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MISSILE SYSTEM PERFORMANCE PARAMETER OPTIMIZATION MODEL

by

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The approach is to find conditions which maximize a "primary response" subject to the constraint that a "secondary response" takes on some specified or desirable value. An algorithm is outlined whereby a user can generate simple two dimensional plots to determine the conditions of constrained maximum primary response subject to the secondary response taking on any value he wishes. He, thus, is able to reduce to simple plotting the complex task of exploring the dual response system.

In certain situations it becomes necessary to apply a double constraint, the second being that the located operating conditions be a certain "distance" from the origin of the independent variables, (or the center of the experimental design).

The procedure applies to optimizing in cases where it is desirable to employ two measures of effectiveness, cost often being the prime candidate for the secondary response and a single measure of performance as the primary response.

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RESPONSE SURFACE EXPLORATION IN PROBLEMS INVOLVING TWO RESPONSES

1. Introduction

Much has been written concerning the exploration of an experimental region using response surface methods. Basically, a polynomial type response function is used to graduate a mechanism given by

$$\eta = g(x_1, x_2, \ldots, x_k)$$

in some experimental region. The most frequently fitted response function and the one to be used here is the quadratic model which gives rise to a fitted response function of the form

$$\hat{y} = b_0 + \underline{x}'\underline{b} + \underline{x}'B\underline{x}, \qquad (1.1)$$

where $\underline{x}$ is a vector of independent or design variables and $\hat{y}$ is the estimated response. The elements in $\underline{b}$ and B represent least squares estimators, the latter being a k x k matrix

$$B = \begin{bmatrix} b_{11} & b_{12}/2 & \cdots & b_{1k}/2 \\ & b_{22} & \cdots & b_{2k}/2 \\ & & & \vdots \\ & & & b_{kk} \end{bmatrix}$$

where the b_{ij} are second order coefficients. The total exploration following the estimation of (1.1) involves finding the stationary point

$$\underline{x}_0 = -B^{-1}\,\underline{b}/2$$

and conducting a canonical analysis to determine the nature of the stationary point. Discussions of these procedures are given in [1], [2], and [5].

Quite often the researcher is confronted with the problem of simultaneous optimization of two or more response variates. It is not unusual in this situation to obtain a solution, $\underline{x}$, which is optimal for one response and far from optimal or even physically impractical for the other(s). The task is then to arrive at some compromise conditions involving the two responses. The problem is a natural one but only a few papers dedicated to it have appeared in the statistical literature. See for example [4] and [6].

2. The Dual Response Problem

Let us suppose that the experimenter has a primary response, with fitted response function given by

$$\hat{y}_p = b_0^{(1)} + \underline{x}'\underline{b}^{(1)} + \underline{x}'B^{(1)}\underline{x} \tag{2.1}$$

and what we shall refer to as a <u>secondary</u> <u>response</u> (although indeed the two responses may be equally important) with response function given by

$$\hat{y}_s = b_0^{(2)} + \underline{x}'\underline{b}^{(2)} + \underline{x}'B^{(2)}\underline{x} \tag{2.2}$$

The expression in (2.2) may have been obtained from the same experiment through the use of multivariate multiple regression or perhaps externally. The latter may be the case when the secondary response is the cost variable in say a yield-cost study. Indeed, the coefficients in (2.2) may possibly not be random variables.

The solution proposed and discussed in the sequel is to find the conditions on $\underline{x}$ which optimize $\hat{y}_p$ subject to $\hat{y}_s = k$, where k is some desirable or acceptable value of the secondary response. (Actually, there are situations in which it is necessary to consider a double constraint. This will be discussed in a later section). To arrive at the solution mentioned above, Lagrangian multipliers are needed. Thus, we consider

$$L = b_0^{(1)} + \underline{b}^{(1)'}\underline{x} + \underline{x}'B^{(1)}\underline{x} - \mu(b_0^{(2)} + \underline{b}^{(2)'}\underline{x} + \underline{x}'B^{(2)}\underline{x} - k)$$

and require solutions for $\underline{x}$ to the set of equations

$$\frac{\partial L}{\partial \underline{x}} = \underline{0}$$

which results in the following:

$$(B^{(1)} - \mu B^{(2)})\underline{x} = \tfrac{1}{2}(\mu \underline{b}^{(2)} - \underline{b}^{(1)}). \tag{2.3}$$

It is important at this point to study the nature of the "stationary point" generated by equation (2.3). We begin by considering the matrix of second partial derivatives, the (i, j) element of which is

$$\frac{\partial^2 L}{\partial x_i \, \partial x_j} \quad (i, j = 1,2,\ldots,k).$$

It follows immediately that

$$M(\underline{x}) = 2(B^{(1)} - \mu B^{(2)}). \tag{2.4}$$

Much of the development that follows is somewhat similar to the approach taken by Draper [3] in Ridge Analysis. In fact, one can consider Ridge Analysis in which it is desired to maximize an estimated response, $\hat{y}$, subject to the constraint $\underline{x}'\underline{x} = R^2$, as a special case of the dual response problem. However, in the dual response problem, the solution must depend on the nature of the matrices $B^{(1)}$ and $B^{(2)}$.

It is well known that if the matrix of second partial derivatives given by equation (2.4) is negative definite, the value of $\underline{x}$ generated by equation (2.3) will give rise to a local maximum on $\hat{y}_p$ (local minimum if the matrix of second partials is positive definite). Therefore, rather than fixing $\hat{y}_s = k$, an appropriate procedure would be to select directly values of the Lagrange multiplier, μ, in the region which gives rise to operating conditions on $\underline{x}$ from (2.3) that result in absolute maxima on $\hat{y}_p$, conditional on being on a surface of the secondary response given by (2.2). In what follows, we make use of the following theorem.

Theorem 2.1: Let $\underline{x}_1$ and $\underline{x}_2$ be solutions to equation (2.3), using μ_1 and μ_2 respectively and let $\hat{y}_{s,1} = \hat{y}_{s,2}$. If the matrix $(B^{(1)} - \mu_1 B^{(2)})$ is negative definite then $\hat{y}_{p,1} > \hat{y}_{p,2}$. It also follows that if $(B^{(1)} - \mu_1 B^{(2)})$ is positive definite, then $\hat{y}_{p,1} < \hat{y}_{p,2}$.

Proof

If $\underline{x}_1$ and $\underline{x}_2$ give rise to the same value of the secondary response, then

$$b_0^{(2)} \underline{x}_1' B^{(2)} \underline{x}_1 + \underline{x}_1' \underline{b}^{(2)} = \underline{x}_2' B^{(2)} \underline{x}_2 + \underline{x}_2' \underline{b}^{(2)} + b_0^{(2)} . \tag{2.5}$$

Consider now $\hat{y}_{p,1} - \hat{y}_{p,2}$. We can write

$$\hat{y}_{p,1} - \hat{y}_{p,2} = \underline{x}_1' B^{(1)} \underline{x}_1 - \underline{x}_2' B^{(1)} \underline{x}_2 + (\underline{x}_1' - \underline{x}_2')\underline{b}^{(1)}.$$

By adding and subtracting $\mu_1 \underline{x}_2' B^{(2)} \underline{x}_2$, we obtain

$$\hat{y}_{p,1} - \hat{y}_{p,2} = \underline{x}_1' B^{(1)} \underline{x}_1 - \underline{x}_2' (B^{(1)} - \mu_1 B^{(2)})\underline{x}_2 - \mu_1 \underline{x}_2' B^{(2)} \underline{x}_2 + (\underline{x}_1' - \underline{x}_2') \underline{b}^{(1)}. \tag{2.6}$$

From equation (2.3) with $\mu = \mu_1$ and $\underline{x} = \underline{x}_1$, we have

$$\underline{x}_1' B^{(1)} \underline{x}_1 = \mu_1 \underline{x}_1' B^{(2)} \underline{x}_1 + \tfrac{1}{2} \mu_1 \underline{x}_1' \underline{b}^{(2)} - \tfrac{1}{2} \underline{x}_1' \underline{b}^{(1)}$$

which from (2.5) becomes

$$\underline{x}_1' B^{(1)} \underline{x}_1 = \mu_1 \hat{y}_s - \mu_1 b_0^{(2)} - \tfrac{1}{2} \mu_1 \underline{x}_1' \underline{b}^{(2)} - \tfrac{1}{2} \underline{x}_1' \underline{b}^{(1)} . \tag{2.7}$$

From (2.5) we also have

$$\underline{x}_2' B^{(2)} \underline{x}_2 = \hat{y}_s - \underline{x}_2' \underline{b}^{(2)} - b_0^{(2)} . \tag{2.8}$$

Hence, from (2.7) and (2.8) it follows that

$$\underline{x}_1' B^{(1)} \underline{x}_1 - \mu_1 \underline{x}_2' B^{(2)} \underline{x}_2 = - \tfrac{1}{2} \mu_1 \underline{x}_1' \underline{b}^{(2)} + \mu_1 \underline{x}_2' \underline{b}^{(2)} - \tfrac{1}{2} \underline{x}_1' \underline{b}^{(1)}.$$

Thus, (2.6) becomes

$$\hat{y}_{p,1} - \hat{y}_{p,2} = (\underline{x}_2' - \tfrac{1}{2} \underline{x}_1') (\mu_1 \underline{b}^{(2)} - \underline{b}^{(1)}) - \underline{x}_2'(B^{(1)} - \mu_1 B^{(2)})\underline{x}_2.$$

From equation (2.3), we have

$$(\underline{x}_2{}' - \tfrac{1}{2}\,\underline{x}_1{}')\,(\mu_1\,\underline{b}^{(2)} - \underline{b}^{(1)}) = 2\underline{x}_2{}'\,(B^{(1)} - \mu_1\,B^{(2)})\,\underline{x}_1 - \underline{x}_1{}'\,(B^{(1)} - \mu_1\,B^{(2)})\,\underline{x}_1$$

and, as a result $\hat{y}_{p,1} - \hat{y}_{p,2} = (\underline{x}_2 - \underline{x}_1)'\,(B^{(1)} - \mu_1\,B^{(2)})\,(\underline{x}_1 - \underline{x}_2)$

$$= -\,(\underline{x}_1 - \underline{x}_2)'\,(B^{(1)} - \mu_1 B^{(2)})\,(\underline{x}_1 - \underline{x}_2) \qquad (2.9)$$

which is positive if $B^{(1)} - \mu_1\,B^{(2)}$ is a negative definite matrix and negative if $B^{(1)} - \mu_1\,B^{(2)}$ is a positive definite matrix.

Theorem (2.1) indicates that in the quest for values of $\underline{x}$ which yield constrained maxima (minima) we can limit ourselves to values of μ which make $B^{(1)} - \mu\,B^{(2)}$ negative definite (positive definite) assuming that such values exist. It shall be demonstrated that this "working region" in μ does often exist and that its location depends on the nature of the matrices $B^{(1)}$ and $B^{(2)}$. Equation (2.9) also indicates

$$\hat{y}_{p,1} - \hat{y}_{p,2} = (\underline{x}_1 - \underline{x}_2)'(B^{(1)} - \mu_2\,B^{(1)})\,(\underline{x}_1 - \underline{x}_2)$$

which implies that while $B^{(1)} - \mu_1\,B^{(2)}$ is negative definite, $B^{(1)} - \mu_2\,B^{(2)}$ cannot be negative definite unless both give rise to the same solution for $\underline{x}$. It will become apparent later that the latter cannot occur.

