property is extended to $\hat{\alpha}_0$ and $\hat{\beta}_0$, then $A_0 = k B_0$ and, as in (3.18), $B_0 = 1/h$. Hence (3.35) becomes

$$C_{00} = \frac{k B_0 - B_0}{G Q} = \frac{(k-1) B_0}{GQ} = \frac{k-1}{GQh}$$

which may be recognized as the scalar multiplier of I_p occurring in the expression for C_{11}.

Suppose that instead of just one additional point, N_2 additional points were taken in the steepest ascent direction. Would the new steepest ascent direction based on the original grid and the N_2 additional points be the same as the old? Again the answer is in the affirmative and this is the content of theorem 3.4 .

<u>Theorem 3.4 .</u> Let $\hat{\beta}$ be determined from the $2^p = N_1$ points of a p-dimensional unit grid. Let $\hat{\alpha}$ be determined from the N_1 initial points and N_2 additional points which lie in the steepest ascent direction. Then

$$\frac{\hat{\beta}_j}{\hat{\beta}_i} = \frac{\hat{\alpha}_j}{\hat{\alpha}_i} \qquad i, j = 1, 2, \ldots, p .$$

Proof: The $N_2 \times p+1$ matrix, X_2, may be written and partitioned as

$$X_2 = \left(\begin{array}{c|cccc} 1 & h_1\hat{\beta}_1 & h_1\hat{\beta}_2 & \cdots & h_1\hat{\beta}_p \\ 1 & h_2\hat{\beta}_1 & h_2\hat{\beta}_2 & \cdots & h_2\hat{\beta}_p \\ . & . & . & & . \\ . & . & . & & . \\ . & . & . & & . \\ 1 & h_{N_2}\hat{\beta}_1 & h_{N_2}\hat{\beta}_2 & & h_{N_2}\hat{\beta}_p \end{array}\right) . \qquad (3.36)$$

Now W_1 may be written as

$$W_1 = \begin{pmatrix} h_1 B_1' \\ h_2 B_1' \\ . \\ . \\ . \\ h_{N_2} B_1' \end{pmatrix} = \begin{pmatrix} h_1 \\ h_2 \\ . \\ . \\ . \\ h_{N_2} \end{pmatrix} B_1' = H B_1' \qquad (3.37)$$

where

$$H = \begin{pmatrix} h_1 \\ h_2 \\ . \\ . \\ . \\ h_{N_2} \end{pmatrix} \quad \text{and} \quad B_1 = \begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ . \\ . \\ . \\ \hat{\beta}_p \end{pmatrix} .$$

Then (3. 36) may be written as

$$X_2 = (W_0, W_1) = (W_0, HB_1') . \qquad (3.38)$$

Now

$$J = X_2 S_1^{-1} = (W_0, HB_1') S_1^{-1} \qquad (3.39)$$

and

S_1^{-1} may be partitioned as

$$S_1^{-1} = \left(\begin{array}{c|cccc} \frac{1}{N_1} & 0 & \cdots & & 0 \\ \hline 0 & \frac{1}{N_1} & 0 & \cdots & 0 \\ \cdot & 0 & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ 0 & 0 & & & \frac{1}{N_1} \end{array}\right) = \begin{pmatrix} C_{00} & 0 \\ 0 & C_{11} \end{pmatrix} . \qquad (3.40)$$

Then using S_1^{-1} as given by (3.40) in (3.39), J may be written as

$$J = (W_0, HB_1') \begin{pmatrix} C_{00} & 0 \\ 0 & C_{11} \end{pmatrix} = (W_0 C_{00}, HB_1' C_{11})$$

so that

$$J' = \begin{pmatrix} C_{00} W' \\ C_{11} B_1 H' \end{pmatrix} . \qquad (3.41)$$

Although explicit expressions may be written for G and Q, it is only necessary to note their dimensions. Now $G = (I + R)^{-1} = (I + X_2 S_1^{-1} X_2')^{-1}$ so that the dimension of G is that of $X_2 S_1^{-1} X_2'$ which is $N_2 \times N_2$. Also, $Q = Y_2 - X_2\hat{\beta}$ has dimension $N_2 \times 1$ so that the product GQ has dimension $N_2 \times 1$. Now substituting the expression (3.41) for J' in the equation for $\hat{\alpha}$ and partitioning $\hat{\alpha}$ as indicated there obtains

$$\hat{\alpha} = \begin{pmatrix} \hat{\alpha}_0 \\ \hline \hat{\alpha}_1 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\alpha}_p \end{pmatrix} = \begin{pmatrix} A_0 \\ A_1 \end{pmatrix} = \begin{pmatrix} B_0 \\ B_1 \end{pmatrix} + \begin{pmatrix} C_{00} W_0' \\ C_{11} B_1 H' \end{pmatrix} GQ . \qquad (3.42)$$

Hence,

$$A_0 = B_0 + C_{00} W_0' GQ$$

and

$$A_1 = B_1 + C_{11} B_1 H' GQ . \qquad (3.43)$$

Now since H' is $1 \times N_2$ and GQ is $N_2 \times 1$, $H'GQ$ is a scalar. Also $C_{11} = \frac{1}{N_1} I_p$ so that

$$A_1 = B_1 + \frac{H'GQ}{N_1} B_1 = B_1 \left(1 + \frac{H'GQ}{N_1} \right) . \qquad (3.44)$$

Let $1 + \frac{H'GQ}{N_1} = k$, so that (3.41) becomes $A_1 = kB_1$, that is

$$\begin{pmatrix} \hat{\alpha}_1 \\ \hat{\alpha}_2 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\alpha}_p \end{pmatrix} = k \begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\beta}_p \end{pmatrix}$$

from which the invariance property follows.

In view of the generalization of theorem 3.2 as given in theorem 3.4, It is to be expected that theorem 3.3 may also be extended. The generalization is given in theorem 3.5. Consider the following conditions:

(a) $$\frac{\hat{\alpha}_j}{\hat{\alpha}_i} = \frac{\hat{\beta}_j}{\hat{\beta}_i} \qquad i, j = 1, 2, \ldots p$$

(b) $$X_2 = \left(\begin{array}{c|cccc} 1 & h_1\hat{\beta}_1 & h_1\hat{\beta}_2 & \cdots & h_1\hat{\beta}_p \\ 1 & h_2\hat{\beta}_1 & h_2\hat{\beta}_2 & \cdots & h_2\hat{\beta}_p \\ \cdot & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & & \\ 1 & h_{N_2}\hat{\beta}_1 & h_{N_2}\hat{\beta}_2 & \cdots & h_{N_2}\hat{\beta}_p \end{array} \right)$$

(c) $$(X_1'X_1)^{-1} = \begin{pmatrix} u & 0 \\ 0 & vI_p \end{pmatrix} .$$

These conditions are the same as those preceding theorem 3.3 except that condition (b) implies that there are N_2 additional points in the direction of steepest ascent instead of just one additional point.

Theorem 3.5. Any two of the above three conditions imply the third.

Proof: X_2, $\hat{\alpha}$, and $\hat{\beta}$ may be partitioned as in theorem 3.4, $(X_1'X_1)^{-1}$ may be partitioned as

$$(X_1' X_1)^{-1} = \left(\begin{array}{c|cccc} u & 0 & \cdot & \cdot & 0 \\ \hline 0 & v & \cdot & \cdot & 0 \\ \cdot & \cdot & & & \\ \cdot & \cdot & & & \\ \cdot & \cdot & & & \\ 0 & 0 & \cdot & \cdot & v \end{array}\right) = \begin{pmatrix} C_{00} & 0 \\ 0 & C_{11} \end{pmatrix}.$$

The proof that (b) and (c) imply (a) is the content of theorem 3.4 with $\frac{1}{N_1}$ replaced by u and v as indicated in the above partitioning of $(X_1' X_1)^{-1}$.

To prove that (a) and (c) imply (b) the equation $\hat{\alpha} = \hat{\beta} + J'GQ$ is written as

$$\begin{pmatrix} A_0 \\ kB_1 \end{pmatrix} = \begin{pmatrix} B_0 \\ B_1 \end{pmatrix} + \begin{pmatrix} u & 0 \\ 0 & vI_p \end{pmatrix} \begin{pmatrix} W_0' \\ X_{21}' \end{pmatrix} G\,Q \qquad (3.45)$$

where A_1 has been replaced by kB_1 according to (a) . Equating corresponding elements of (3.45) there results

$$A_0 = B_0 + u W_0' GQ \qquad (3.46)$$

and

$$kB_1 = B_1 + v I_p X_{21}' G Q. \qquad (3.47)$$

Equation (3.47) may be written as

$$\left(\frac{k - 1}{v} \right) B_1 = X_{21}' G Q \qquad (3.48)$$

or

$$M X_{21} = \ell B_1' \qquad (3.49)$$

where $M = (GQ)'$ has dimension $1 \times N_2$ and ℓ is the scalar

$\frac{k-1}{v}$. Evidently, the elements x_{ij} of X_{21} are of the form $x_{ij} = a_{ij}\hat{\beta}_i$. Let $M = (m_1, m_2, \ldots m_{N_2})$. Then (3.49) may be written as

$$(m_1, m_2, \ldots m_{N_2}) \begin{pmatrix} a_{11}\hat{\beta}_1 & a_{12}\hat{\beta}_2 & \ldots & a_{1p}\hat{\beta}_p \\ a_{21}\hat{\beta}_1 & a_{22}\hat{\beta}_2 & \ldots & a_{2p}\hat{\beta}_p \\ \cdot & \cdot & & \\ \cdot & \cdot & & \\ \cdot & \cdot & & \\ a_{N_2 1}\hat{\beta}_1 & a_{N_2 2}\hat{\beta}_2 & \ldots & a_{N_2 p}\hat{\beta}_p \end{pmatrix} = (\ell\hat{\beta}_1, \ell\hat{\beta}_2, \ldots \ell\hat{\beta}_p). \quad (3.50)$$

Now (3.50) must be true for all M and in particular must hold as M ranges over the unit vectors

$$u_1 = (1, 0, \ldots 0),$$
$$u_2 = (0, 1, \ldots 0),$$

and

$$\vdots$$

$$u_{N_2} = (0, 0, \ldots 1).$$

When $M = u_1$, equating the corresponding elements of (3.50) yields

$$a_{11}\hat{\beta}_1 = \ell\hat{\beta}_1$$
$$a_{12}\hat{\beta}_2 = \ell\hat{\beta}_2$$
$$\vdots$$
$$a_{1p}\hat{\beta}_p = \ell\hat{\beta}_p$$

so that $a_{11} = a_{12} = \ldots = a_{1p}$.

More generally, when $M = u_i$,

$$a_{i1}\hat{\beta}_1 = \ell\hat{\beta}_1$$

$$a_{i2}\hat{\beta}_2 = \ell\hat{\beta}_2$$

$$\vdots$$

$$a_{ip}\hat{\beta}_p = \ell\hat{\beta}_p$$

so that $a_{i1} = a_{i2} = \ldots a_{ip}$.

Since this is true for $i = 1, 2, \ldots N_2$, the a_{ij} in any row are alike. Hence X_{21} has the form

$$\begin{pmatrix} a_1\hat{\beta}_1 & a_1\hat{\beta}_2 & \ldots & a_1\hat{\beta}_p \\ a_2\hat{\beta}_1 & a_2\hat{\beta}_2 & \ldots & a_2\hat{\beta}_p \\ \vdots & \vdots & & \\ a_{N_2}\hat{\beta}_1 & a_{N_2}\hat{\beta}_2 & \ldots & a_{N_2}\hat{\beta}_p \end{pmatrix} = \begin{pmatrix} a_1 B_1' \\ a_2 B_1' \\ \\ \\ a_{N_2} B_1' \end{pmatrix} = A B_1' .$$

which is of the form of (b).