2.1 $B^{(2)}$ Positive Definite

Suppose that the stationary point of the secondary response results in a minimum, implying that $B^{(2)}$ is positive definite. Consider the quadratic form with matrix given by $M(\underline{x})$, i.e.,

$$q = \underline{u}'(B^{(1)} - \mu\,B^{(2)})\,\underline{u}$$

Since $B^{(2)}$ is symmetric positive definite, there exists a nonsingular matrix R (Rao [7]) such that

$$R'\,B^{(1)}R = \mathrm{diag}(\lambda_1,\ \lambda_2,\ \ldots\ \lambda_k)$$

and

$$R' B^{(2)} R = I_k.$$

Performing the transformation

$$\underline{u}' = \underline{v}' R'$$

we have

$$q = \underline{v}' \text{ diag } (\lambda_1 - \mu, \lambda_2 - \mu, \ldots, \lambda_k - \mu) \underline{v}. \tag{2.10}$$

The λ's are merely the eigenvalues of the real, symmetric matrix

$$D_2^{(-\frac{1}{2})} Q' B^{(1)} Q D_2^{(-\frac{1}{2})} = S. \tag{2.11}$$

Here Q is the orthogonal matrix for which

$$Q' B^{(2)} Q = D_2 \tag{2.12}$$

and D_2 is the diagonal matrix containing the eigenvalues of $B^{(2)}$. We use the notation $D_2^{(-\frac{1}{2})}$ to denote a diagonal matrix containing the reciprocals of the square roots of the eigenvalues of $B^{(2)}$. From equation (2.10), it is clear that we can insure a negative definite $M(\underline{x})$ if $\mu > \lambda_k$ (positive definite if $\mu < \lambda_1$) where $\lambda_1, \lambda_2, \ldots, \lambda_k$ are the eigenvalues of the matrix S arranged in ascending order. In what follows, it becomes apparent that this indeed defines the working region for μ and, in fact, any $\mu_i > \lambda_k$ yields $\underline{x}_i$ which gives rise to an absolute maximum $\hat{y}_{p,i}$ (absolute minimum for $\mu_i < \lambda_1$) conditional on being on a surface of secondary response given by

$$\hat{y}_{s,i} = b_0 + \underline{x}_i' \underline{b}^{(2)} + \underline{x}_i' B^{(2)} \underline{x}_i.$$

It turns out that by choosing μ values in this region one generates $\underline{x}$'s which give all possible values of $\hat{y}_s$.

The following theorem will be useful in obtaining an understanding of the relationship between the Lagrangian multiplier, μ, and the resulting estimated value of the secondary response function.

Theorem 2.2 : Let $\underline{x}$ be a solution to (2.3) where $B^{(2)}$ is positive definite. Then $\frac{\partial^2 \hat{y}_s}{\partial \mu^2} \geqslant 0$ with the equality holding only in the limit as μ approaches $\pm \infty$.

Proof :

Differentiating both sides of equations (2.2) and (2.3) with respect to μ yields

$$\frac{\partial \hat{y}_s}{d \mu} = \underline{b}_2' \frac{\partial \underline{x}}{\partial \mu} + 2\, \underline{x}'\, B^{(2)} \frac{d \underline{x}}{\partial \mu} \tag{2.13}$$

and

$$(B^{(1)} - \mu B^{(2)}) \frac{d \underline{x}}{\partial \mu} = \tfrac{1}{2} \underline{b}_2 + B^{(2)} \underline{x}. \tag{2.14}$$

Upon taking the second partial in (2.13) and (2.14) with respect to μ, one can write

$$\frac{\partial^2 \hat{y}_s}{\partial \mu^2} = \underline{b}_2' \frac{\partial^2 \underline{x}}{\partial \mu^2} + 2 \left[\underline{x}'\, B^{(2)} \frac{\partial^2 \underline{x}}{\partial \mu^2} + \frac{\partial \underline{x}'}{\partial \mu} B^{(2)} \frac{\partial \underline{x}}{\partial \mu} \right] \tag{2.15}$$

$$(B^{(1)} - \mu B^{(2)}) \frac{\partial^2 \underline{x}}{\partial \mu^2} = 2\, B^{(2)} \frac{\partial \underline{x}}{\partial \mu} \tag{2.16}$$

Upon premultiplying (2.14) by $\frac{\partial^2 \underline{x}'}{\partial \mu^2}$ and (2.16) by $\frac{\partial \underline{x}'}{\partial \mu}$ and subtracting the resulting equations we find that

$$\tfrac{1}{2} \underline{b}_2' \frac{\partial^2 \underline{x}}{\partial \mu^2} = 2 \frac{\partial \underline{x}'}{\partial \mu} B^{(2)} \frac{\partial \underline{x}}{\partial \mu} - \underline{x}'\, B^{(2)} \frac{\partial^2 \underline{x}}{\partial \mu^2} \quad . \tag{2.17}$$

Substituting the expression for $\underline{b}_2' \frac{\partial^2 \underline{x}}{\partial \mu^2}$ from (2.17) into (2.15) results in

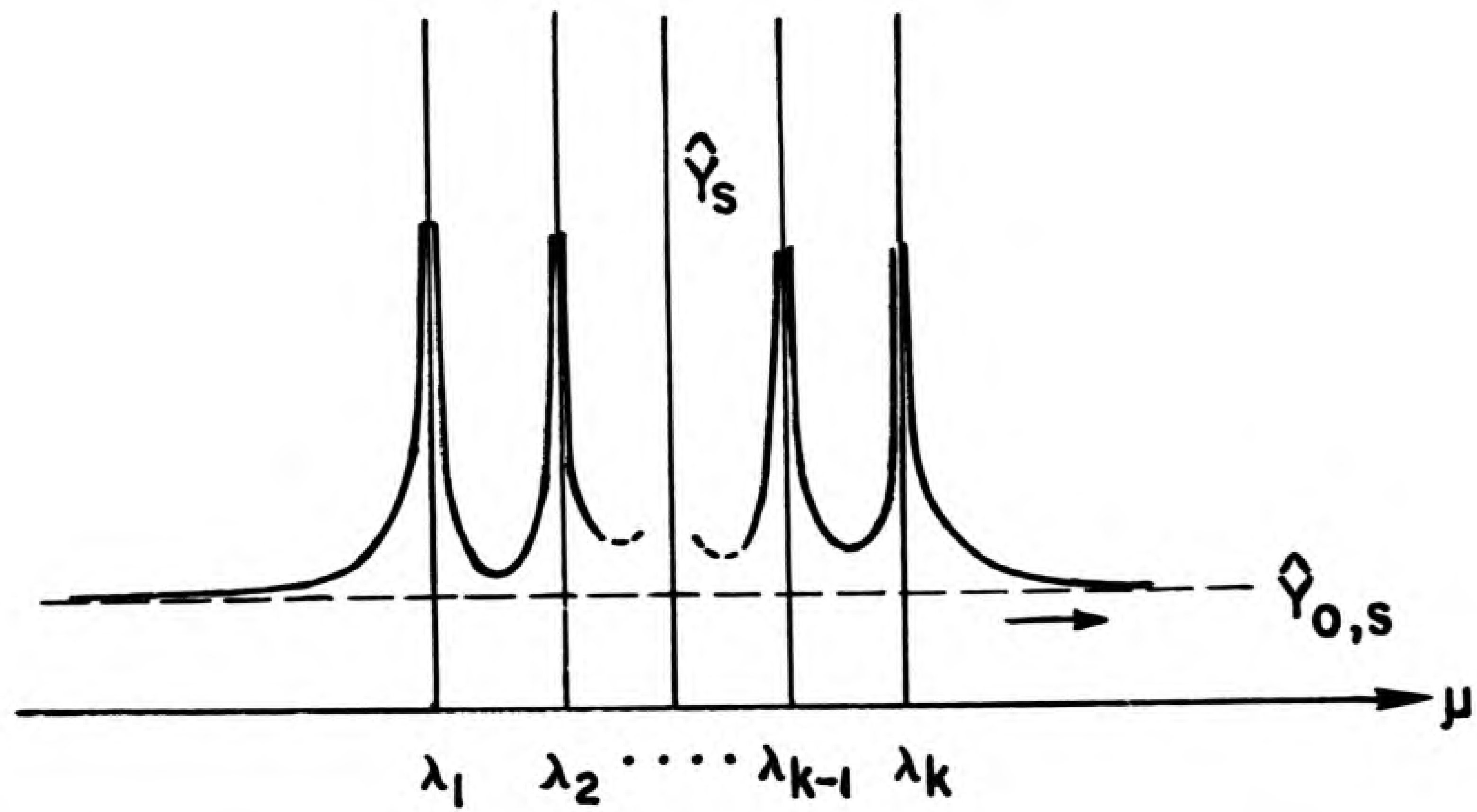

Fig. 2.1 PLOT OF $\hat{Y}_s$ AGAINST μ.

$$\frac{\partial^2 \hat{y}_s}{\partial \mu^2} = 6 \frac{\partial \underline{x}'}{\partial \mu} B^{(2)} \frac{\partial \underline{x}'}{\partial \mu}$$

which, of course, is positive except when $\frac{\partial \underline{x}}{\partial \mu} = \underline{0}$. From (2.3) and (2.14) $\frac{d \underline{x}}{\partial \mu} = 0$ only in the limit as μ approaches either plus or minus infinity.

It is important to note that the relationship between $\hat{y}_s$ and μ is of the form illustrated in Figure (2.1). In the figure, $\hat{y}_{s,0}$ is the value of the estimated secondary response function at its stationary point, the latter being a point of minimum response. The existence of the asymptotes is easily seen since from (2.3)

$$\lim_{\mu \to \infty} \underline{x} = -\frac{B^{(2)^{-1}} \underline{b}^{(2)}}{2} = \underline{x}_{s,0}$$

which is the center or stationary point for the secondary system. As μ approaches λ_i $(i = 1,2,...,k)$, $\hat{y}_s$ approaches infinity since

$$|B^{(1)} - \lambda_i B^{(2)}| = 0. \qquad (i = 1,2,...,k)$$

Hence, the asymptotes at the λ_i .

Theorems (2.1) and (2.2) indicate that the "working region" for μ resulting in a maximization of $\hat{y}_p$, subject to specific values of $\hat{y}_s$ is $\mu > \lambda_k$ and $\mu < \lambda_1$ for minimization. In a practical situation, interest would only be centered upon that part of the working region that generates values of $\hat{y}_s$ and thus $\underline{x}$ in the region of the experiment which generated either or both response functions. The procedure of determining operating conditions can be reduced to one of constructing a few simple graphs. Numerical examples of this procedure are given in a later section following the discussion of the problem for the case where $B^{(2)}$ is negative definite.