In order to prove that (a) and (b) imply (c), the symmetric matrix S_1^{-1} is partitioned as

$$\left(\begin{array}{c|ccc} C_{00} & C_{01} & \ldots & C_{0p} \\ \hline C_{10} & C_{11} & \ldots & C_{1p} \\ \vdots & \vdots & & \\ C_{p0} & C_{p1} & \ldots & C_{pp} \end{array}\right) = \begin{pmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{pmatrix} .$$

Now $J = (W_0, HB_1') \begin{pmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{pmatrix}$ so that

$J' = \begin{pmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{pmatrix} \begin{pmatrix} W_0' \\ B_1H' \end{pmatrix}$. Hence

$$\begin{pmatrix} A_0 \\ A_1 \end{pmatrix} = \begin{pmatrix} B_0 \\ B_1 \end{pmatrix} + \begin{pmatrix} C_{00}W_0' + C_{01}B_1H' \\ C_{10}W_0' + C_{11}B_1H' \end{pmatrix} GQ \quad . \qquad (3.51)$$

It follows that

$$A_0 = B_0 + C_{00}W_0'GQ + C_{01}B_1H'GQ \qquad (3.52)$$

and that

$$A_1 = B_1 + C_{10}W_0'GQ + C_{11}B_1H'GQ \, . \qquad (3.53)$$

Now by (a), $A_1 = kB_1$ so that (3.53) becomes

$$kB_1 = B_1 + C_{10}W_0'GQ + C_{11}B_1H'GQ \, . \qquad (3.54)$$

Since (3.54) must be true for all vectors B_1, $C_{10} = 0$ so that (3.54) becomes

$$kB_1 = B_1 + C_{11}B_1H'GQ \, . \qquad (3.55)$$

Now $H'GQ$ is a scalar so that (3.55) may be written

$$(kI - H'GQC_{11}) \, B_1 = B_1 \quad \text{which}$$

implies that

$$kI - H'GQC_{11} = I.$$

It follows that

$$C_{11} = \frac{(k-1)}{H'GQ} \, I \quad \text{so that} \quad C_{11}$$

is a scalar matrix as in (c) .

If the invariance property is extended to include $\hat{\alpha}_0$ and $\hat{\beta}_0$ then H must be chosen so that $B_0 H = W_0$. Then since $C_{01} = 0$, equation (3. 52) becomes

$$k B_0 = B_0 + C_{00} W_0{}' G Q . \quad \text{Hence}$$

$$C_{00} = \frac{(k-1) B_0}{W_0{}' G Q} = \frac{(k-1) B_0}{Q' G' W_0} = \frac{(k-1) B_0}{Q' G' B_0 H}$$

$$= \frac{(k-1)}{H' G Q}$$ which is the scalar multiplier of I in the expression for C_{11} above.

The Predicted Response

Thus far the invariance property has been investigated but no expression for the response at an additional point has been given. Suppose that a p-dimensional unit grid has been employed to estimate $\hat{\beta}$ and that in addition to the $N_1 = 2^p$ grid points, an additional point $x = (x_1, x_2, \ldots, x_p)$ is used. It is convenient then to distinguish between:

(a) . y, the observed response at x,

(b) . $\hat{y}_1$, the least squares prediction of η at x on the basis of the N_1 points, and

(c) . $\hat{y}_2$, the least squares prediction of η at x on the basis of the $N_1 + 1$ points.

Clearly, $\hat{y}_1 = X\hat{\beta}$ and $\hat{y}_2 = X\hat{\alpha}$. Now suppose that the additional point is in the steepest ascent direction so that in matrix notation, $X_2 = (1, h\hat{\beta}_1, \ldots, h\hat{\beta}_p) = (1, h B_1')$. Now

$$\begin{aligned} \hat{y}_2 &= X_2 \hat{\alpha} = X_2 (\hat{\beta} + J' GQ) \\ &= X_2 \hat{\beta} + X_2 S_1^{-1} X_2' G (y - X_2 \hat{\beta}) \\ &= \hat{y}_1 + R(I + R)^{-1} (y - \hat{y}_1) . \end{aligned} \quad (3.56)$$

Now R is a positive scalar written

$$R = X_2 S_1^{-1} X_2' = (1, hB_1') \begin{pmatrix} \frac{1}{N_1} & 0 \\ 0 & \frac{I_p}{N_1} \end{pmatrix} \begin{pmatrix} 1 \\ hB_1 \end{pmatrix} = \frac{1}{N_1} (1 + h^2 B_1' B_1).$$

Denote the quantity $R(I + R)^{-1} = \dfrac{R}{1 + R}$ by k^2 so that $0 < k^2 < 1$.

Then by (3.56) ,

$$\hat{y}_2 = \hat{y}_1 + k^2 (y - \hat{y}_1) \quad (3.57)$$

so that

$$\hat{y}_2 - \hat{y}_1 = k^2 (y - \hat{y}_1) \text{ and } 0 < \frac{\hat{y}_2 - \hat{y}_1}{y - \hat{y}_1} < 1 . \quad (3.58)$$

It is to be noted that $R = X_2 S^{-1} X_2'$ is simply the sum of squares of the elements of the additional point divided by the number of points in the initial design. The result (3.58) is more general than has been indicated since it is valid whenever the design matrix has the form $X_1' X_1 = pI$. Further, the additional point is not restricted to the steepest ascent line but may be arbitrary. In these circumstances

$$R = X_2(X_1'X_1)^{-1}X_2' = \frac{X_2X_2'}{p}$$ which is a positive scalar.

Then (3. 56) becomes

$$\hat{y}_2 = \hat{y}_1 + \frac{\frac{X_2X_2}{p}}{\frac{p + X_2X_2'}{p}}(y - \hat{y}_1) = \hat{y}_1 + \frac{X_2X_2'}{p + X_2X_2'}(y - \hat{y}_1). \tag{3.59}$$

Hence (3. 58) is valid in the general case.

The expression (3. 58) symbolizes a condition which intuition could have foretold. It states that the observation y and the prediction on the basis of $N_1 + 1$ points, $\hat{y}_2$, either are both greater than the prediction on the basis of N_1 points, $\hat{y}_1$, or they are both less than $\hat{y}_1$. It also implies that $\hat{y}_2$ is always between y and $\hat{y}_1$.

These facts can be more elegantly stated if (3. 57) is written as

$$\hat{y}_2 = k^2 y + (1 - k^2)\hat{y}_1 . \tag{3.60}$$

from which $\hat{y}_2$ may be recognized to be a convex combination of y and $\hat{y}_1$. In addition, since $k^2 = \frac{X_2'X_2}{N_1}$, the further along the steepest ascent path the additional observation is taken, the greater is the weight placed upon it. Figure 1 indicates the relative positions of y, $\hat{y}_1$, and $\hat{y}_2$ in a two dimensional factor space.

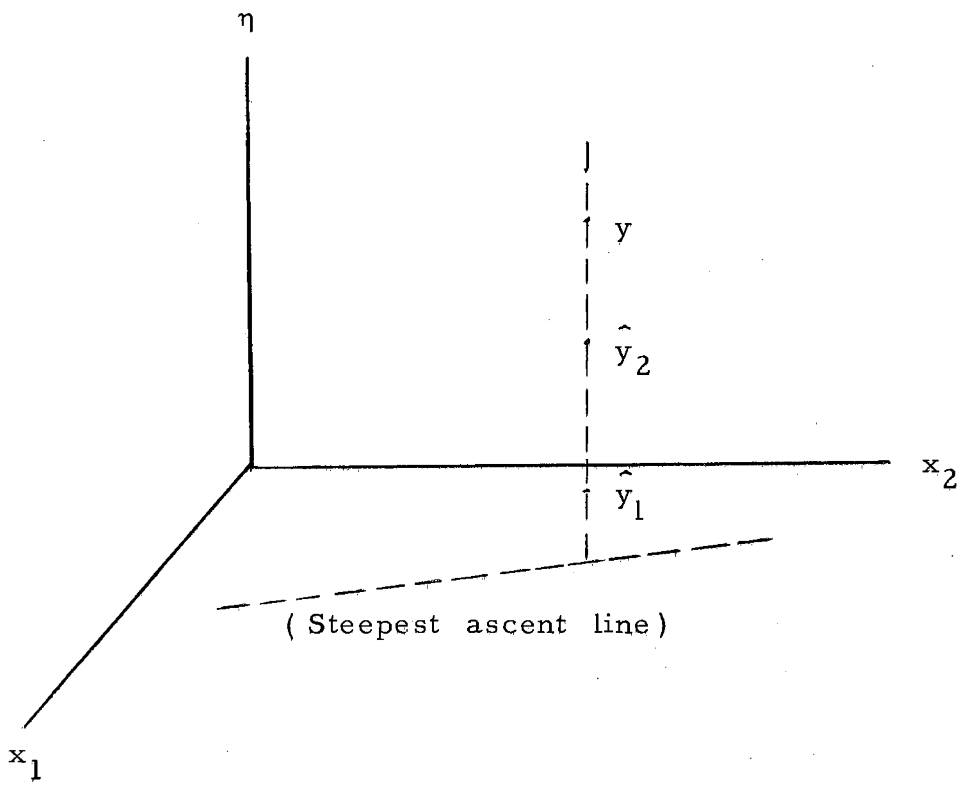

Figure 1. Relative Magnitude of Observed and Predicted Responses

A judicious choice of the location of the first experiment on the steepest ascent line is a problem to which some space will be given subsequently. Apparently the step size along the steepest ascent line is something about which the experimenter is supposed to have some feeling. To be more concrete, suppose the experimenter wishes to take a step of such a size that the predicted yield will increase by an amount Π .

Now at the origin, $x = (0, \ldots, 0)$ so that $X = (1, 0, \ldots, 0)$ and

$$\hat{y} = X\hat{\beta} = \hat{\beta}_0 \, . \qquad (3.61)$$

It is desired to determine h so that at $x = (h\hat{\beta}_1, \ldots, h\hat{\beta}_p)$ the response has increased by an amount Π, that is

$$\hat{y} = (1, hB_1') \begin{pmatrix} B_0 \\ B_1 \end{pmatrix} = \Pi + \hat{\beta}_0 . \qquad (3.62)$$

Then $\hat{\beta}_0 + hB_1'B_1 = \Pi + \hat{\beta}_0$ so that

$$h = \frac{\Pi}{B_1'B_1} . \qquad (3.63)$$

Hence an increase in response by the amount Π is predicted at the point

$$x = \frac{\Pi}{B_1'B_1} (\hat{\beta}_1, \ldots, \hat{\beta}_p) = \frac{\Pi B_1'}{B_1'B_1} . \qquad (3.64)$$

Upper and Lower Bounds for $\frac{\beta_{11}}{\beta_{22}}$

Usually the experimenter has some prior information regarding the response under consideration. He is quite likely to know whether the response has a maximum or a minimum in the region of interest and he may even know the shape of the factor space contours. The following discussion indicates a position along the steepest ascent line where the first experiment may be run in order to utilize prior information.

Consider the response

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

and the least squares prediction

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_{12} x_1 x_2 \qquad (3.65)$$

where the β's are estimated by means of a unit grid. It may readily be verified that

$$E(\hat{\beta}_0) = \beta_0 + \beta_{11} + \beta_{22}$$

$$E(\hat{\beta}_1) = \beta_1$$

$$E(\hat{\beta}_2) = \beta_2$$

$$E(\hat{\beta}_{12}) = \beta_{12}$$

so that

$$E(y - \hat{y}) = E[(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{22} x_2^2 + e)$$

$$- (\beta_0 + \beta_{11} + \beta_{22} + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2)]$$

$$= \beta_{11} x_1^2 + \beta_{22} x_2^2 - \beta_{11} - \beta_{22} . \quad (3.66)$$

Hence the difference between the observed response and the predicted response at a point (x_1, x_2) is an unbiased estimate of

$\beta_{11} x_1^2 + \beta_{22} x_2^2 - \beta_{11} - \beta_{22}$.

The gradient line at the origin has the equation $x_2 = \beta_2/\beta_1 \; x_1$ so that a point on the gradient line may be written as $(h\beta_1, h\beta_2)$. Then the difference $y - \hat{y}$ at the point $(h\beta_1, h\beta_2)$ is an estimate of $\beta_{11} h^2 \beta_1^2 + \beta_{22} h^2 \beta_2^2 - \beta_{11} - \beta_{22}$.

That is,

$$E(y - \hat{y})\Big|_{(h\beta_1, h\beta_2)} = \beta_{11} h^2 \beta_1^2 + \beta_{22} h^2 \beta_2^2 - \beta_{11} - \beta_{22} . \quad (3.67)$$

The quantities β_1 and β_2 have been estimated by $\hat{\beta}_1$ and $\hat{\beta}_2$.

β_{11} and β_{22} are unknown while the choice of h remains with the investigator. Suppose h is chosen so that $h^2\hat{\beta}_1^2 - 1 > 0$ and $h^2\hat{\beta}_2^2 - 1 < 0$. Also let the observed response at $(h\hat{\beta}_1, h\hat{\beta}_2)$ be larger than that predicted there so that $y - \hat{y} > 0$. Then

$$\beta_{11}(h^2\hat{\beta}_1^2 - 1) + \beta_{22}(h^2\hat{\beta}_2^2 - 1) > 0 . \qquad (3.68)$$

Further, if $\beta_{22} > 0$, (3.68) may be written

$$\frac{\beta_{11}}{\beta_{22}} > - \frac{h^2\hat{\beta}_2^2 - 1}{h^2\hat{\beta}_1^2 - 1} \qquad (3.69)$$

whereas if $\beta_{22} < 0$,

$$\frac{\beta_{11}}{\beta_{22}} < - \frac{h^2\hat{\beta}_2^2 - 1}{h^2\hat{\beta}_1^2 - 1} . \qquad (3.70)$$

Now the right side of (3.69) and (3.70) is positive so that in the first case it serves as a lower bound to the ratio β_{11}/β_{22} while in the second case it serves as an upper bound to the ratio β_{11}/β_{22}.

Now consider the combination $h^2\hat{\beta}_1^2 - 1 > 0$, $h^2\hat{\beta}_2^2 - 1 > 0$, $\beta_{11} < 0$, and $\beta_{22} < 0$. Then (3.68) leads to

$$\frac{\beta_{11}}{\beta_{22}} < - \frac{h^2\hat{\beta}_2^2 - 1}{h^2\hat{\beta}_1^2 - 1} . \qquad (3.71)$$

Now the right side of (3.71) is negative while the left side is positive so that evidently this combination of signs cannot occur.

Now take $(h^2\hat{\beta}_1^2 - 1) > 0$, $(h^2\hat{\beta}_2^2 - 1) > 0$, $\beta_{11} > 0$, and $\beta_{22} > 0$. Then (3.68) leads to

$$\frac{\beta_{11}}{\beta_{22}} > - \frac{h^2\hat{\beta}_2^2 - 1}{h^2\hat{\beta}_1^2 - 1} . \qquad (3.72)$$

Since it is known at the outset that $\frac{\beta_{11}}{\beta_{22}}$ is positive and since the right side is negative, (3.72) yields no new information.

Denote $\left| \frac{h^2\hat{\beta}_2^2 - 1}{h^2\hat{\beta}_1^2 - 1} \right|$ by t. Let U (t) denote an upper bound of t and U (-t) denote an upper bound of -t. Let the symbol L ($\pm$ t) be used in a similar fashion. Also let N indicate that no new information is available and let I indicate that a particular combination of signs cannot occur. With this notation, table II summarizes all possible sign combinations for $y > \hat{y}$. When $y < \hat{y}$ it is merely necessary to interchange N with I and L with U .

A knowledge of the ratio β_{11}/β_{22} can be useful in some instances. If interaction is present the axes of the contour system will be rotated through an angle θ where $\tan 2\theta = \frac{\beta_{12}}{\beta_{11} - \beta_{22}}$.

If β_{11}/β_{22} is close to 1, then θ is close to 45° or 135°

depending on the sign of β_{12}. If the experimenter feels that no interaction is present then $\beta_{12} = 0$. In this case it can be shown that the eccentricity, ρ, of the elliptical contours is given by $\rho = \sqrt{|d^2 - 1|}$ where $d = \beta_{11} / \beta_{22}$. Hence a measure of the degree of elongation of the contour system is available.

TABLE II

UPPER AND LOWER BOUNDS FOR β_{11}/β_{22}

$y - \hat{y}$	$h^2\hat{\beta}_1^2 - 1$	$h^2\hat{\beta}_2^2 - 1$	β_{11}	β_{22}	β_{11}/β_{22}
+	+	+	+	+	N
+	+	+	+	-	U (-t)
+	+	+	-	+	L (-t)
+	+	+	-	-	I
+	+	-	+	+	L (t)
+	+	-	+	-	N
+	+	-	-	+	I
+	+	-	-	-	U (t)
+	-	+	+	+	U (t)
+	-	+	+	-	I
+	-	+	-	+	N
+	-	+	-	-	L (t)
+	-	-	+	+	I
+	-	-	+	-	L (-t)
+	-	-	-	+	U (-t)
+	-	-	-	-	N

In the case where $\beta_{12} = 0$, equation (3.74) gives the equation of the line from the origin to the true maximum as

$$x_2 = \frac{\beta_2}{\beta_1} \; \frac{\beta_{11}}{\beta_{22}} \; x_1 .$$

An estimate of the ratio β_{11}/β_{22} can be used to adjust the slope $\hat{\beta}_2/\hat{\beta}_1$ of the path of steepest ascent.

Gradient Properties

Consider the response $y = \eta + e$ where

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{22} x_2^2 . \qquad (3.73)$$

Now

$$\frac{\partial \eta}{\partial x_1} = \beta_1 + 2\beta_{11} x_1 + \beta_{12} x_2$$

and

$$\frac{\partial \eta}{\partial x_2} = \beta_2 + \beta_{12} x_1 + 2 \beta_{22} x_2 .$$

If these are set equal to 0 and solved for x_1 and x_2, there results

$$x_1 = \frac{2\beta_1 \beta_{22} - \beta_2 \beta_{12}}{\beta_{12}^2 - 4\beta_{11} \beta_{22}}$$

and

$$x_2 = \frac{2\beta_2 \beta_{11} - \beta_1 \beta_{12}}{\beta_{12}^2 - 4\beta_{11} \beta_{22}} \qquad (3.74)$$

which are the coordinates of the maximum of η. Since the coordinates of the maximum will often be referred to, let it be agreed to denote them by (x_1^*, x_2^*).

The path in the factor space which leads to the coordinates of the true maximum is along the line

$$x_2 = \frac{x_2^*}{x_1^*} \; x_1, \text{ provided } \beta_{12}^2 - 4\beta_{11}\beta_{22} \neq 0 .$$

The gradient path is normal to the factor space contours at the origin and has the equation $x_2 = \beta_2/\beta_1 \; x_1$. Unfortunately, only in very special instances will the gradient pass through the coordinates of the maximum. Evidently these paths will coincide whenever

$$\frac{\beta_2}{\beta_1} = \frac{2\beta_2\beta_{11} - \beta_1\beta_{12}}{2\beta_1\beta_{22} - \beta_2\beta_{12}} , \qquad (3.75)$$

which reduces to

$$2\beta_1\beta_2(\beta_{22} - \beta_{11}) + \beta_{12}(\beta_1^2 - \beta_2^2) = 0 . \qquad (3.76)$$

This is satisfied whenever

(a) $\beta_{22} = \beta_{11}$ and $\beta_1 = \beta_2$,

(b) $\beta_{22} = \beta_{11}$ and $\beta_{12} = 0$, or

(c) $\beta_2 = 0$ and $\beta_{12} = 0$.

In each of these cases, it is geometrically evident that the gradient line at the origin passes through the center of the contour system. In (a), the line $x_2 = \pm x_1$ passes through the center of the system and the line $x_2 = \mp x_1$ is tangent at the origin. In case (b), the contour system is circular while in case (c), the center is on the x_1 axis.

In general, the factor space contour system will not be one of the special cases discussed in the previous paragraph. The experimenter would indeed be extremely fortunate if the contour system were such that the maximum on the line $x_2 = \frac{\beta_2}{\beta_1} x_1$ was close to the true maximum. In accordance with the steepest ascent technique, experimentation may be continued at the points of a second grid, the center of which is located at the maximum of the first steepest ascent path. Further experimentation is then performed along the line determined from the second grid. It is relevant therefore to find an expression for the maximum response attainable on the gradient and for the coordinates of the point where this maximum occurs. It is also relevant to find the equation of the gradient at this maximum point.

Theorem 3.6. The maximum value of η subject to $x_2 = mx_1$ occurs at the point

$$x_1 = -\frac{a}{2b}$$

$$x_2 = -\frac{ma}{2b} \qquad (3.77)$$

and is given by

$$\eta = \beta_0 - \frac{a^2}{2b} \qquad (3.78)$$

where

$$a = \beta_1 + m\beta_2 \quad \text{and} \quad b = \beta_{11} + m\beta_{12} + m^2\beta_{22} . \qquad (3.79)$$

Proof: On substituting mx_1 for x_2 in (3.73), there results

$$\eta = \beta_0 + \beta_1 x_1 + \beta_2 m x_1 + \beta_{11} x_1^2 + \beta_{12} x_1^2 m + \beta_{22} m^2 x_1^2$$

$$= \beta_0 + (\beta_1 + m\beta_2)\, x_1 + (\beta_{11} + m\beta_{12} + m^2\beta_{22})\, x_1^2 . \quad (3.80)$$

Then finding $\frac{d\eta}{dx_1}$ and setting it equal to 0, there results

$$\frac{d\eta}{dx_1} = \beta_1 + m\beta_2 + 2(\beta_{11} + m\beta_{12} + \beta_{22}m^2)\, x_1 = 0$$

so that

$$x_1 = - \frac{\beta_1 + m\beta_2}{2(\beta_{11} + m\beta_{12} + m^2\beta_{22}}$$

$$x_2 = - \frac{m(\beta_1 + m\beta_2)}{2\beta_{11} + m\beta_{12} + m^2\beta_{22}}$$

thereby verifying (3.77). Using (3.80),

$$\eta = \beta_0 - \frac{a^2}{2b} + \frac{a^2}{4b^2} \cdot b = \beta_0 - \frac{a^2}{2b} \qquad (3.81)$$

thereby establishing (3.78).

In particular, the line $x_2 = mx_1$ is the gradient line when

$m = \frac{\beta_2}{\beta_1}$. In this case the maximum response occurs at the point

$$x_1 = - \frac{\beta_1(\beta_1^2 + \beta_2^2)}{2(\beta_1^2\beta_{11} + \beta_1\beta_2\beta_{12} + \beta_2^2\beta_{22}}$$

$$x_2 = - \frac{\beta_2(\beta_1^2 + \beta_2^2)}{2(\beta_1^2\beta_{11} + \beta_1\beta_2\beta_{12} + \beta_2^2\beta_{22}} \qquad (3.82)$$

and is given by

$$\eta = \beta_0 - \frac{(\beta_1^2 + \beta_2^2)^2}{2(\beta_1^2\beta_{11} + \beta_1\beta_2\beta_{12} + \beta_2^2\beta_{22})} \qquad (3.83)$$

Theorem 3.7. The gradient line at the point on the line $x_2 = mx_1$ where η is maximized, is perpendicular to the line $x_2 = mx_1$.