2.2 $B^{(2)}$ Negative Definite

When $B^{(2)}$ is negative definite, the stationary point for the secondary response function is a point of maximum response. Much of the development given in the previous section carries over, with a few modifications that deserve some attention. Consider again the matrix M(x) given in equation (2.4) and the associated quadratic form $q = \underline{u}' (B^{(1)} - \mu B^{(2)})\underline{u}$. Again, there exists an orthogonal matrix Q for which

$$Q' B^{(2)} Q = D_2 \tag{2.18}$$

where D_2 is a diagonal matrix containing negative values. Let the matrix $D_2^* = - D_2$ and make the transformation

$$\underline{u} = Q D_2^{*(-\frac{1}{2})} \underline{y},$$

where $D_2^{*(-\frac{1}{2})}$ is diagonal containing reciprocals of square roots of the diagonal elements of D_2^*. Therefore, the quadratic form q can be written as

$$q = \underline{y}' \left[P' B^{(1)} P + \mu I \right] \underline{y} \tag{2.19}$$

where $P = Q D_2^{*(-\frac{1}{2})}$. The matrix $P' B^{(1)} P$ is real symmetric and thus there exists an orthogonal O for which

$$O' \left[P' B^{(1)} P \right] O = \Lambda^* \tag{2.20}$$

where Λ^* is a diagonal matrix of eigenvalues of $P' B^{(1)} P$. We can then make the orthogonal transformation

$$\underline{y} = O \underline{z} \tag{2.21}$$

and as a result

$$q = \underline{z}' [\Lambda^* + \mu I] \underline{z} \tag{2.22}$$

If we call Λ the diagonal matrix containing the eigenvalues of the symmetric matrix

$$S = D_2^{(-\frac{1}{2})} Q' B^{(1)} Q D_2^{(-\frac{1}{2})},$$

which is real in spite of the fact that $D_2^{(-\frac{1}{2})}$ contains purely imaginary values,

$$\Lambda^* = - \Lambda, \tag{2.23}$$

thus

$$q = \underline{z}' [\mu I - \Lambda] \underline{z}. \tag{2.24}$$

So in order to render q negative definite, and thus find $\underline{x}$ from (2.3) which maximize $\hat{y}_p$ subject to a constraint on $\hat{y}_s$, we are led to choosing values of μ which are <u>smaller than the smallest eigenvalue of S</u>. On the other hand, if our desire is to minimize $\hat{y}_s$, we find conditions by choosing μ <u>larger than the largest eigenvalue of S</u>.

A theorem analogous to Theorem 2.2 is again helpful in showing that constrained absolute maxima (minima) are obtained by choosing $\mu < \lambda_1$ $(\mu > \lambda_k)$.

<u>Theorem 2.3</u>: Let $\underline{x}$ be a solution to (2.3) with $B^{(2)}$ negative definite. Then $\frac{\partial^2 \hat{y}_s}{\partial \mu^2} \leq 0$, with the equality holding in the limit as μ approaches $\pm \infty$.

<u>Proof</u>: The proof is similar to that of Theorem 2.2

As a result, the nature of the plot of $\hat{y}_s$ against μ is an inverted version of that given in Figure 2.1. That is, $\hat{y}_s$ will approach $-\infty$ as μ approaches an eigenvalue of S. For values of μ smaller than λ_1, $\hat{y}_s$ will increase with decreasing μ and asymptote to $\hat{y}_{s,0}$ which is its maximum value. Hence, the "working region" is $\mu < \lambda_1$ for constrained maximization of $\hat{y}_p$ and $\mu > \lambda_k$ for constrained minimization of $\hat{y}_p$.

3. Summary and Example for Case where $B^{(2)}$ is Definite

Perhaps the best way to summarize the results obtained when $B^{(2)}$ is definite is to outline the procedure which would be followed when it is of interest to obtain operating conditions resulting in a constrained optimum primary response variable. Following this outline will be a numerical example.

Once the parameters of the two response functions have been obtained, the eigenvalues of the matrix S should be determined. If one is interested in the constrained maximization of $\hat{y}_p$ and $B^{(2)}$ is positive definite, then values of $\mu > \lambda_k$ should be substituted into equation (2.3) and stationary values of $\underline{x}$ generated. These values of $\underline{x}$ represent points of absolute maximum response conditional on the estimated secondary response being given by equation (2.2). If minimization is desired, then values of $\mu < \lambda_1$ should be chosen. If $B^{(2)}$ is negative definite, values of $\mu < \lambda_1$ provide constrained maxima and values of $\mu > \lambda_k$ provide constrained minima.

Exploration of the dual response system can be carried out simply and concisely by constructing plots of x_1 vs. $\hat{y}_s$, x_2 vs. $\hat{y}_s$, ..., x_k vs. $\hat{y}_s$, and $\hat{y}_s$ vs. $\hat{y}_p$. When these simple two dimensional graphs are available to the experimenter, it will be possible for him to make a decision regarding what operating conditions should be used. In particular, for any value of the secondary response chosen, values of the x's are found which give rise to the maximum (or minimum) primary response.

One must be careful, of course, to consider as reliable only those results corresponding to values within or on the periphery of the experimental region. In addition, caution must be exercised in placing heavy reliance on results where either or both response functions are derived from empirical data that may have large random errors associated with them. (This too is a hazard with Ridge Analysis as pointed out by Draper.)

3.1 A Numerical Example

Consider a dual response surface problem where y_p and y_s depend on three independent variables x_1, x_2, and x_3. The following two response functions were fit to a set of experimental data

$$\hat{y}_p = 65.39 + 9.24x_1 + 6.36x_2 + 5.22x_3 - 7.23x_1^2 - 7.76x_2^2 - 13.11x_3^2 - 13.68x_1 x_2 - 18.92x_1 x_3 - 14.68x_2 x_3.$$

$$\hat{y}_s = 56.42 + 4.65x_1 + 8.39x_2 + 2.56x_3 + 5.25x_1^2 + 5.62x_2^2 + 4.22x_3^2 + 8.74x_1 x_2 + 2.32x_1 x_3 + 3.78x_2 x_3$$

giving

$$B^{(2)} = \begin{bmatrix} 5.25 & 4.37 & 1.16 \\ & 5.62 & 1.89 \\ \text{sym} & & 4.22 \end{bmatrix}$$

with eigenvalues of $B^{(2)}$ being (10.553, 3.557, 0.979). Thus, the secondary response function yields a stationary point which is a point of minimum response, with the stationary point and the estimated response at the stationary point being

$$\underline{x}_{s,0} = - B^{(2)^{-1}} \frac{\underline{b}^{(2)}}{2} = \begin{bmatrix} 0.5194 \\ -1.178 \\ 0.0814 \end{bmatrix}, \quad \hat{y}_{s,0} = 52.79$$

For the primary response function

$$B^{(1)} = \begin{bmatrix} -7.23 & -6.84 & -9.46 \\ & -7.76 & -7.34 \\ \text{sym} & & -13.11 \end{bmatrix}$$ (eigenvalues are 0.1765, -2.6304 -25.6460)

with $$\underline{x}_{p,0} = - \frac{B^{(1)^{-1}} \underline{b}^{(1)}}{2} = \begin{bmatrix} -8.077 \\ 3.8862 \\ 3.8516 \end{bmatrix}, \quad \hat{y}_{p,0} = 50.4849$$

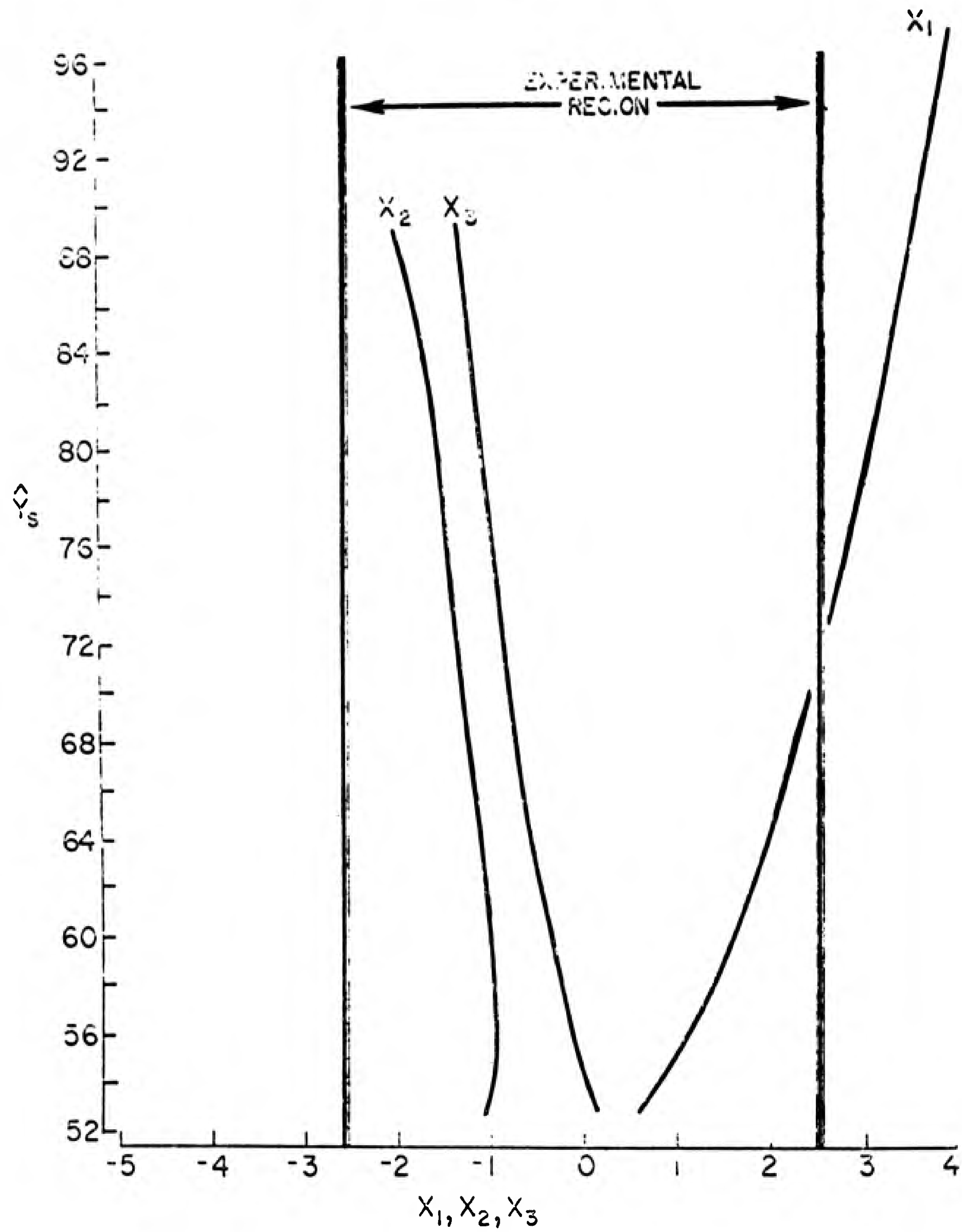

Fig. 3.1 CONDITIONS OF CONSTRAINED MAXIMA ON PRIMARY RESPONSE FOR FIXED VALUES OF $\hat{Y}_s$.