Proof: The maximum point may be shifted to the origin by the translation

$$z_1 = x_1 - h$$
$$z_2 = x_2 - k \qquad (3.84)$$

where

$$h = -\frac{a}{2b} \quad \text{and} \quad k = -\frac{ma}{2b} \qquad (3.85)$$

are the coordinates of the maximum point as given in theorem 3.6. Then equation (3.73) transforms to

$$\eta = \beta_0' + \beta_1' z_1 + \beta_2' z_2 + \beta_{11} z_1^2 + \beta_{12} z_1 z_2 + \beta_{22} z_2^2 \qquad (3.86)$$

where β_1' and β_2' are given by

$$\beta_1' = \beta_1 + 2\beta_{11}h + \beta_{12}k$$
$$\beta_2' = \beta_2 + \beta_{12}h + 2\beta_{22}k. \qquad (3.87)$$

Hence the gradient line at the origin in the z space is

$$z_2 = \frac{\beta_2 + \beta_{12}h + 2\beta_{22}k}{\beta_1 + 2\beta_{11}h + \beta_{12}k} z_1. \qquad (3.88)$$

Using (3.85) and (3.79), the numerator of this equation may be written

$$\beta_2 + \beta_{12}h + 2\beta_{22}k = \beta_2 - \frac{\beta_{12}a}{2b} - \frac{2\beta_{22}ma}{2b}$$

$$= \frac{2\beta_2 b - a\beta_{12} - 2ma\beta_{22}}{2b}$$

$$= \frac{2\beta_2(\beta_{11} + m\beta_{12} + \beta_{22}m^2) - (\beta_1 + m\beta_2)\beta_{12} - 2m(\beta_1 + m\beta_2)\beta_{22}}{2\,b}$$

$$= \frac{(2\beta_2\beta_{11} + m\beta_2\beta_{12} - \beta_1\beta_{12} - 2m\beta_{22}\beta_1)}{2\,b} .$$

The denominator of (3.88) may be written

$$\beta_1 - \frac{2\beta_{11}a}{2b} - \frac{\beta_{12}ma}{2b} = \frac{2\beta_1 b - 2\beta_{11}a - \beta_{12}ma}{2\,b}$$

$$= \frac{2\beta_1(\beta_{11} + m\beta_{12} + \beta_{22}m^2) - 2\beta_{11}(\beta_1 + m\beta_2) - m\beta_{12}(\beta_1 + m\beta_2)}{2\,b}$$

$$= \frac{m(\beta_1\beta_{12} + 2\beta_1\beta_{22}m - 2\beta_2\beta_{11} - m\beta_2\beta_{12})}{2\,b} .$$

Therefore equation (3.88) becomes

$$z_2 = \frac{2\beta_2\beta_{11} + m\beta_2\beta_{12} - \beta_1\beta_{12} - 2m\beta_{22}\beta_1}{-m(2\beta_2\beta_{11} + m\beta_2\beta_{12} - \beta_1\beta_{12} - 2m\beta_{22}\beta_1)}\, z_1 \qquad (3.89)$$

and provided the denominator is not zero,

$$z_2 = -\frac{1}{m}\, z_1 . \qquad (3.90)$$

The condition that the denominator is not zero implies that $m \neq 0$ and $m \neq \frac{\beta_1\beta_{12} - 2\beta_2\beta_{11}}{\beta_2\beta_{12} - 2\beta_1\beta_{22}}$. As $m \to 0$, $\frac{1}{m} \to \infty$, so that the gradient lines approach perpendicularity. As may be seen by (3.75), if $m = \frac{\beta_1\beta_{12} - 2\beta_2\beta_{11}}{\beta_2\beta_{12} - 2\beta_1\beta_{22}}$, then the line $x_2 = mx_1$ goes through the true maximum. Substituting x_1 and x_2 as given by (3.84) in (3.90), there results

$$x_2 + \frac{ma}{2b} = -\frac{1}{m}\left(x_1 + \frac{a}{2b}\right) \qquad (3.91)$$

Since the slope of this line and the line $x_2 = mx_1$ are negative reciprocals, the lines are perpendicular.

In particular, theorem 3.7 applies when $m = \frac{\beta_2}{\beta_1}$, so that the second gradient line is perpendicular to the first.

An examination of equation (3.75) has shown that only under very special circumstances will the gradient at the origin pass through the true maximum. Now the same can be said of any other point, and in particular, the point where the response is maximized on the gradient line through the origin, the coordinates of which, are given by (3.77). Hence, a second gradient line at the maximum of the first could be expected to pass through the true maximum only under special conditions.

It may be asked if there are points on the gradient line through the origin where a second gradient line passes through the true maximum. That the answer is in the affirmative can be seen from figure 2. Evidently, there are two such points, those two points where the gradient line intersects the axes of the elliptical contour system.

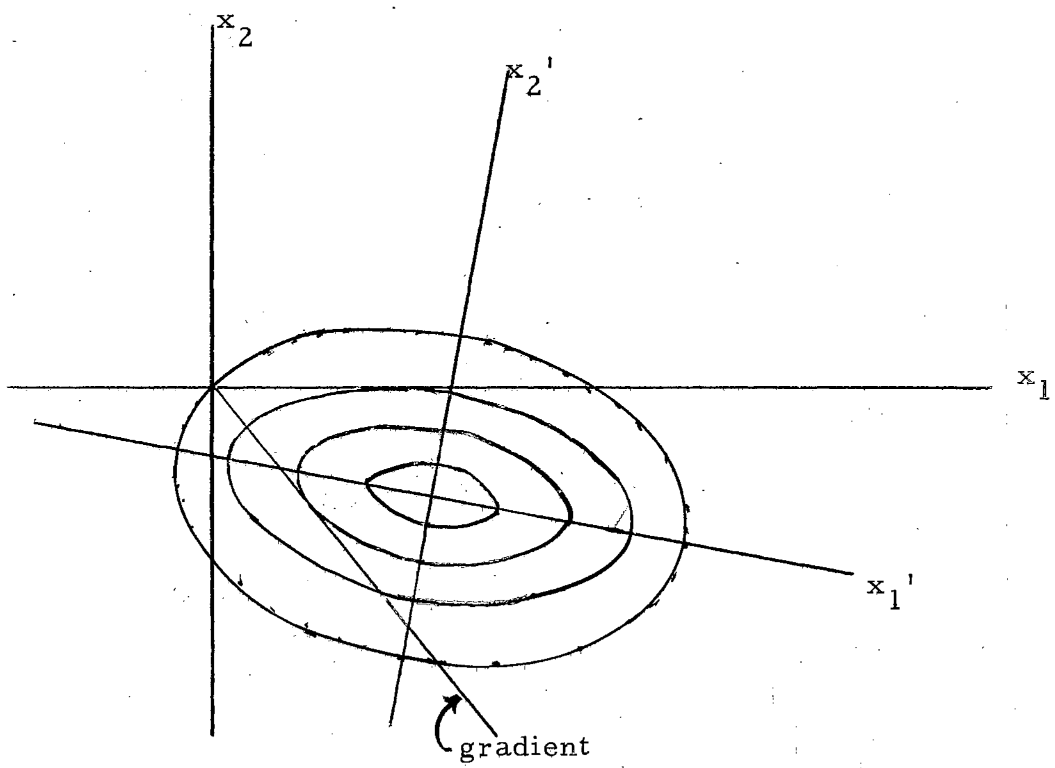

Figure 2. Intersection of the Gradient With the Axes of the Contour System .

If a point on the gradient be denoted by $(h\beta_1, h\beta_2)$, then the slope of the line joining this point to the true maximum may be equated to the slope of the gradient at the point $(h\beta_1, h\beta_2)$. The resulting quadratic equation when solved for h gives

$$h = \frac{(\beta_{11} + \beta_{22}) \pm \sqrt{(\beta_{11} - \beta_{22})^2 + \beta_{12}^2}}{\beta_{12}^2 - 4\beta_{11}\beta_{22}} \qquad (3.92)$$

In general, the gradient line at the maximum point of the gradient line through the origin, does not pass through the true maximum. Is there any line such that the gradient at the maximum passes through the true maximum? That there are three such lines is the content of theorem 3.8 .

<u>Theorem 3.8 .</u> Let (x_1^*, x_2^*) be the coordinates of the maximum response attainable on the line $x_2 = mx_1$. If the gradient at (x_1^*, x_2^*) passes through the coordinates of the true maximum, then m has one of the values

$$m_1 = \frac{2\beta_{11}\beta_2 - \beta_{12}\beta_1}{2\beta_{22}\beta_1 - \beta_{12}\beta_2} , \tag{3.93}$$

$$m_2 = \frac{(\beta_{22} - \beta_{11}) + \sqrt{(\beta_{11} - \beta_{22})^2 + \beta_{12}^2}}{\beta_{12}} , \tag{3.94}$$

or

$$m_3 = \frac{(\beta_{22} - \beta_{11}) - \sqrt{(\beta_{11} - \beta_{22})^2 + \beta_{12}^2}}{\beta_{12}} \tag{3.95}$$

Proof: In accordance with (3.77) , the maximum response attainable on the line $x_2 = mx_1$ occurs at the point

$- \frac{a}{2b}$, $- \frac{ma}{2b}$ where a and b are given by (3.79). According to theorem (3.7) , the gradient at the point (x_1^*, x_2^*) is perpendicular to the line $x_2 = mx_1$. The equation of the line perpendicular to the line $x_2 = m x_1$ at the point $- \frac{a}{2b}$, $- \frac{ma}{2b}$

has the equation

$$x_2 = -\frac{1}{m} x_1 - \frac{a(m^2 + 1)}{2mb} \qquad (3.96)$$

If this line is to pass through the true maximum, then the point

$$x_1^* = \frac{2\beta_1\beta_{22} - \beta_2\beta_{12}}{\beta_{12}^2 - 4\beta_{11}\beta_{22}}$$

$$x_2^* = \frac{2\beta_2\beta_{11} - \beta_1\beta_{12}}{\beta_{12}^2 - 4\beta_{11}\beta_{22}}$$

must satisfy (3.96) . Imposing this condition and substituting in the values of a and b, there results

$$\begin{aligned} & m^3 [\beta_{12}(\beta_2\beta_{12} - 2\beta_{22}\beta_1)] + \\ & m^2[4\beta_1\beta_{22}(\beta_{22} - \beta_{11}) + 2\beta_2\beta_{12}(2\beta_{11} - \beta_{22}) - \beta_1\beta_{12}^2] + \\ & m [4 \beta_{11}\beta_2(\beta_{11} - \beta_{22}) + 2\beta_1\beta_{12}(2\beta_{22} - \beta_{11}) - \beta_2\beta_{12}^2] + \\ & \beta_{12}(\beta_1\beta_{12} - 2\beta_{11}\beta_2) = 0 . \end{aligned} \qquad (3.97)$$

Consider the line determined by (0, 0) and (x_1^*, x_2^*) . Obviously the coordinates of the maximum on this line are the coordinates of the true maximum so that trivially the gradient at this point goes through the true maximum. Hence one of the roots of (3.97) is m_1 as given in (3.93) . Using m_1 in the synthetic division process yields the depressed equation

$$\beta_{12}m^2 + 2(\beta_{11} - \beta_{22}) m - \beta_{12} = 0, \qquad (3.98)$$

the roots of which are m_2 and m_3 as given by (3.94) and (3.95).

Since m_1 is the slope of the line from the origin to the true maximum in the factor space, it is natural to expect m_2 and m_3 to have geometrical significance. It is easily verified that $m_2 m_3 = -1$ so that the lines $x_2 = m_2 x_1$ and $x_2 = m_3 x_1$ must be mutually perpendicular. Since the axes of the contour system in the factor space are also mutually perpendicular, it is reasonable to look for some relationship between the axes of the contour system and the lines which have slopes m_2 and m_3. The relationship is given in theorem 3.9.

<u>Theorem 3.9 .</u> The lines $x_2 = m_2 x_1$ and $x_2 = m_3 x_1$ are parallel to the axes of the contour system.

Proof: By analytic geometry the angle of rotation of a conic is given by :

$$\tan \theta = \frac{1 - \cos 2\theta}{\sin 2\theta} \qquad (3.99)$$

where

$$\tan 2\theta = \frac{\beta_{12}}{\beta_{11} - \beta_{22}} .$$

Now

$$\sin 2\theta = \frac{\beta_{12}}{\sqrt{(\beta_{11} - \beta_{22})^2 + \beta_{12}^2}} \qquad (3.100)$$

and

$$\cos 2\theta = \frac{\beta_{11} - \beta_{22}}{\sqrt{(\beta_{11} - \beta_{22})^2 + \beta_{12}^2}} \; . \qquad (3.101)$$

Substituting (3.100) and (3.101) in (3.99) there results

$$\tan \theta = \frac{\beta_{22} - \beta_{11} + \sqrt{(\beta_{11} - \beta_{22})^2 + \beta_{12}^2}}{\beta_{12}} = m_2 \; .$$

Since m_2 has the same slope as one of the axes, m_3 must have the same slope as the other .

The geometrical significance of the roots of the cubic equation (3.97) now becomes clear. The roots m_2 and m_3 are the slopes of lines passing through the origin which are parallel to the axes of the contour system. The maximum response is attained at the point of intersection of the line with an axis of the contour system. The gradient is coincident with the axis and hence passes through the center of the contour system. The situation is illustrated in figure 3.

An interesting situation arises when the axis of rotation passes through the origin. Suppose that the contour system in figure 3 is rotated until x_1' coincides with the line $x_2 = m_1 x_1$. Then m_1 and m_2 are equal so that the lines $x_2 = m_1 x_1$ and $x_2 = m_2 x_1$ coincide. Further, since the x_1' axis passes through the origin and is normal to the contours, it must coincide with the gradient at the origin. Hence, $\beta_2/\beta_1 = m_2 = m_1$. These statements, which are geometrically evident, may readily be verified by the methods of analytic geometry.

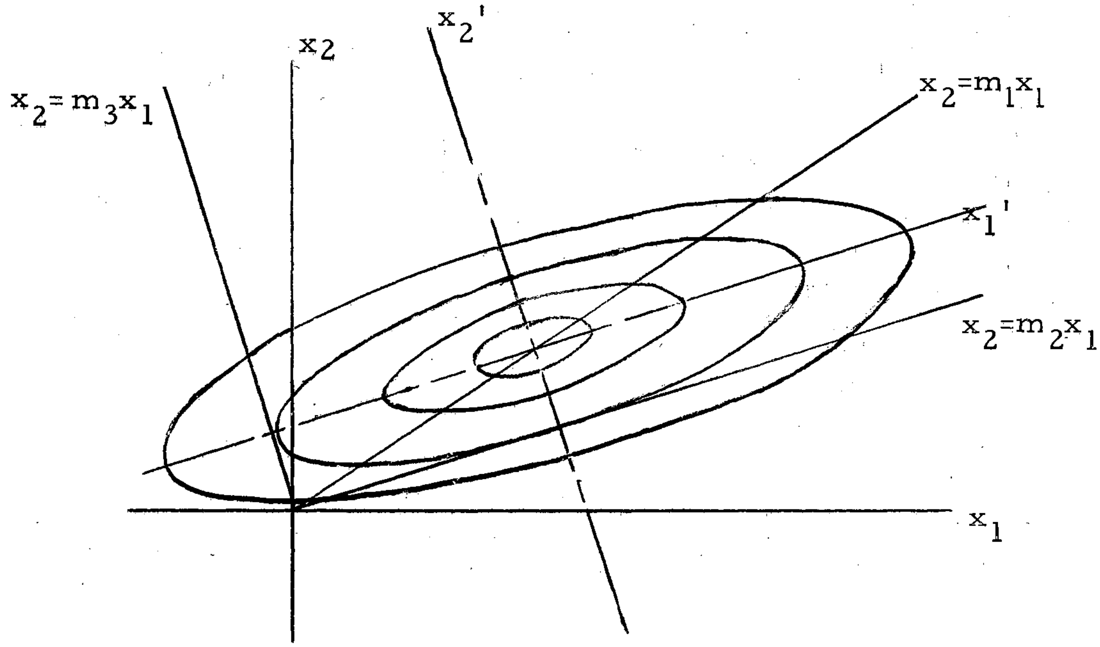

Figure 3. Relationship Between m_1, m_2, m_3, and the Contour System Axes .

CHAPTER IV

THE CHOICE OF SCALE

The most important decision that must be made by an experimenter using the steepest ascent technique occurs at the very outset of the investigation. He must decide where to run the experiments. The seemingly trivial nature of this statement may account in part for the lack of attention that it has received.

For purposes of illustration, suppose it is felt that the maximum yield obtained in a certain chemical process depends upon the controllable operating conditions of temperature and pressure. Obviously, the combinations of temperature and pressure should be chosen so that differences in the responses will be large enough to be clearly recognized. It is to be expected that, since investigators are human and possess varying degrees of experience, they will make different choices of the factor levels for the initial experiments. Unfortunately, as will be shown later, each different choice of factor levels leads to a different path for further experimentation.

Once the levels are chosen, the pressure and temperature variables are coded so that the rectangular array of experimental points map into the corner points of a unit grid. Hence the initial choice of levels determines the coding. The path of steepest ascent is calculated in terms of the coded variables. It is then decoded and written in terms of temperature and pressure. The investigator then proceeds to vary the temperature and pressure in additional experiments along the decoded path. This, in effect, is the procedure used in the field and is outlined by Box and Wilson (1), Davies (2) , and Cochran and Cox (3) . The crucial nature of the choice of levels and the effect of further experimentation along the decoded path is treated in the following discussion.

The Lack of Scale Invariance of the Steepest Ascent Path

Definition 4. 1 . The space of the uncoded variables in which the experiments are performed will be called the process space and will be denoted by P .

In this section the following notation will be used:

$z = (z_1, z_2, \ldots, z_p)$ will denote a point in P,

Z will denote the design matrix of the model,

Z_1 will denote the design matrix of the initial experimental points, and

Z_2 will denote the design matrix of an additional experimental point or additional experimental points.

As an example, suppose that the response in P is

$$y = \delta_0 + \delta_1 z_1 + \delta_2 z_2 + \delta_{11} z_1^2 + \delta_{12} z_1 z_2 + \delta_{22} z_2^2 + e.$$

This may be written as

$$y = (1, z_1, z_2, z_1^2, z_1 z_2, z_2^2) \begin{pmatrix} \delta_0 \\ \delta_1 \\ \delta_2 \\ \delta_{11} \\ \delta_{12} \\ \delta_{22} \end{pmatrix} + e$$

$$= Z\Delta + e .$$

If the initial experimental points in P are (-2, -3), (-2, 3), (2, -3) and (2, 3), then

$$Z_1 = \begin{pmatrix} 1 & -2 & -3 \\ 1 & -2 & 3 \\ 1 & 2 & -3 \\ 1 & 2 & 3 \end{pmatrix} .$$

If an additional experiment is run at $z = (5, 6)$, then $Z_2 = (1, 5, 6)$.

Definition 4.2 . The space of the coded process space variables will be called the design space and will be denoted by D.

The symbols x, X, X_1 and X_2 will be used in D in the same fashion as the symbols z, Z, Z_1, and Z_2 are used in P.

In order to map the points of a p-dimensional rectangle in P into a unit grid whose center is at the origin in D, a translation followed by a change of scale must be used. No loss of generality will occur if it is assumed that the center of the rectangle in P has already been translated to the origin in P. With this assumption the mapping of the rectangular grid in P to the unit grid in D can be accomplished by a change in scale alone.

<u>Definition 4.3 .</u> The transformation which maps the unit grid points of D into the grid points of P will be denoted by T_1.

As an example suppose that $p = 2$ and that the process points are (-40, -20) , (-40, 20), (40, -20) and (40, 20), then the mapping required to transform the unit grid points into the process points is represented by the equation

$$(1, z_1, z_2) = (1, x_1, x_2) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 40 & 0 \\ 0 & 0 & 20 \end{pmatrix}.$$ In this example

T_1 is the matrix $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 40 & 0 \\ 0 & 0 & 20 \end{pmatrix}$. It is to be noticed that T_1 is associated with the decoding and is specified at the moment that the experimenter chooses the process space grid points.

Whereas T_1 will be used with the $1 \times p + 1$ matrices X_1 and Z_1, T will be used with the $1 \times q$ matrices X and Z. For example, suppose that

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

$$= X\beta + e.$$

In this case the transformation $Z = XT$ may be written out as

$$(1, z_1, z_2, z_{11}, z_1 z_2, z_{22}) = (1, x_1, x_2, x_{11}, x_1 x_2, x_{22})\,\text{diag.}\,(1, t_1, t_2, t_1^2, t_1 t_2, t_2^2).$$

Evidently the matrix T_1 determines the matrix T.

It is necessary to distinguish between the steepest ascent line fitted to the unit grid in D, its map in P, and the steepest ascent line in P calculated from the process grid points.

Definition 4.4 . The steepest ascent line calculated in D from a unit grid will be denoted by L_d. The transform of L_d will be denoted by L_t. The steepest ascent line in P calculated from the experimental grid points will be denoted by L_p.

It is indeed unfortunate that it is generally necessary to distinguish between L_t and L_p. That this is true is the content of theorem 4.1.

Theorem 4.1. A necessary and sufficient condition that $L_t = L_p$ is that

$$T_1 = \text{diag.} \ (1, t I_p) \ . \qquad (4.1)$$

Proof: In order to prove necessity let the response in D be given by

$$y = X \beta + e \qquad (4.2)$$

where X is $1 \times q$ and β is $q \times t$. Let $T_1 = \text{diag.}(1, t_1, \ldots t_p)$.

Now L_d is determined by the equations

$$x_j = \frac{\hat{\beta}_j}{\hat{\beta}_1} x_1, \quad j = 2, 3, \ldots, p. \qquad (4.3)$$

According to (4.1), $x_j = z_j/t_j$, $j = 0, 1, \ldots, p$

so that (4.3) becomes

$$\frac{z_j}{t_j} = \frac{\hat{\beta}_j}{\hat{\beta}_1}\frac{z_1}{t_1} \text{ or } z_j = \frac{t_j}{t_1}\frac{\hat{\beta}_j}{\hat{\beta}_1} z_1 \quad j = 2, 3, \ldots, p \quad (4.4)$$

Equation (4.4) determines the line L_t. It is necessary to find the expression for L_p. Since $Z = XT$, $X = ZT^{-1}$ which may be substituted in (4.2) to obtain

$$y = Z T^{-1} \beta + e = Z \Delta + e \quad (4.5)$$

where $\Delta = T^{-1} \beta$. It is desired to find $\hat{\Delta}$ in the equation

$$\hat{y} = Z \hat{\Delta} \quad (4.6)$$

where Z is $1 \times p+1$ and $\hat{\Delta}$ is $p+1 \times 1$. According to least squares,

$$\hat{\Delta} = (Z_1' Z_1)^{-1} Z_1' Y_1$$

$$= (T_1 X_1' X_1 T_1)^{-1} T_1 X_1' Y_1$$

$$= (N T_1^2)^{-1} T_1 X_1' Y_1 = N^{-1} T_1^{-1} X_1' Y_1$$

$$= T_1^{-1} \hat{\beta}$$

where $N = 2^p$. Then the line L_p is determined by the equations

$$z_j = \frac{\frac{\hat{\beta}_j}{t_j}}{\frac{\hat{\beta}_1}{t_1}} z_1 = \frac{t_1 \hat{\beta}_j}{t_j \hat{\beta}_1} z_1, \quad j = 2, 3, \ldots, p. \quad (4.8)$$

Hence if the line L_p is to be the same as the line L_t, then by (4.4) and (4.8) ,

$$\frac{t_j}{t_1} \frac{\hat{\beta}_j}{\hat{\beta}_1} = \frac{t_1 \hat{\beta}_j}{t_j \hat{\beta}_1} , \qquad j = 2, 3, \ldots , p$$

which implies that

$$t_1 = t_2 = \ldots , = t_p .$$

That T_1 = diag. $(1, t I_p)$ is a sufficient condition follows from equations (4.4) and (4.8) .