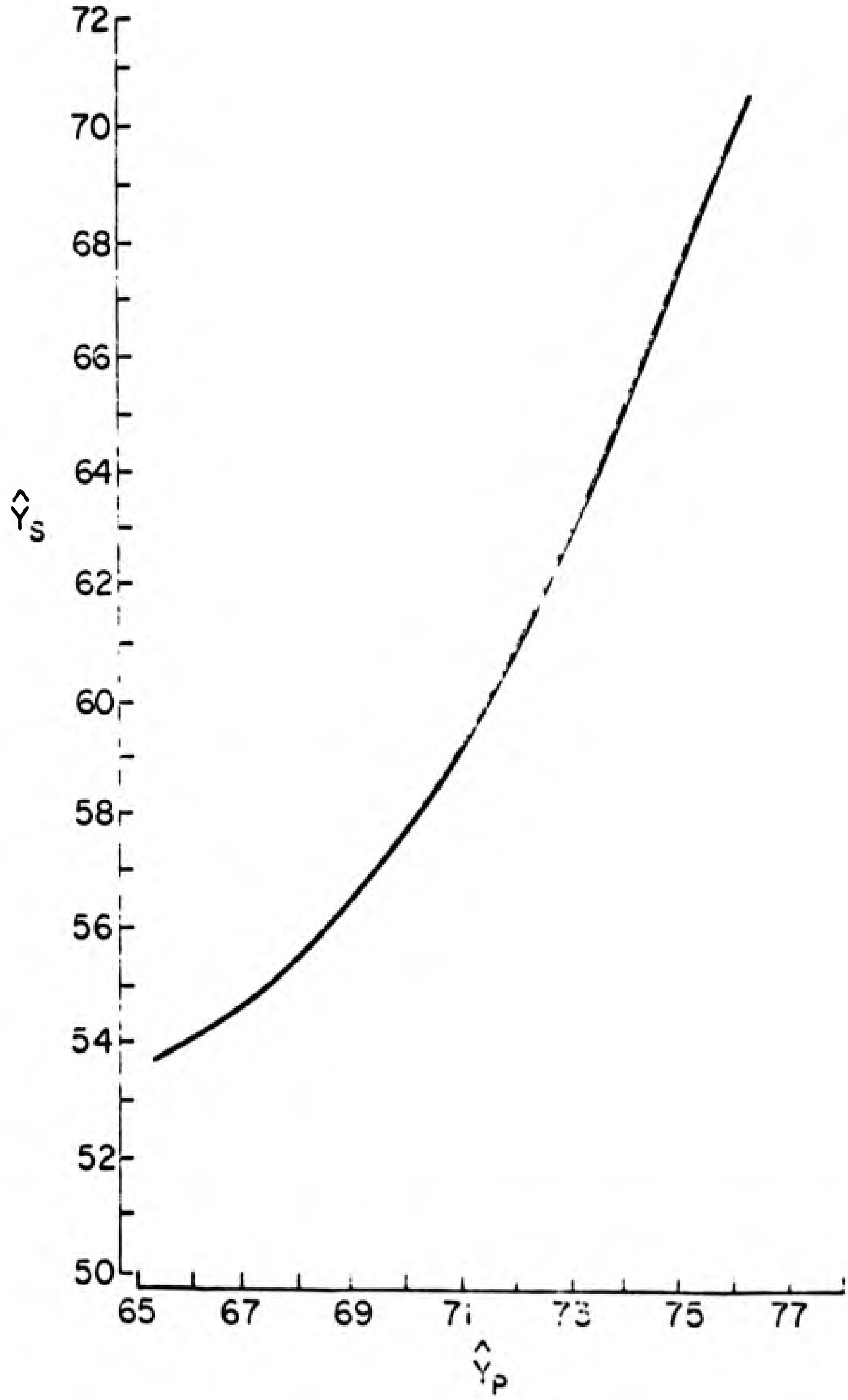

Fig. 3.2 MAXIMUM ESTIMATED PRIMARY RESPONSE AT SPECIFIC VALUES OF THE SECONDARY RESPONSE.

From these results, it follows that the primary response system is a "saddle system" with center at $\underline{x}_{p,0}$ which is outside the experimental region. The goal of the investigation was to determine operating conditions which maximize $\hat{y}_p$ but do not allow $\hat{y}_s$ to become too large. It was felt that values of the secondary response larger than about 65 would probably be excessive. Recall that the matrix S is given by

$$S = D_2^{(-\frac{1}{2})} Q' B^{(1)} Q D_2^{(-\frac{1}{2})}$$

For this example, we have

$$S = \begin{bmatrix} 0.3078 & 0 & 0 \\ 0 & 0.5302 & 0 \\ 0 & 0 & 1.0105 \end{bmatrix} \begin{bmatrix} 0.64276 & 0.69381 & 0.32478 \\ -0.34969 & -0.11148 & 0.93021 \\ 0.68159 & -0.71147 & 0.17097 \end{bmatrix} B^{(1)} Q D_2^{(-\frac{1}{2})}$$

$$= \begin{bmatrix} -2.0338 & -1.4100 & -0.7715 \\ -1.4100 & -1.4566 & -1.3899 \\ -0.7715 & -1.3899 & -1.4861 \end{bmatrix}$$

The eigenvalues of S are

$$\lambda = -4.0617 \qquad \lambda_2 = -0.9945 \qquad \lambda_3 = 0.08017$$

Equation (2.3) was used with $\mu > 0.08017$ to generate values of $\underline{x}$ representing points of constrained maximum primary response. Corresponding values of $\hat{y}_p$ and $\hat{y}_s$ were computed and the plots given in Figures 3.1 and 3.2 were constructed. Figure 3.1 indicates the locus of operating conditions giving absolute maxima on the primary response for various fixed values of the estimated secondary response. Figure 3.2 gives the value of the maximum estimated primary response for values of the estimated secondary response. In this example, the operating conditions which maximize $\hat{y}_p$, conditional on $\hat{y}_s = 65.0$ are found in Figure 3.1 to be

$$x_1 = 2.07; \; x_2 = -1.15; \; x_3 = -0.6$$

with an estimated primary response found in Figure 3.2 to be approximately 74.

These two dimensional plots can be very revealing in exploring dual response systems and the method of course can be used for any number of independent variables. A computer algorithm can be easily altered to handle the case where $B^{(2)}$ is negative definite. One merely needs to change all the signs from negative to positive of the eigenvalues of $B^{(2)}$ in forming D to avoid imaginary values. Then all of the signs of the elements in the resulting S matrix should be changed and the λ's obtained as the eigenvalues of this matrix are appropriate. Points of maximum $\hat{y}_p$ are then obtained by choosing $\mu < \lambda_1$ and points of minimum $\hat{y}_p$ are obtained by choosing $\mu > \lambda_k$.

4.0 $B^{(2)}$ Indefinite

When $B^{(2)}$ is indefinite, situations exist for which it is impossible to obtain a solution to the dual response optimization problem as it is currently stated. This will become obvious to the reader who attempts to maximize a two dimensional primary response system that is ellipsoidal in nature with a minimum at the center, given some specific value of a secondary variable with the latter having a saddle point system, i.e., $B^{(2)}$ is indefinite. No solution is found without further constraints.

In the case of a $B^{(2)}$ which is indefinite and the desire is a constrained maximization of $\hat{y}_p$ (constrained minimization is discussed in section 5.0), a solution exists if the primary response system yields a maximum at the center, i.e., $B^{(1)}$ is negative definite. Likewise, a constrained minimization is possible if the primary system yields a minimum at the center (constrained maximization is discussed in section 5.0). For the former case, consider the matrix of second partial derivatives $M(\underline{x}) = 2(B^{(1)} - \mu B^{(2)})$. To make $M(\underline{x})$ negative definite, we require that the quadratic form

$$q = \underline{u}' [\mu B^{(2)} + (- B^{(1)})] \underline{u}$$

be positive definite. Again, we make use of the fact that there exists a nonsingular matrix R for which

$$R' B^{(2)} R = \text{diag}(\lambda_1, \ldots, \lambda_k)$$

$$R' (- B^{(1)}) R = I_k,$$

the roles of $B^{(1)}$ and $B^{(2)}$ having been reversed. The λ's are the eigenvalues of the matrix

$$S^* = D_1^{(-\frac{1}{2})} P' B^{(2)} P D_1^{(-\frac{1}{2})}, \tag{4.1}$$

where P is the orthogonal matrix for which

$$P' [- B^{(1)}] P = D_1$$

and $D_1^{(-\frac{1}{2})}$ contains reciprocals of the square roots of eigenvalues of $(- B^{(1)})$.

Letting $\underline{u} = R\, \underline{v}$, we have

$$q = \underline{v}' [\mu\, \text{diag}(\lambda_1, \ldots, \lambda_k) + I_k]\, \underline{v}.$$

The values of μ required to insure a local maximum on $\hat{y}_p$ are those for which $\mu \lambda_i > -1$ ($i = 1,2,\ldots,k$) and, as a result, are the values of μ to employ in (2.3). From the definition of S^* and since $B^{(2)}$ is indefinite, the signs of the λ's will be mixed. Thus, the appropriate values of μ to use are given by the inequality

$$- \frac{1}{\lambda_1} > \mu > - \frac{1}{\lambda_k} \tag{4.2}$$

Again, a plot of $\hat{y}_s$ against μ in the working region of μ, is very revealing. Figure 4.1 indicates the appearance of this plot. In this case, the asymptotes will not be at $\mu = \lambda_i$ but rather at $\mu = -\frac{1}{\lambda_i}$ ($i = 1,2,\ldots,k$), where a solution to equation (2.3) does not exist. To show this, we first consider

$$|B^{(1)} - \mu B^{(2)}| = (-\mu)^k |B^{(2)} + \frac{1}{\mu} (- B^{(1)}|.$$

Thus, we have

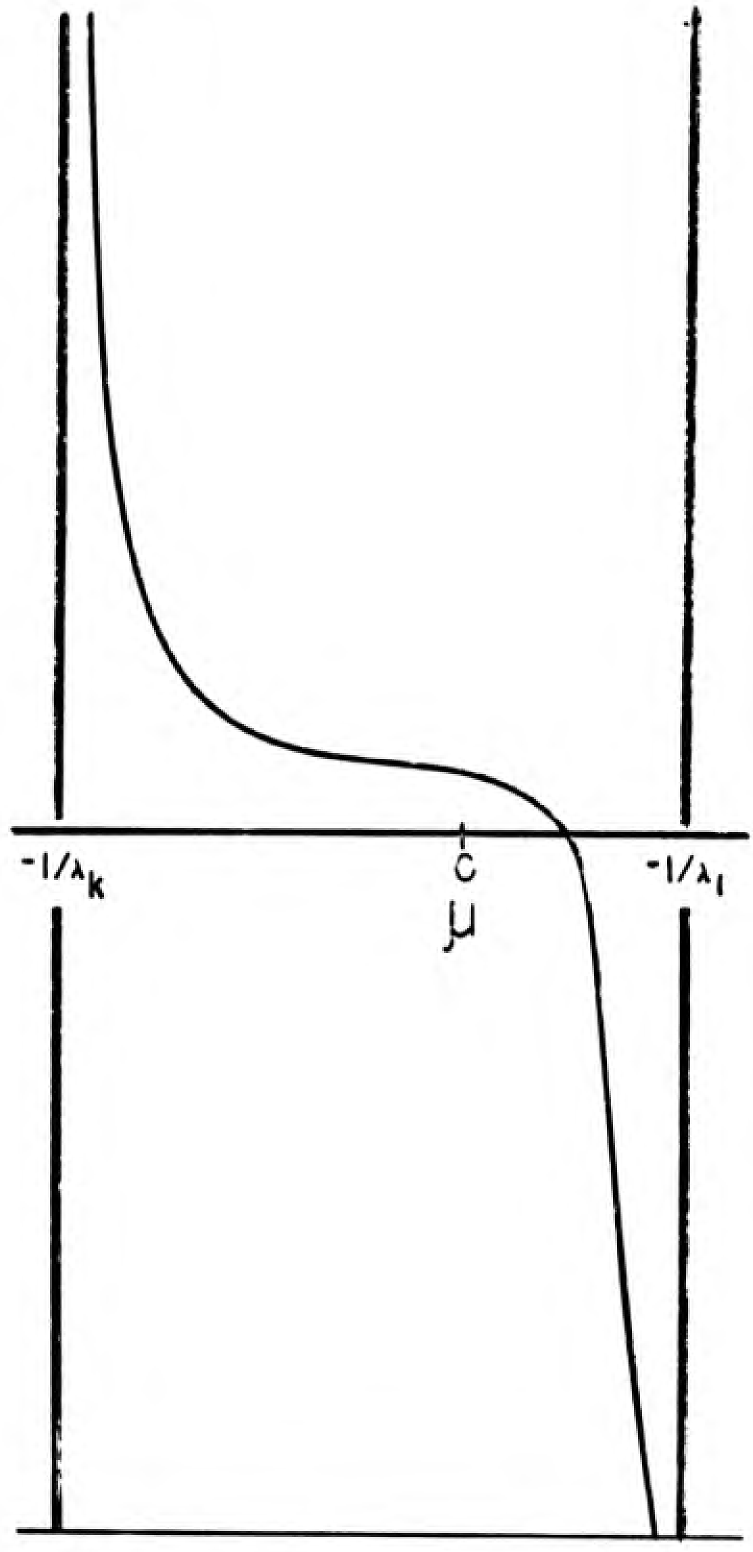

Fig. 4.1 TYPICAL PLOT OF $\hat{Y}_s$ AGAINST μ FOR $B^{(2)}$ INDEFINITE AND $B^{(1)}$ NEGATIVE DEFINITE IN THE WORKING REGION OF μ.

$$|D_1^{(-\frac{1}{2})}|\,|P'|\,|B^{(1)} - \mu B^{(2)}|\,|P|\,|D_1^{(-\frac{1}{2})}| = (-\mu)^k |S^* + \frac{1}{\mu} I|.$$

Thus, if $\mu = -\frac{1}{\lambda_i}$, $|S^* + \frac{1}{\mu} I| = 0$ and thus $|B^{(1)} - \mu B^{(2)}| = 0$.

The first derivative $\frac{\partial y_s}{\partial \mu}$ is negative in the working region of μ, i.e., in the region given by equation (4.2), for we can write, by combining equations (2.13) and (2.14)

$$\frac{\partial y_s}{\partial \mu} = \frac{1}{2}(\underline{b}^{(2)'} + 2\underline{x}'B^{(2)})(B^{(1)} - \mu B^{(2)})(\underline{b}^{(2)} + 2B^{(2)}\underline{x}).$$

The derivative cannot be other than negative in this region since $B^{(1)} - \mu B^{(2)}$ is negative definite and $(\underline{b}^{(2)} + 2B^{(2)})\underline{x}$ can only be zero when μ is infinite.

Again, the methodology involves choosing values of μ, this time in the region given by equation (4.2), generating $\underline{x}$ values from (2.3), computing $\hat{y}_s$ and $\hat{y}_p$ and plotting graphs similar to those in Figures (3.1) and (3.2) to describe the dual response system in the experimental region and using these plots to arrive at appropriate operating conditions.

If $B^{(1)}$ is positive definite, operating conditions can be found which <u>minimize</u> $\hat{y}_p$ for specific values of $\hat{y}_s$. The procedure involves using values of μ in equation (2.3) for which $\mu\lambda_i < 1$ $(i=1,2,\ldots,k)$ where again the λ's are eigenvalues of the matrix S^* as given in (4.1). In this case, P is the orthogonal matrix for which

$$P'B^{(1)}P = D_1.$$

So the range of μ to use in this case is given by

$$\frac{1}{\lambda_1} < \mu < \frac{1}{\lambda_k} \qquad (4.3)$$

CONTRACT NUMBER DAAH01-71-C-0026

5.0 Double Constraint Exploration

In the previous sections, we have considered the exploration of the dual response system with the goal of finding conditions that optimize the primary response with a simple constraint, namely, that the secondary response takes on a specific value. However, the experimenter will encounter many situations where mathematically the solution is valid but the recommended operating conditions $\underline{x}$ fall outside the region of the experiment that generated the estimated response functions and thus, would not be considered reliable. In the example given in section 3.1, the method would not have been successful if the operating conditions given in Figure 3.1 for $\hat{y}_s = 65$ had fallen outside the experimental region.

It seems that an appropriate procedure to follow would be to apply the <u>additional constraint</u> $\sum_{i=1}^{k} x_i^2 = R^2$ (using $\underline{x} = \underline{0}$ as the origin in the design variables) and employ the procedure where R is small enough to insure a solution inside the region of the designed experiment.

In fact, if $B^{(2)}$ is indefinite, there are cases when such a procedure is necessary. The solution to the problem as it has now been stated is obtained by employing, again, the method of Lagrangian multipliers. Hence, we consider the function

$$L = \hat{y}_p - \mu(\hat{y}_s - k) - \gamma(\underline{x}'\underline{x} - R^2). \qquad (5.1)$$

The equation $\frac{\partial L}{\partial \underline{x}} = \underline{0}$ implies that

$$(B^{(1)} - \mu B^{(2)} - \gamma I)\, \underline{x} = \frac{1}{2}(\mu\, \underline{b}^{(2)} - \underline{b}^{(1)}). \qquad (5.2)$$

Perhaps the most effective method for solving (5.2) is to choose values of μ and γ directly, making appropriate choices to insure that the values of $\underline{x}$ represent operating conditions where the maximum (or minimum) on $\hat{y}_p$ is achieved. For a given value of μ, the matrix of second partials

$$M(\underline{x}) = 2(B^{(1)} - \mu B^{(2)} - \gamma I)$$

is made negative definite (and thus, a local maximum achieved) by selecting $\gamma > \lambda_k$, where λ_k is the largest eigenvalue of the matrix $B^{(1)} - \mu B^{(2)}$. [See Draper [3]]. Values of $\gamma < \lambda_1$ should be taken for local minima. In fact, for $\mu = 0$, the problem reduces to Ridge Analysis where the locus of coordinates generated by (5.2) represents points of absolute maxima on $\hat{y}_p$ without the constraint on $\hat{y}_s$.

The choice of μ essentially defines the direction taken as one moves away from $\underline{x} = \underline{0}$. Again, various two dimensional plots describe the dual response system. This will become apparent in the following section.

5.1 Example

Two responses were fit to a set of experimental data involving k = 2 independent variables. The two response functions were found to be the following:

$$\hat{y}_p = 53.69 + 7.26x_1 - 10.33x_2 + 7.22x_1^2 + 6.43x_2^2 + 11.36x_1 x_2.$$

$$\hat{y}_s = 82.17 - 1.01x_1 - 8.61x_2 + 1.40x_1^2 - 8.76x_2^2 - 7.20x_1 x_2.$$

The method can be used for any value of k, the number of independent variables. The above example was used so that the response contours can be drawn for illustrative purposes. The center of the primary and secondary systems are given by

$$\underline{x}_{p,0} = \begin{bmatrix} -3.7197 \\ 4.0891 \end{bmatrix} \qquad \underline{x}_{s,0} = \begin{bmatrix} -0.439 \\ -0.311 \end{bmatrix}$$

$B^{(1)}$ has eigenvalues given by 12.5187 and 1.1313 and thus, $x_{p,0}$ represents a point of minimum response. The eigenvalues of B(2) are -9.9063 and 2.5463 and so the secondary response system is hyperbolic in nature. Figure 5.1 shows the dual response system. Of course, in this example, it is impossible to find conditions which maximize y_p subject to specific values of y_s. However, by applying the additional restriction that $\underline{x}'\underline{x} = R^2$ equation (5.2) can be used with different values of μ and various values of γ exceeding the largest eigenvalue of $B^{(1)} - \mu B^{(2)}$ to generate values of $\underline{x}$ satisfying the constraints and giving rise to optimal operating conditions. The two dimensional plots in Figures (5.2), (5.3) and (5.4) are helpful in providing an exploration of the system and providing a recommendation for future operating conditions.

Suppose for example that we wish to find conditions in the experimental region which maximize $\hat{y}_p$ but we also require $84 < \hat{y}_s < 88$. Figures (5.2) and (5.3) indicate 'candidates' for operating conditions. The $\mu = 0$ line represents maximization of y_p subject only to $\underline{x}'\underline{x} = R^2$. The line $\mu = -2$ at $R = 1.0$ appears to be the proper choice. Figure 5.4 gives the values of the coordinates, $x_1 = 0.85$ and $x_2 = -0.6$, with the estimated responses at these conditions given from Figures (5.2) and (5.3) as

$$y_p = 67, \quad \hat{y}_s = 87.8$$

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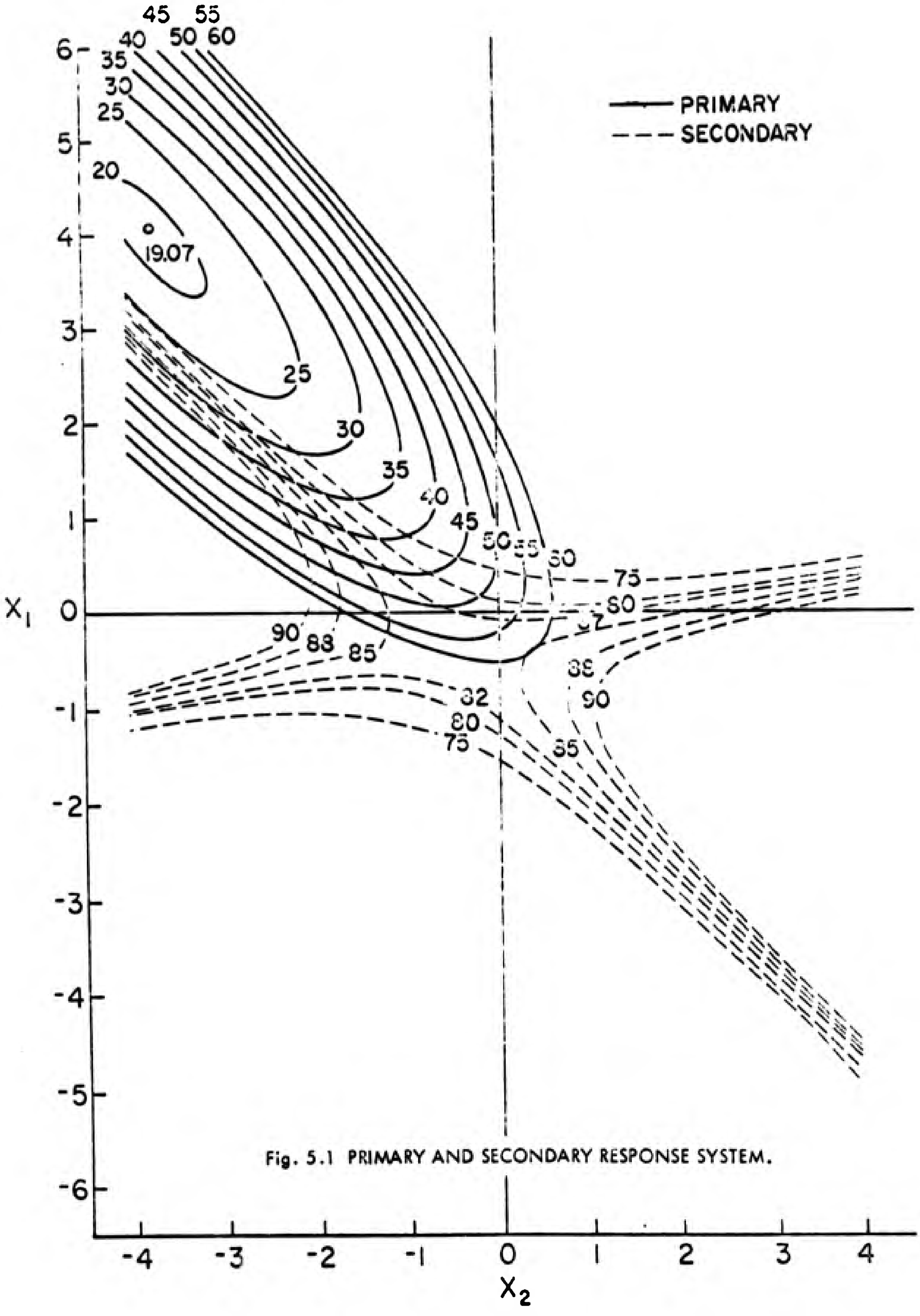

Fig. 5.1 PRIMARY AND SECONDARY RESPONSE SYSTEM.