It is instructive to examine the steepest ascent procedure in the light of theorem 4.1. The experimenter determines T_1 at the outset. In theory, experimentation along the path of steepest ascent is an attempt to proceed in a direction which is normal to the factor space contours at the center of the experiment. Now the lines L_p and L_t cannot both be normal to the contours at the same point in P. A little reflection convinces one that it is the line L_p which is trying to estimate the gradient at the center of the rectangle in P. However, the method of steepest ascent calls for further experimentation on L_t. The situation is shown in figure 4.

Experimentation Along the Transformed Path of Steepest Ascent

The lack of scale invariance exhibited by the steepest ascent line and the invariance property of the steepest ascent line, previously examined in chapter III , combine in the present instance to make matters still more bizarre.

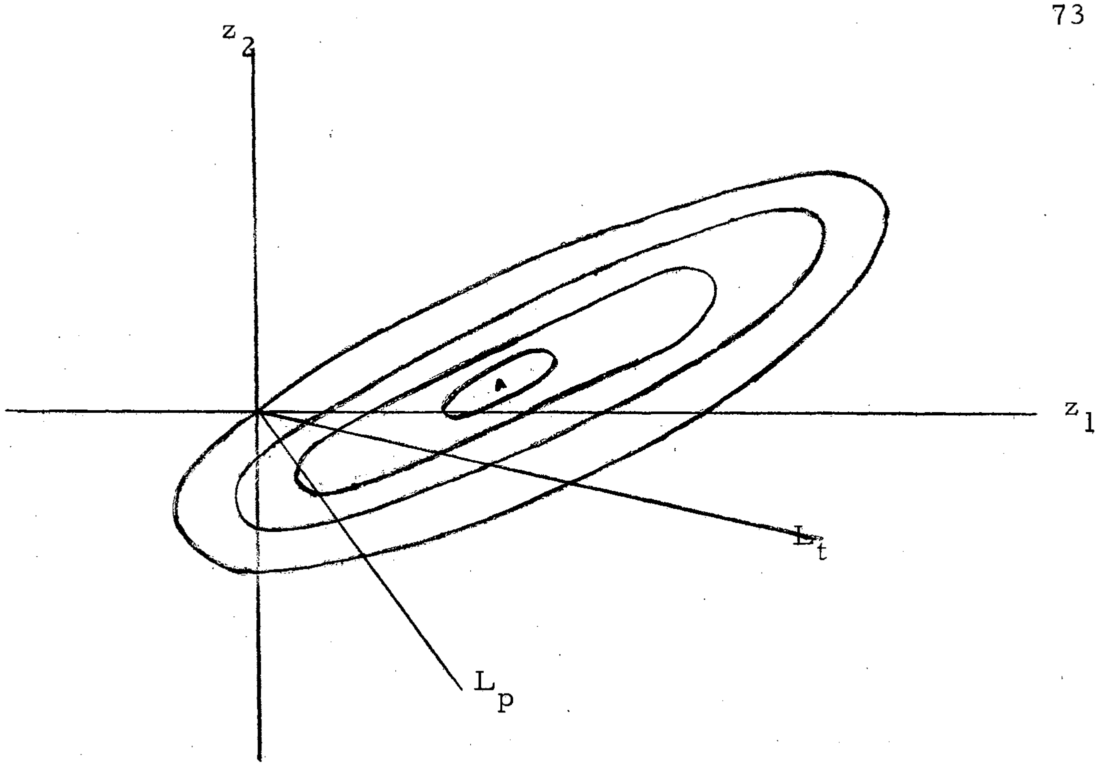

Figure 4. The Effect of a Change of Scale on the Steepest Ascent Path .

It is known from chapter III that if an additional point is run on the line L_d and a new path calculated, the new path will still be the line L_d . The additional point on L_d maps by T_1 to an additional point on L_t. Suppose that in P a second steepest ascent path is calculated by use of the process points and the additional point on L_t. What is the new steepest ascent line in the space P? In order to answer this question it is necessary to examine the property of invariance using a p-dimensional rectangular grid instead of a p - dimensional unit grid as in chapter III.

<u>Theorem 4, 2 .</u> The steepest ascent line L_p is invariant if the additional point is on the line L_t.

Proof: The additional point on L_t is the map of an additional point on L_d. Let the point on L_d be written in matrix form as

$$X_2 = (1, h\hat{\beta}_1, \ldots h\hat{\beta}_p) = (1, h B_1') . \qquad (4.9)$$

The additional point is mapped from D to P by

$$Z_2 = X_2 \; T_1 . \qquad (4.10)$$

T_1 may be partitioned as

$$T_1 = \begin{pmatrix} 1 & 0 \\ 0 & \text{diag.}(t, \ldots t_p) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & T_{11} \end{pmatrix} . \qquad (4.11)$$

Substituting X_2 as given in (4.9) in (4.10) and partitioning T_1 as in (4.11), there results

$$Z_2 = (1, hB_1') \begin{pmatrix} 1 & 0 \\ 0 & T_{11} \end{pmatrix} = (1, hB_1' T_{11}) . \qquad (4.12)$$

As in theorem 4.1, the equation $y = X\beta + e$ in D becomes the equation $y = Z \Delta + e$ in P where

$$\Delta = T^{-1} \beta .$$

Let

$$\hat{\Delta} = \begin{pmatrix} \hat{\delta}_0 \\ \hline \hat{\delta}_1 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\delta}_p \end{pmatrix} = \begin{pmatrix} \hat{\Delta}_0 \\ \hat{\Delta}_1 \end{pmatrix}$$ be calculated from the initial experimental

points. Let $\hat{\alpha} = \begin{pmatrix} \hat{\alpha}_0 \\ \hline \hat{\alpha}_1 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\alpha}_p \end{pmatrix} = \begin{pmatrix} \hat{A}_0 \\ \hat{A}_1 \end{pmatrix}$ be the revision of $\hat{\Delta}$

based on the initial experimental points and the additional point Z_2 on L_t. Then according to (3.11) ,

$$\hat{\alpha} = \hat{\Delta} + J' G Q \qquad (4.13)$$

where the symbols J, G, and Q are used as in theorem 3, 7 . By definition

$$J = Z_2 (Z_1'Z_1)^{-1} \quad \text{so that} \quad J' = (Z_1' Z_1)^{-1} Z_2' . \qquad (4.14)$$

$$\text{Now } (Z_1' Z_1)^{-1} = (T_1 X_1' X_1 T_1)^{-1} = \frac{(T_1^2)^{-1}}{N}$$

$$= \frac{1}{N} \begin{pmatrix} 1 & 0 \\ 0 & (T_{11}^2)^{-1} \end{pmatrix} \text{ where } N = 2^p. \qquad (4.15)$$

Substituting the expression for Z_2 as given in (4.12) and the expression for $(Z_1' Z_1)^{-1}$ as given in (4.15) into the expression for J' as given in (4.14), there results

$$J' = \frac{1}{N} \begin{pmatrix} 1 & 0 \\ 0 & (T_{11}^2)^{-1} \end{pmatrix} \begin{pmatrix} 1 \\ hT_{11}B_1 \end{pmatrix} = \frac{1}{N} \begin{pmatrix} 1 \\ hT_{11}^{-1}B_1 \end{pmatrix}$$

$$= \frac{1}{N} \begin{pmatrix} 1 \\ h \hat{\Delta}_1 \end{pmatrix} . \qquad (4.16)$$

Substituting the value of J' as given in (4.16) into the expression for $\hat{a}$ given in (4.13) and noting that $G\,Q$ is a scalar, there results

$$\begin{pmatrix} \hat{A}_0 \\ \hat{A}_1 \end{pmatrix} = \begin{pmatrix} \hat{\Delta}_0 \\ \hat{\Delta}_1 \end{pmatrix} + \frac{G\,Q}{N} \begin{pmatrix} 1 \\ h\,\hat{\Delta}_1 \end{pmatrix} . \tag{4.17}$$

It follows that

$$\hat{A}_1 = \hat{\Delta}_1 + \frac{G\,Q}{Nh}\,\hat{\Delta}_1 = \hat{\Delta}_1\left(1 + \frac{G\,Q}{N\,h} \right) = k\,\hat{\Delta}_1 \tag{4.18}$$

where the scalar $k = 1 + \dfrac{G\,Q}{N\,h}$. Hence $\hat{A}_1$ is a scalar multiple of $\hat{\Delta}_1$ so that the path L_p remains unchanged

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The theorem 4.2 generalizes so that the line L_p remains invariant regardless of how many additional points are taken on L_t.

<u>Theorem 4.3 .</u> The steepest ascent line L_p is invariant if N_2 additional points are taken on L_t .

Proof: The N_2 additional points on L_d , written in matrix notation as

$$X_2 = \left(\begin{array}{c|cccc} 1 & h_1\hat{\beta}_1 & h_1\hat{\beta}_2 & \cdots & h_1\hat{\beta}_p \\ 1 & h_2\hat{\beta}_1 & h_2\hat{\beta}_2 & \cdots & h_2\hat{\beta}_p \\ \cdot & \cdot & & & \\ \cdot & \cdot & & & \\ \cdot & \cdot & & & \\ 1 & h_{N_2}\hat{\beta}_1 & h_{N_2}\hat{\beta}_2 & \cdots & h_{N_2}\hat{\beta}_p \end{array} \right) = (W_0, HB_1') ,$$

map to N_2 additional points on L_t. This may be written as

$$Z_2 = X_2 T_1 = (W_0, H B_1') \begin{pmatrix} 1 & 0 \\ 0 & T_{11} \end{pmatrix} = (W_0, HB_1' T_{11}). \quad (4.19)$$

Let $\hat{a}$ and $\hat{\Delta}$ be as in theorem 4.2. Then

$$J' = (Z_1' Z_1)^{-1} Z_2' = \frac{1}{N} \begin{pmatrix} 1 & 0 \\ 0 & (T_{11}^2)^{-1} \end{pmatrix} \begin{pmatrix} W_0' \\ T_{11} B_1 H' \end{pmatrix}$$

$$= \frac{1}{N} \begin{pmatrix} W_0' \\ T_{11}^{-1} B_1 H' \end{pmatrix} . \quad (4.20)$$

Substituting this expression for J' into the equation $\hat{a} = \hat{\Delta} + J'GQ$, there results

$$\begin{pmatrix} \hat{A}_0 \\ \hat{A}_1 \end{pmatrix} = \begin{pmatrix} \hat{\Delta}_0 \\ \hat{\Delta}_1 \end{pmatrix} + \frac{1}{N} \begin{pmatrix} W_0' \\ T_{11}^{-1} B_1 H' \end{pmatrix} GQ. \quad (4.21)$$

Hence

$$\hat{A}_1 = \hat{\Delta}_1 + \frac{1}{N} T_{11}^{-1} B_1 H' G Q . \quad (4.22)$$

Now $H'GQ$ is a scalar so that (4.22) becomes

$$\hat{A}_1 = \hat{\Delta}_1 + \frac{H'GQ}{N} T_{11}^{-1} B_1 = \hat{\Delta}_1 + \frac{H'GQ}{N} \hat{\Delta}_1$$

$$= \hat{\Delta}_1 \left(1 + \frac{H'GQ}{N} \right) = k \hat{\Delta}_1 \quad (4.23)$$

where $k = 1 + \dfrac{H'GQ}{N}$. Hence $\hat{A}_1$ is a scalar multiple of $\hat{\Delta}_1$ and the path L_p remains unchanged.

The Choice Between the Lines L_d and L_p

It is clear from the preceding theorems that in P, the path of steepest ascent and the path upon which the experiments are being run, are generally distinct. Since experimentation along the path L_t is customary rather than mandatory, it is fair to ask which path comes closest to the true maximum. The answer depends upon the structure of η in the equation $y = \eta + e$. The complexity of the problem increases with the dimension p and the degree of η. In order to simplify the problem and visualize the geometry involved, let η be of second degree in the variables x_1 and x_2.