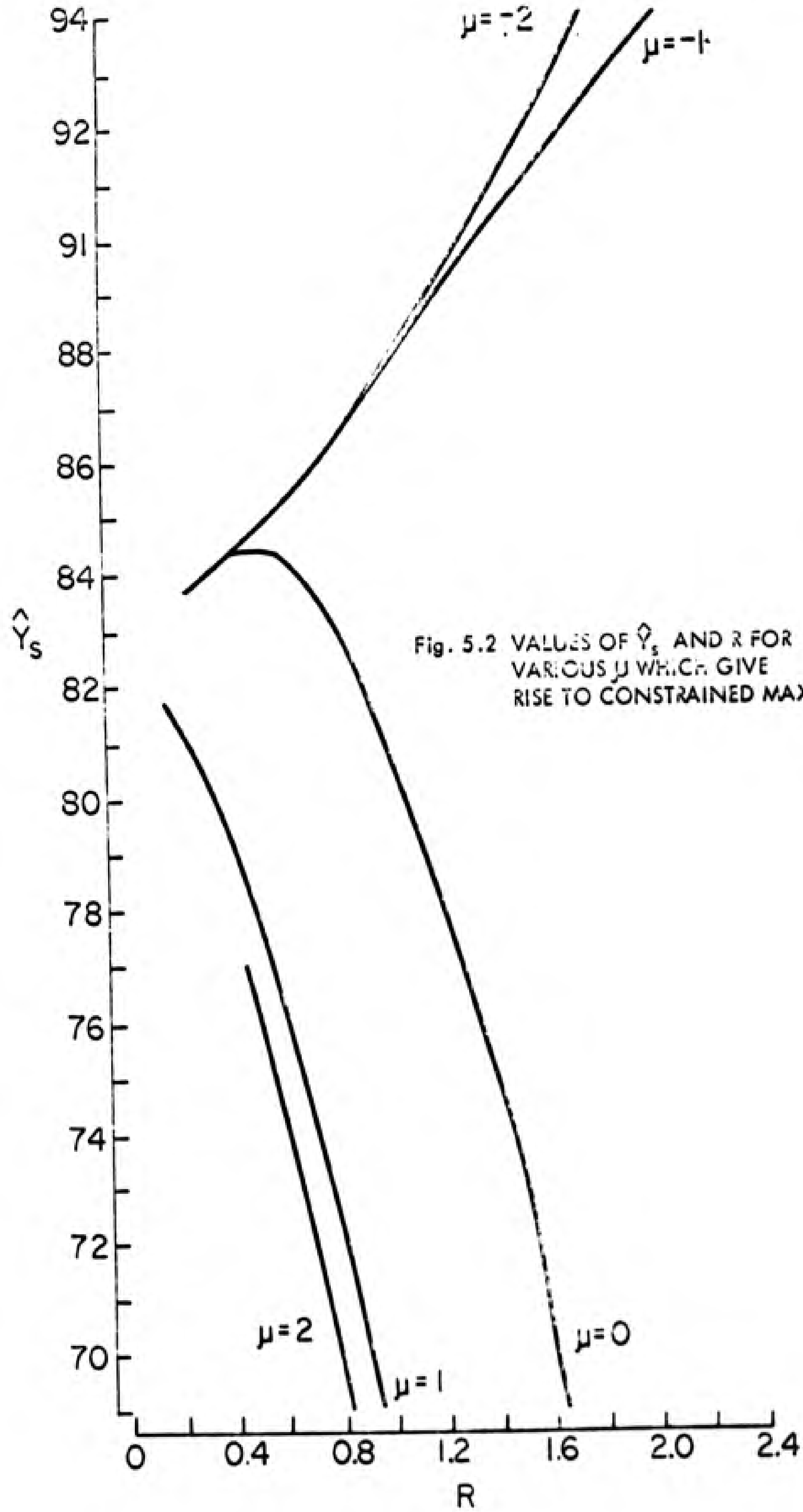

Fig. 5.2 VALUES OF $\hat{Y}_s$ AND R FOR VARIOUS μ WHICH GIVE RISE TO CONSTRAINED MAXIMA.

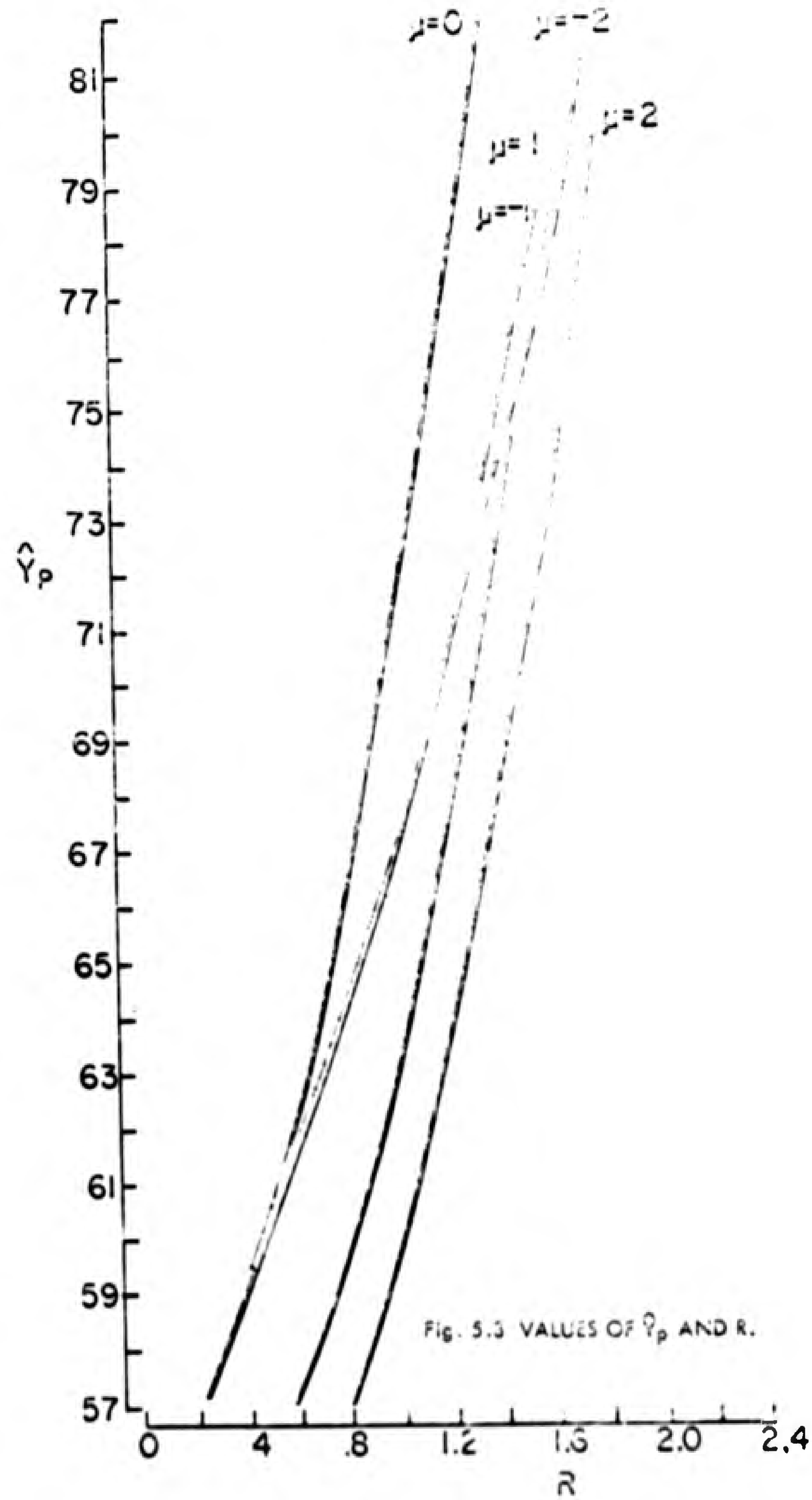

Fig. 5.3 VALUES OF $\hat{Y}_p$ AND R.

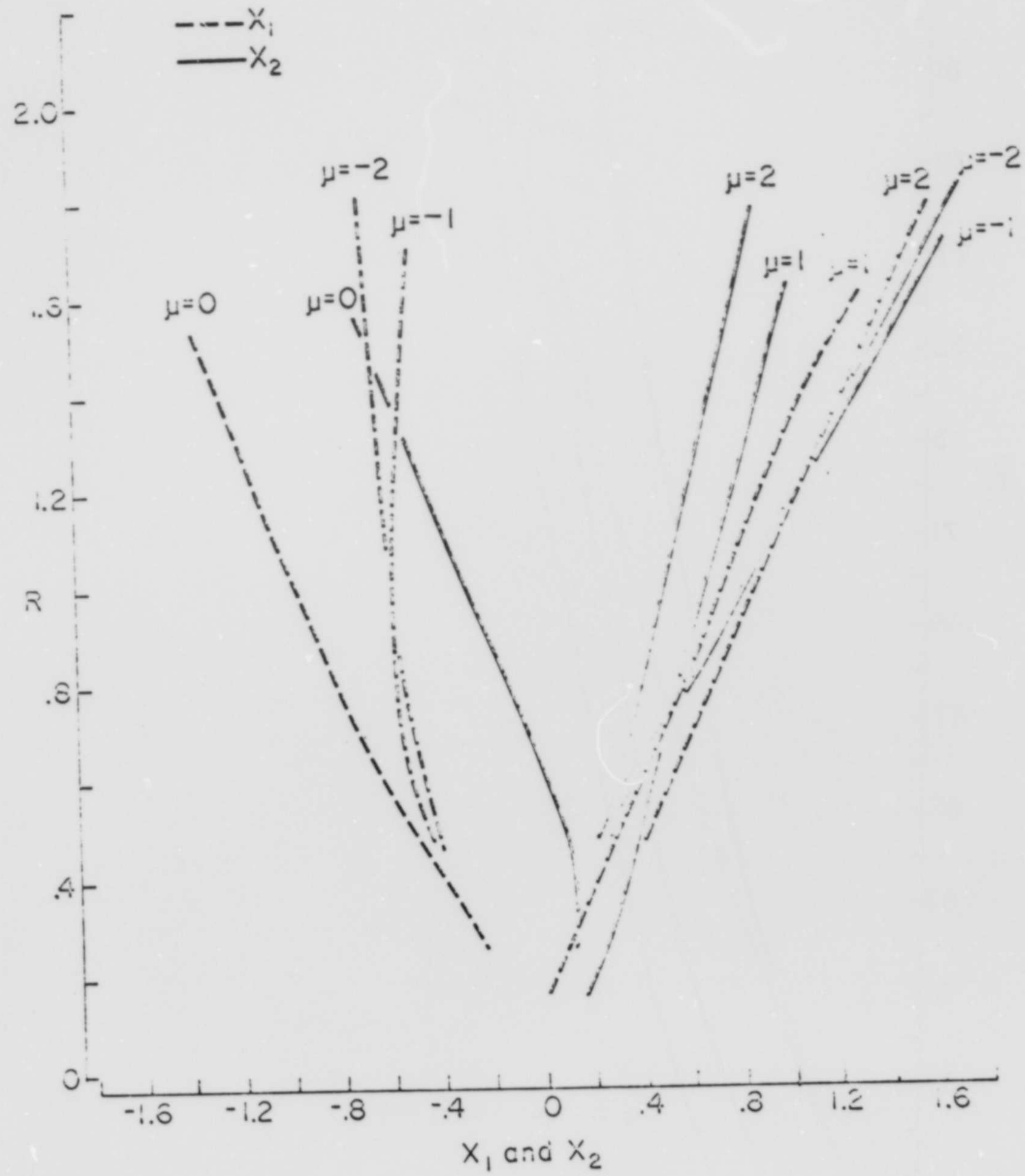

Fig. 5.4 OPERATING CONDITIONS FOR VARIOUS R.

APPENDIX - COMPUTER PROGRAM

DOCUMENTATION OF PROGRAM

(a) Subroutines

The program includes two main programs (MRSA) and (INDEF) and the following subroutines:

1. CORRE
2. ORDER
3. MINV
4. MULTR
5. GMPRD
6. EIGEN
7. MSTR
8. MPRD
9. TPRD
10. LINEQ
11. OBSER
12. DATA
13. PUREE
14. OPTUM

The first nine subroutines are well known IBM scientific subroutines. The function of the other subroutines are given in the listing of the program.

(b) Execution of the Program

The following cards are needed for execution after the programs and subroutines have been stored. (Note sample deck)

CARD	DESCRIPTION		
1.	// XEQ MRSA 1		
2.	*LOCALMRSA,CORRE,LINEQ,PUREE,MULTR,ORDER,OBSER,MPRD,OPTUM,GMPRD,TPRD		
3.	Cols. 1 - 8	Description of Problem	(FORMAT 8A1)
	9 - 11	Number of Observations	(FORMAT I3)
	12 - 14	Number of Independent Variables	(FORMAT I3)
4-n+3	Data cards in the following form		
	$y_1\ y_2\ x_1, x_2, \ldots, x_k$		(FORMAT 12F6.0)
n+4	Cols. 1 - 5	Increment on μ	
	6 - 10	Upper bound on μ	
n+5	blank		
n+6	blank		

(c) Additional Comments

Prior to storing the program the variables MX and MY should be defined with the appropriate values. MX is the number for the printer and MY is the number for the card reader.

The format statement for the input data is statement one in subroutine OBSER.

If there are more than 6 concomitant variables the appropriate dimension statements must be changed.

In card 3, number of independent variables, this implies the total number of variables in the response system, e.g., a two concomitant variable system has five independent variables, i.e., x_1, x_2, x_1^2, x_2^2, x_1x_2. The variable y_1 is primary and y_2 is secondary. If any design point has repeated observations, these must be read in succession.

The increment on μ is determined by the user. A recommendation is 0.1. The upper bound on μ is difficult to determine and should be set at something arbitrary (but large). Then the user can stop the output when he wishes.

(d) INDEF

If the matrix $B^{(2)}$ is indefinite, the program will say $B^{(2)}$ is indefinite and stop. The user must then read in the following cards

CARD		
1	// XEQ INDEF	
2	Cols. 1 - 5 is number of independent variables	(FORMAT I5)
3	Regression coefficients for y_1	(FORMAT 8F10.0)
4	Regression coefficients for y_2	(FORMAT 8F10.0)
5-	Cols. 1 - 5 μ values	
	6 - 10 Increment on γ	
	11 - 15 Upper bound on γ	
	Repeat if desired for additional μ values	

(e) Additional Comments

Regression coefficients are obtained as output from the main program and read in the order:

$b_0, b_1, \ldots, b_k, b_{11}, b_{22}, \ldots, b_{kk}, b_{12}, b_{13}, \ldots, b_{1k}, b_{23}, \ldots, b_{2k}, \ldots, b_{k-1,k}$.