Under the transformation

$$z_1 = t_1 x_1$$

$$z_2 = t_2 x_2 ,$$

the response in D, which is written

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

is written in P as

$$y = \delta_0 + \delta_1 z_1 + \delta_2 z_2 + \delta_{11} z_1^2 + \delta_{12} z_1 z_2 + \delta_{22} z_2^2 + e$$

where $\delta_0 = \beta_0, \delta_1 = \beta_1 / t_1, \ldots \delta_{22} = \beta_{22}/t_2^2$.

The coordinates of the maximum of η in P are by (3.74) ,

$$z_1^* = \frac{2\delta_1\delta_{22} - \delta_2\delta_{12}}{\delta_{12}^2 - 4\delta_{11}\delta_{22}}$$

$$z_2^* = \frac{2\delta_2\delta_{11} - \delta_1\delta_{12}}{\delta_{12}^2 - 4\delta_{11}\delta_{22}} . \qquad (4.24)$$

The equation of the line joining $(0, 0)$ to (z_1^*, z_2^*) is then

$$z_2 = \frac{2\delta_2\delta_{11} - \delta_1\delta_{12}}{2\delta_1\delta_{22} - \delta_2\delta_{12}} z_1. \qquad (4.25)$$

Definition 4.5 . Let the line joining the origin to the point in the P space where the response is maximized be called L_m. There have been three lines defined in P, the lines L_t, L_p, and L_m . Their equations in terms of the β 's are

$$L_t: \quad z_2 = \frac{t_2 \hat{\beta}_2}{t_1 \hat{\beta}_1} z_1 , \qquad (4.26)$$

$$L_p: \quad z_2 = \frac{t_1 \hat{\beta}_2}{t_2 \hat{\beta}_1} z_1, \qquad (4.27)$$

and

$$L_m: \quad z_2 = \frac{t_2 (2\beta_2\beta_{11} - \beta_1\beta_{12})}{t_1 (2\beta_1\beta_{22} - \beta_2\beta_{12})} z_1. \qquad (4.28)$$

The various angles that these lines make with one another may be found by use of the formula

$$\tan \theta = \frac{m_2 - m_1}{1 + m_1 m_2}$$ where θ, m_1, and m_2 are the

conventional symbols of analytic geometry. One might be inclined to choose the path for which the angle between the path and the line to the maximum is minimized. Alternatively, with the aid of equation (3.78), a comparison could be made between the maximum value of η attainable on L_t and the maximum value of η attainable on L_p. Each of the above approaches are algebraically involved and shed little light upon the strategy that the experimenter should adopt. For this reason the discussion will be of a geometrical nature taking full advantage of the simplicity of a two dimensional factor space.

Frequently the investigator will feel that he knows, in a general way, the orientation of the contour system. Naturally he will choose the initial experimental points to be in harmony with his conjecture. Thus, if the experimenter's conception of the contour system is as in figure 5, he would be quite likely to feel that the rectangular grid shown there is appropriate.

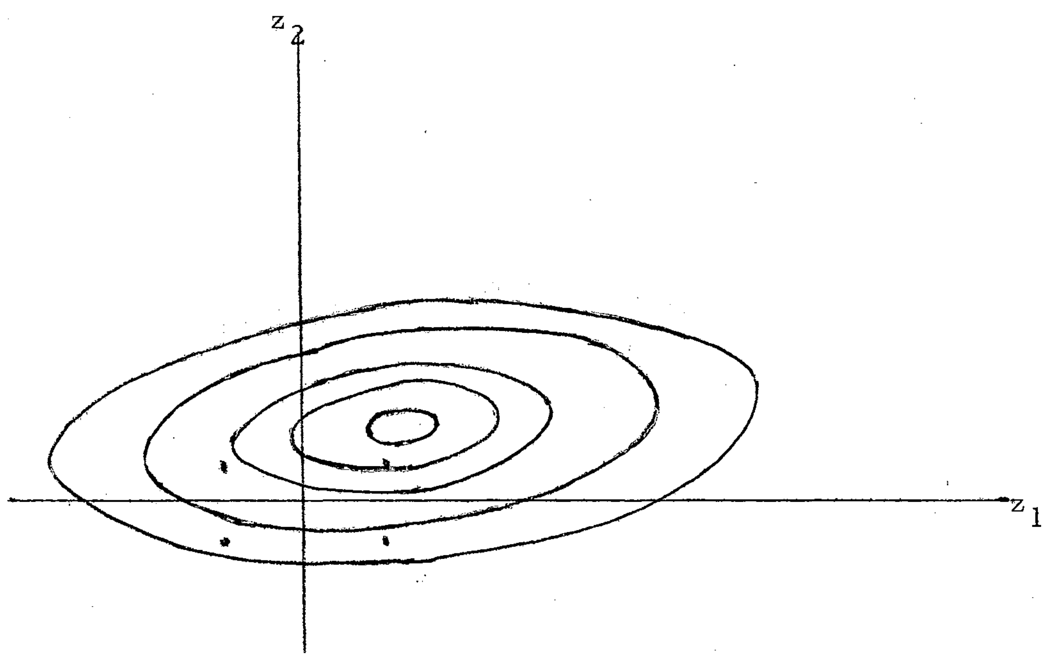

Figure 5. An Appropriate Grid for Horizontal Elongated Contours.

The mapping of the unit grid points in D to the rectangle in P may be written

$$z_1 = t_1 x_1$$

$$z_2 = t_2 x_2$$

where, in accordance with figure 5, $t_1 > t_2$.

Let the true maximum of a horizontal elongated contour system be in the first quadrant and assume that the slope of the major axis is positive. Under these conditions there are four distinct cases which may arise. The first case is shown in figure 6.

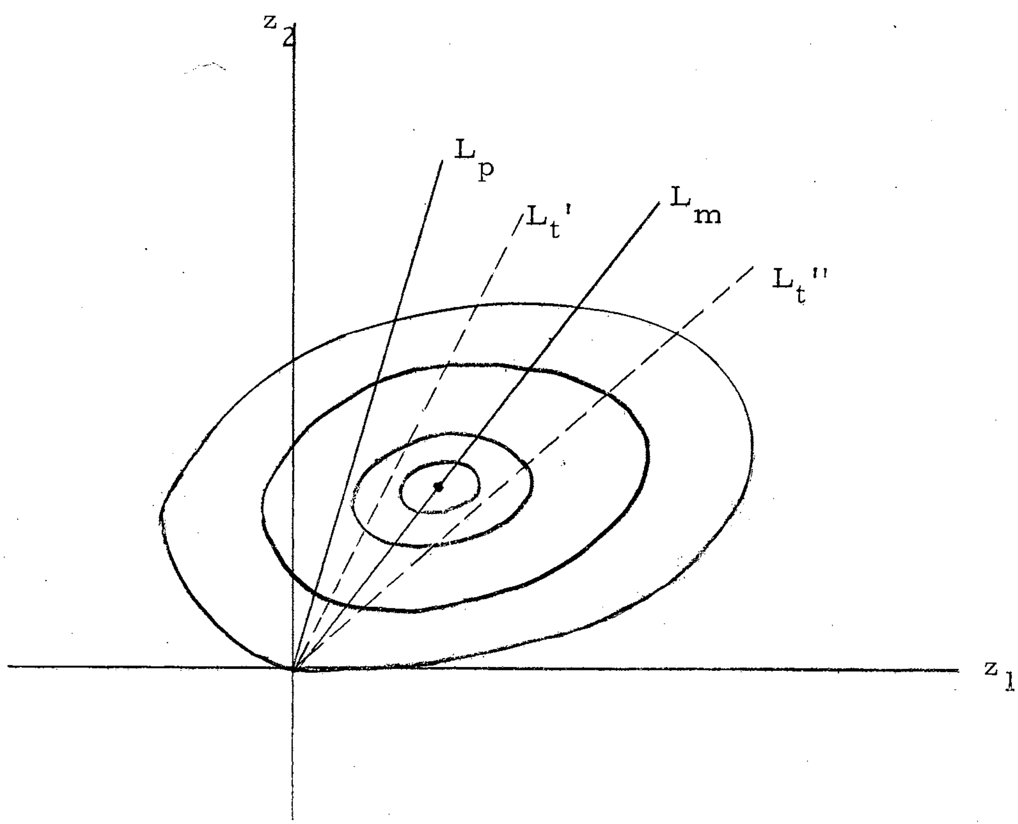

Figure 6. The Slope of L_p is Positive; There is no Basis for a Decision.

The line L_t can have either of the positions indicated in figure 6 by L_t' or L_t''. The choice as to which path to take is left to the judgement of the experimenter.

In figure 7 the line L_p lies between the line to the true maximum and the line L_t. Hence, the experimenter should choose the line L_p for further experimentation.

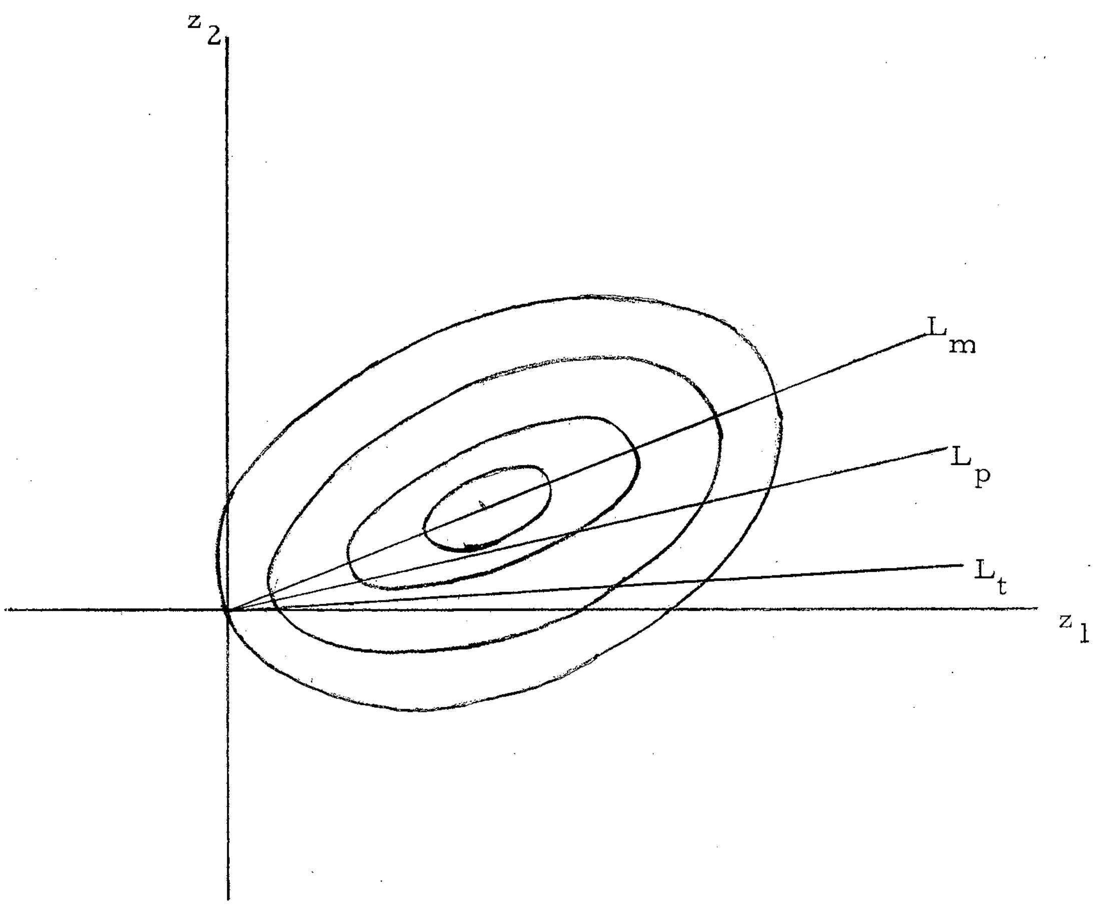

Figure 7. The Slope of L_p is Positive; the Line L_p Should be Chosen .

In the third case, the slopes of the lines L_t and L_p are both negative as shown in figure 8 .

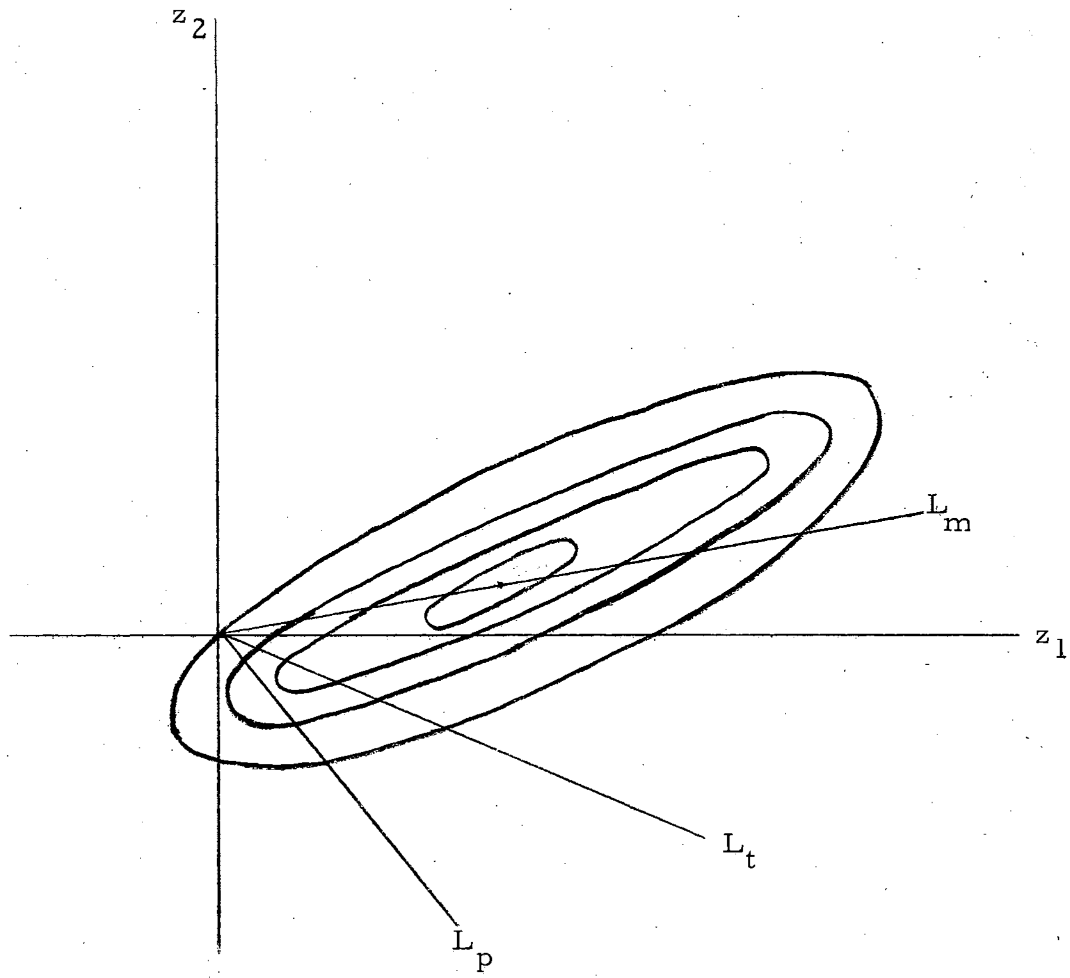

Figure 8. The Slope of L_p is Negative; the Line L_t Should be Chosen.

The line L_t should be chosen as a path for further experimentation since it lies between L_p and L_m.

In figure 9 the slopes of L_t and L_p are negative. L_p should be chosen as a path for further experimentation since it lies between L_t and L_m.

Similar analyses are applicable to the various other orientations of the contour system axes which the experimenter may suspect.

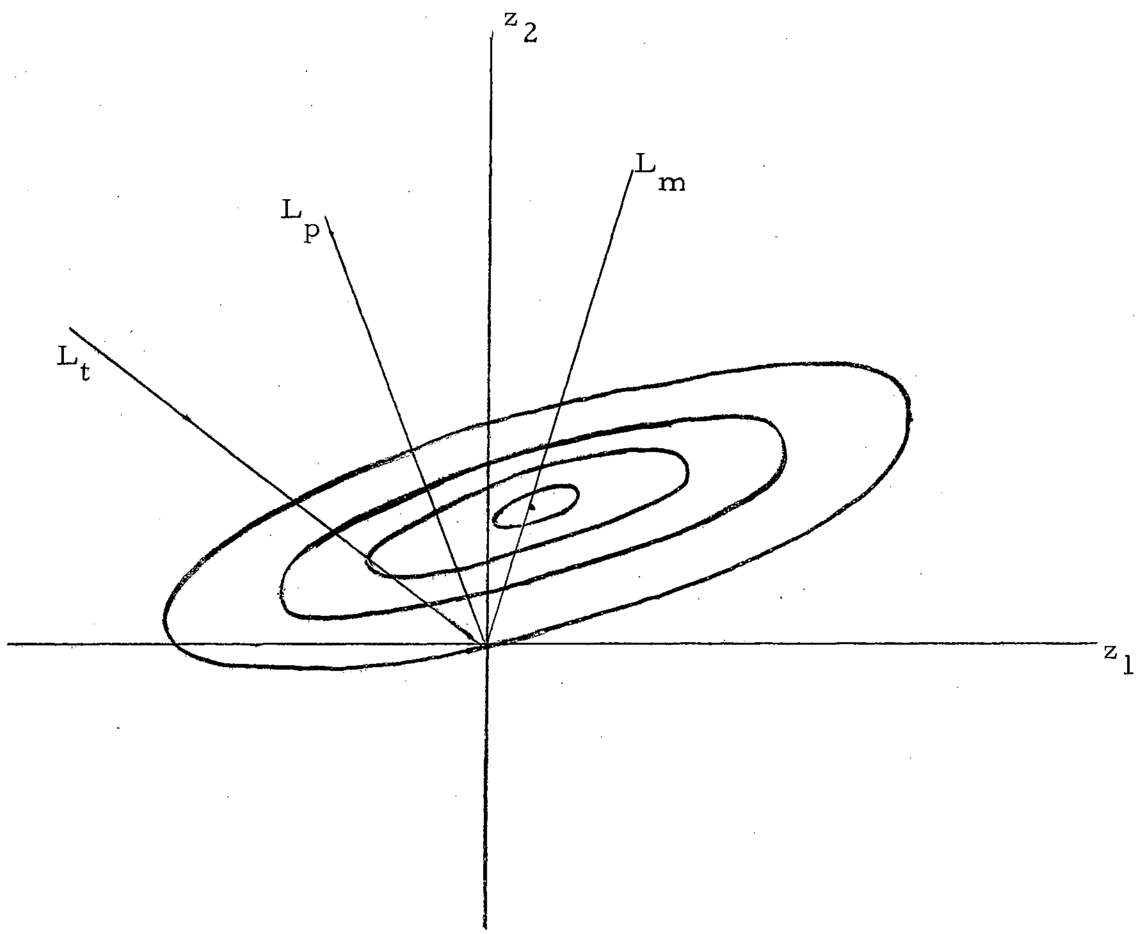

Figure 9. The Slope of L_p is negative; the Line L_p Should be Chosen.

The foregoing remarks are applicable to a p-dimensional factor space. Should information regarding the orientation of any one of the p axes become available, the preceding arguments remain valid.

CHAPTER V

SUMMARY

The method of steepest ascent is part of a general technique which has been proposed to locate a maximum, minimum, or stationary point in the factor space. The use of the steepest ascent method is often accompanied by scant knowledge of its properties. In this study various properties of the steepest ascent path are investigated. Particular attention is given to the estimation of the coefficients of the fitted plane which determine the path of steepest ascent, the direction of additional paths calculated by the use of points on the first path, and the behavior of the steepest ascent path when subjected to a change of scale.

Conclusions

In chapter II several theorems are presented which are concerned with the coefficients of the plane fitted to a quadratic response function. This plane is fitted by the method of least squares from a rectangular grid in the factor space. It is shown that the linear coefficeints of the fitted plane are unbiased estimates of the first order partial derivatives of the response function evaluated at the center of the grid.

It is shown that, in the absence of experimental error, a p-dimensional hyperplane passes through the responses at the 2^p points in the factor space provided that there are no cross product terms in the quadratic response function. This surprising fact is used to divide the factor space into three-point sets, the set where the predicted response $\hat{y}$ equals the observed response y, the set where $y > \hat{y}$, and the set where $y < \hat{y}$.

Also it is shown that decreasing the variance of $\hat{\beta}_1$ or $\hat{\beta}_2$ by increasing the design size results in an increase in the bias of these estimators. Since mean square error is dependent on both bias and variance, a study is made of the relationship between design size and mean square error. A design size is given which will minimize the mean square error in the case where a quadratic response model is chosen, when in truth, the response function is cubic.

In chapter III it is shown that the revised path of steepest ascent, calculated by means of the initial grid and additional points on the initial steepest ascent line, is the same as the initial path of steepest ascent. This property of the steepest ascent line, termed invariance, is shown to hold when an arbitrary number of additional points are added to the initial steepest ascent line. It is shown that the three conditions, invariance, location on the path of steepest ascent, and the use of a square grid, are so related that any two of them imply the third. These results make it impossible to obtain a different path of steepest ascent by this approach.

An expression is obtained for $\hat{y}_2$ in terms of $\hat{y}_1$ and y where $\hat{y}_2$ is the response predicted on the basis of $N + 1$ points, $\hat{y}_1$ is the response predicted on the basis of N points, and y is the observed response. It is shown that $\hat{y}_2$ is a convex combination of y and $\hat{y}_1$.

If the contours are elliptic and a point exists in the factor space where the response is maximized, a method is given whereby upper and lower bounds to the ratio β_{11}/β_{22} may be estimated. Some properties of the gradient line are examined. The coordinates of the maximum response attainable on the gradient line and the value of the response at that point are given.

Chapter IV deals with the behavior of the steepest ascent line when it is subjected to a change of scale. Necessary and sufficient conditions are given for the steepest ascent line to be invariant under a change of scale.

It is shown that if points along the transform of the steepest ascent path in the space of the coded variables are used, together with the initial experimental points, to calculate a revised path of steepest ascent, the revised path will be the same as the initial path.

Examples are given which demonstrate the manner in which prior knowledge of the general orientation of the contour system may be used in making a choice between the transform of the coded steepest ascent line and the steepest ascent line in the uncoded variables.

Areas for Future Research

As additional experiments are performed along the path of steepest ascent, the transformed path of steepest ascent, or indeed any line, additional information becomes available at each point. This information is, of course, contained in the value of the observation at the additional point. A reasonable strategy would be to use this information to revise the path before proceeding to the next point. Although the unexpected invariance property seems to be an obstacle to such a strategy, further work should be done in this area.

Instead of experimenting along some path believed to be desirable, it might be just as well to estimate all of the unknown parameters initially and proceed along the path to the maximum calculated from the estimated parameters. For example, in the case of a quadratic response in two variables, the six unknown parameters could be estimated by means of an initial six point design in the factor space. As a competing strategy, the unknown parameters could be estimated by means of the initial design points and points along the line of steepest ascent. In the example of the six unknown parameters, the full quadratic could be estimated upon the completion of the second experiment on the steepest ascent line. The difficulty lies in finding an adequate basis for comparing these strategies.

The discussion in chapter IV concerning the choice between the lines L_p and L_t was restricted severely. The more general case, in which the location of the true maximum and the orientation of the contour system are arbitrary, needs attention. This problem should be analyzed both from an algebraic and a geometric viewpoint.

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