Recommendations for μ values are 0, ± 0.25, ± 0.5, ± 1.0, ± 1.25, ± 1.5, ± 2.0, ± 3.0, ± 50. The same comments on the increment and upper bound on γ apply as before on μ. This program will stop automatically at $\mu = 50$.

```
// DUP
*DELETE             MRSA
// FOR
*ARITHMETIC TRACE
*TRANSFER TRACE
*IOCS(CARD,1132 PRINTER,DISK)
*LIST SOURCE PROGRAM
*ONE WORD INTEGERS
C     THE MAIN PROGRAM FOR RESPONSE SURFACE ANALYSIS
      DIMENSION PR(8)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE
C        NUMBER OF VARIABLES,M.
      DIMENSION XBAR(29),STD(29),ISAVE(29),RY(29),SB(29)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE
C        PRODUCT OF M*M.
      DIMENSION RX(841),D(841),W(841)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL N,
C        WHERE N EQUALS THE NUMBER OF OBSERVATIONS.
      DIMENSION B(100),T(100)
C        THE FOLLOWING DIMENSIONS MUST BE GREATER THAN OR EQUAL TO THE
C        PRODUCT OFMD*MD,WHERE MD EQUALS THE NUMBER OF LINEAR X TERMS.
      DIMENSION SX(36),  BMATR(6,6),  BMATS(36)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO THE
C        PRODUCT OF (MD+1) * MD/2.
      DIMENSION BMATE(21)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO
C        (M+1)*M/2.
      DIMENSION R(435)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 10.
      DIMENSION ANS(11),VEC(11)
C        THE FOLLOWING DIMENSION MUST BE GREATER THAN OR EQUAL TO 2 TIMES
C        TIMES THE PRODUCT OF (MD+1) * MD/2.
      DIMENSION BMATM(2,21),BC(2,36)
      DIMENSION BO(6)
      COMMON MY,IN
      DEFINE FILE 1(100,100,U,IN)
    1 FORMAT(8A1,2I3)
    2 FORMAT('1','DUAL RESPONSE SURFACE ANALYSIS..'8A1//6X,'Y',I2///)
    3 FORMAT(//9H VARIABLE,5X,4HMEAN,6X,8HSTANDARD,6X,11HCORRELATION,4X,
     110HREGRESSION,4X,10HSTD. ERROR,5X,8HCOMPUTED/24X,9HDEVIATION,7X,6H
     2X VS Y,7X,11HCOEFFICIENT,3X,12HOF REG.COEF.,3X,7HT VALUE)
    4 FORMAT('0',1HY,3X,6F14.5)
    5 FORMAT(//,10H DEPENDENT)
    6 FORMAT(///10H INTERCEPT,13X,F13.5//23H MULTIPLE CORRELATION  ,F13.
     15,10X,10HR SQUARE  ,F13.5,//23H STD. ERROR OF ESTIMATE,F13.5//)
    7 FORMAT(1H1,21X,39HANALYSIS OF VARIANCE FOR THE REGRESSION//5X,19HS
     1OURCE OF VARIATION,7X,7HDEGREES,7X,6HSUM OF,10X,4HMEAN,13X,7HF VAL
     2UE/30X,10HOF FREEDOM,4X,7HSQUARES,9X,7HSQUARES)
    8 FORMAT(/30H ATTRIBUTABLE TO REGRESSION    ,I6,3F16.5)
    9 FORMAT(/5X,5HTOTAL,19X,I6,F16.5)
   11 FORMAT(/,15X,18HTABLE OF RESIDUALS//9H CASE NO.,5X,7HY VALUE,5X,10
     1HY ESTIMATE,6X,8HRESIDUAL
   12 FORMAT I6,F15.5,2F14.5
   14 FORMAT(//52H THE MATRIX IS SINGULAR.  THIS SELECTION IS SKIPPED.)
   24 FORMAT(////1X,' THE RESPONSE ESTIMATE AT THE STATIONARY POINT IS D
     1EFINED BY')
   25 FORMAT(1X,'YO = ',F10.5)
   32 FORMAT (/30H          LACK OF FIT          ,I8,2F16.5/30H
     1PURE ERROR          ,I8,2F16.5)
```

```
   33 FORMAT ('0',1HX,2X,111,2X,6F14.5)
   34 FORMAT ('0',1HX,1X,2I1,2X,6F14.5)
   35 FORMAT (/30H            LACK OF FIT          ,I8,3F16.5/30H
     1PURE ERROR          ,I8,2F16.5)
   36 FORMAT(/30H             LINEAR              ,I8,3F16.5)
   37 FORMAT(/30H DEVIATION FROM REGRESSION     ,I6,2F16.5)
   38 FORMAT(/30H             QUADRATIC           ,I8,3F16.5)
   39 FORMAT (1H1,34HTHE STATIONARY POINT IS DEFINED BY)
   40 FORMAT(1X,1HX,I2,1H=,F10.5)
   42 FORMAT(/////1X,'EIGENVALUES OF THE B MATRIX')
   43 FORMAT (1X,5HLAMDA,1X,I2,1H=,F10.5)
   45 FORMAT (1X,6HVECTOR,I3,/(10F10.5))
   47 FORMAT(/////1X,12HEIGENVECTORS)
   65 FORMAT('0','PSEUDO EIGENVALUES')
   66 FORMAT('0','PSEUDO EIGENVECTORS')
   67 FORMAT(1X,'P LAMDA',1X,I2,'=',F10.5)
   68 FORMAT(1X,'P VECTOR',1X,I3,/(10F10.5) )
  301 FORMAT(//'0','B2 IS INDEFINITE')
  700 FORMAT('1','THE S MATRIX')
  701 FORMAT('0',10F10.5)
  704 FORMAT(//,'0','B2 IS NEGATIVE DEFINITE')
  706 FORMAT(//,'0','B2 IS POSITIVE DEFINITE')
      MX=3
      MY=2
      IN=1
      MV=0
C         READ PROBLEM PARAMETER CARD
  100 READ(MY,1)PR,N,K
C         PR.........PROBLEM NUMBER  MAY BE ALPHAMERIC
C         N..........NUMBER OF OBSERVATIONS
C         K..........NUMBER OF INDEPENDENT VARIABLES
      M=K+2
      IO=0
      X=0.0
      XM=K+1
      ML=-.5+SQRT(.25+2.*XM)
      DO 101 I=1,K
  101 ISAVE(I)=I+2
      MD=ML-1
      ME = MD-1
      CALL OBSER(M,ISAVE,2,MD,N)
      IN=1
      CALL CORRE (N,M,IO,X,XBAR,STD,RX,R,D,B,T)
      DO 200 I=1,2
      WRITE(MX,2)PR,I
      NRESI=1
      CALL ORDER (XM,R,I,K,ISAVE,RX,RY)
      LN = MD
      LM = 1
      LP=1
      DO 82 LO = 1,MD
      DO 81 L = LM,LN
      SX(LP) = RX(L)
   81 LP=LP+1
      LM=LM+K
      LN=LN+K
   82 CONTINUE
      CALL MINV (RX,K,DET,B,T)
      MM=XM
      CALL LINEQ (N,MD,D,SX,RY,ISAVE,SSAR,MM)
```

```
C        TEST SINGULARITY OF THE MATRIX INVERTED
      IF DET  112, 110, 112
  110 WRITE  MX,14
      GO TO 200
  112 CALL MULTR (N,K,XBAR,STD,D,RX,RY,ISAVE,B,SB,T,ANS)
C        FORMING AND STORING THE B MATRIX TO BE USED TO OBTAIN THE
C        STATIONARY POINT IN ARRAY BMATS AND STORING THE UPPER
C        TRIANGULAR PORTION IN ARRAY BMATE TO BE USED TO OBTAIN THE
C        EIGENVALUES.
      IB=1
      IC=1
      ID=2
      DO 75 J=1,K
   75 BC(I,J)=B(J)
      DO 21 J = ML,K
      BMATR(IB,IB)=B(J)
      IB = IB +1
      IF (J-ML-MD) 21,22,22
   22 BMATR(IC,ID)=B(J)/2.
      ID = ID + 1
      IF (ID-ML) 21,23,23
   23 IC = IC + 1
      ID = IC
      IF (IC-ID) 21,26,21
   26 ID = ID + 1
   21 CONTINUE
      DO 29 III = 1,MD
      DO 29 JJJ = 1,MD
   29 BMATR(JJJ,III) = BMATR(III,JJJ)
      KKK = 1
      LLL = 1
      DO 27 JJJ = 1,MD
      DO 27 III = 1,MD
      BMATS (KKK) = BMATR(III,JJJ)
      KKK = KKK + 1
      IF (III-JJJ) 28,28,27
   28 BMATE (LLL) = BMATR(III,JJJ)
      BMATM(I,LLL)=BMATE(LLL)
      LLL = LLL + 1
   27 CONTINUE
C        PRINT MEANS, STANDARD DEVIATIONS, INTERCORRELATIONS BETWEEN
C        X AND Y, REGRESSION COEFFICIENTS, STANDARD DEVIATIONS OF
C        REGRESSION COEFFICIENTS, AND COMPUTED T.VALUES
      WRITE  MX,3
      J=1
      L=ISAVE(J)
      DO 116 LL=1,MD
      WRITE(MX,33)LL,XBAR(L),STD(L),RY(J),B(J),SB(J),T(J)
      J=J+1
      L=L+1
  116 CONTINUE
      DO 117 LL=1,MD
      WRITE(MX,34)LL,LL,XBAR(L),STD(L),RY(J),B(J),SB(J),T(J)
      J=J+1
      L=L+1
  117 CONTINUE
      DO 118 LL=1,MD
      DO 118 LK=2,MD
      IF(LL-LK) 119,118,118
  119 WRITE(MX,34) LL,LK,XBAR(L),STD(L),RY(J),B(J),SB(J),T(J)
```

```
      L=L+1
      J=J+1
  118 CONTINUE
      WRITE  MX,5
      L ISAVE MM
      WRITE(MX,4) XBAR(L),STD(L)
C        PRINT INTERCEPT, MULTIPLE CORRELATION COEFFICIENT, AND
C        STANDARD ERROR OF ESTIMATE
      ANS(11)=ANS(2)*ANS(2)
      BO(I)=ANS(1)
      WRITE (MX,6) ANS(1),ANS(2),ANS(11),ANS(3)
C        PRINT ANALYSIS OF VARIANCE FOR THE REGRESSION
      WRITE  MX,7
      L ANS 8
C     CALCULATION OF THE STATIONARY POINT
      LA = 1
      CALL MINV (BMATS,MD,DET,T,SB)
      CALL GMPRD(BMATS,B,T,MD,MD,LA)
      DO 41 MMM = 1,MD
   41 T(MMM) = T(MMM) * (-.5)
      YO= ANS(1)
      DO 15 J=1,MD
   15 YO=.5 * (B(J) * T(J) ) + YO
      CALL EIGEN (BMATE,SB,MD,MV)
      CALL PUREE (IHRX,PE,ML,N,ISAVE,I)
C     OBTAINING MEAN SQUARES AND F VALUES FOR THE ANOVA TABLE
      IRX = L-IHRX
      ORX=ANS(7) - PE
      ORXA = ORX/IRX
      ORXB = PE/IHRX
      ORXM=ORXB
      IF(PE) 18,19,18
   19 ORXB=ORXA
   18 ORXC = ORXA/ORXB
      ORXF = ANS(6) / ORXB
      QUAD = ANS(4) - SSAR
      MQDF = K-MD
      SSMS = SSAR/MD
      QUAMS = QUAD/MQDF
      SSARF = SSMS/ORXB
      QUADF = QUAMS/ORXB
      WRITE(MX,8) K,ANS(4),ANS(6),ORXF
      WRITE (MX,36) MD,SSAR,SSMS,SSARF
      WRITE(MX,38) MQDF,QUAD,QUAMS,QUADF
      WRITE(MX,37) L,ANS(7),ANS(9)
      IF(PE)30,20,30
   20 WRITE(MX,32)IRX,ORX,ORXA,IHRX,PE,ORXM
      GO TO 31
   30 WRITE(MX,35)IRX,ORX,ORXA,ORXC,IHRX,PE,ORXM
   31 L=N-1
      SUM ANS 4 &ANS 7
      WRITE  MX,9  L,SUM
      WRITE(MX,39)
      DO 51 II = 1,MD
   51 WRITF(MX,40) II,T(II)
      WRITE(MX,24)
      WRITE(MX,25) YO
      WRITE(MX,42)
      DO 46 J=1,MD
      II = J + (J*J-J) / 2
```

```
   46 WRITE(MX,43) J, BMATE (II)
      IF (MV) 52,52,61
   52 WRITE(MX,47)
      LL = 0
      DO 48 J = 1,MD
      DO 49 KK=1,MD
      LL = LL + 1
   49 VEC(KK) = SB(LL)
   48 WRITE (MX,45) J,  (VEC(KK) ,KK= 1,MD )
   61 IF(NRESI) 200,200,120
C          PRINT TABLE OF RESIDUALS
  120 WRITE(MX,2)PR,I
      WRITE  MX,11
      MM ISAVE K&1
      IN=1
      DO  140 II 1,N
      CALL DATA (M,W)
      SUM ANS 1
      DO 130 J 1,K
      L ISAVE J
  130 SUM=SUM+W(L)*B(J)
      RESI W MM -SUM
  140 WRITE  MX,12  II,W MM ,SUM,RESI
  200 CONTINUE
C                    TEST FOR DEFINITENESS OF B2
      MENDS=(MD*(MD+1))/2
      DO 91 LLL=1,MENDS
      BMATS(LLL)=BMATM(2,LLL)
   91 RX(LLL)=BMATM(1,LLL)
      CALL EIGEN (BMATS,SB,MD,MV)
      CALL MSTR(BMATS,BMATE,MD,1,2)
      BO(3)=0.
      DO 62 J=2,MD
      JJ=J-1
      IF(BMATE(J))73,72,72
   72 IF(BMATE(JJ))77,74,74
   74 IF(J-MD)62,76,62
   73 IF(BMATE(JJ))79,77,77
   79 IF(J-MD)62,80,62
   62 CONTINUE
   77 WRITE(MX,301)
      GO TO 300
   80 BMATE(J)=-BMATE(J)
      BO(3)=1.
      WRITE(MX,704)
      GO TO 705
   76 WRITE(MX,706)
C                    FORMING OF THE S MATRIX
  705 DO 78 J=1,MD
      BMATE(J)=SQRT(BMATE(J))
   78 BMATE(J)=1./BMATE(J)
      CALL MPRD(SB,BMATE,BMATS,MD,MD,0,2,MD)
      CALL TPRD(BMATS,RX,R,MD,MD,0,1,MD)
      CALL MPRD(R,BMATS,T,MD,MD,0,0,MD)
      CALL MSTR(T,D,MD,0,1)
      WRITE(MX,700)
      LL=0
      DO 702 J=1,MD
      DO 703 KK=1,MD
      LL=LL+1
```

```
  703 VEC(KK)=T(LL)
  702 WRITE(MX,701) (VEC(KK),KK=1,MD)
      CALL EIGEN(D,W,MD,MV)
      CALL MSTR(D,T,MD,1,2)
      WRITE(MX,65)
      DO 63 J=1,MD
   63 WRITE(MX,67)J,T(J)
      WRITE(MX,66)
      LL=0
      DO 69 J=1,MD
      DO 70 KK=1,MD
      LL=LL+1
   70 VEC(KK)=W(LL)
   69 WRITE(MX,68)J,(VEC(KK),KK=1,MD)
      CALL OPTUM (BMATM,D,MD,RC,T,MX,RO)
  300 CALL EXIT
      END
// DUP
*STORE      WS  UA  MRSA
```

```
// DUP
*DELETE             CORRE
// FOR
*TRANSFER TRACE
*ARITHMETIC TRACE
*ONE WORD INTEGERS
**CORRE
      SUBROUTINE CORRE  N,M,IO,X,XBAR,STD,RX,R,B,D,T                    CORRE   1
      DIMENSION X 1 ,XBAR 1 ,STD 1 ,RX 1 ,R 1 ,B 1 ,D 1 ,T 1            CORRE   2
      COMMON MY,IN
C         INITIALIZATION                                                CORRE   3
      DO 100 J 1,M                                                      CORRE   4
      B J  0.0                                                          CORRE   5
  100 T J  0.0                                                          CORRE   6
      K  M*MGM /2                                                       CORRE   7
      DO 102 I 1,K                                                      CORRE   8
  102 R I  0.0                                                          CORRE   9
      FN N                                                              CORRE  10
      L 0                                                               CORRE  11
      IF IO  105, 127, 105                                              CORRE  12
C         DATA ARE ALREADY IN CORE                                      CORRE  13
  105 DO 108 J 1,M                                                      CORRE  14
      DO 107 I 1,N                                                      CORRE  15
      L LG1                                                             CORRE  16
  107 T J  T J GX L                                                     CORRE  17
      XBAR J  T J                                                       CORRE  18
  108 T J  T J /FN                                                      CORRE  19
      DO 115 I 1,N                                                      CORRE  20
      JK 0                                                              CORRE  21
      L I-N                                                             CORRE  22
      DO 110 J 1,M                                                      CORRE  23
      L LGN                                                             CORRE  24
      D J  X L -T J                                                     CORRE  25
  110 B J  B J GD J                                                     CORRE  26
      DO 115 J 1,M                                                      CORRE  27
      DO 115 K 1,J                                                      CORRE  28
      JK JKG1                                                           CORRE  29
  115 R JK  R JK GD J *D K                                              CORRE  30
      GO TO 205                                                         CORRE  31
C         READ OBSERVATIONS AND CALCULATE TEMPORARY                     CORRE  32
C         MEANS FROM THESE DATA IN T J                                  CORRE  33
  127 IF N-M  130, 130, 135                                             CORRE  34
  130 KK N                                                              CORRE  35
      GO TO 137                                                         CORRE  36
  135 KK M                                                              CORRE  37
  137 DO 140 I 1,KK                                                     CORRE  38
      CALL DATA  M,D                                                    CORRE  39
      DO 140 J 1,M                                                      CORRE  40
      T J  T J GD J                                                     CORRE  41
      L LG1                                                             CORRE  42
  140 RX L  D J                                                         CORRE  43
      FKK KK                                                            CORRE  44
      DO 150 J 1,M                                                      CORRE  45
      XBAR J  T J                                                       CORRE  46
  150 T J  T J /FKK                                                     CORRE  47
C         CALCULATE SUMS OF CROSS-PRODUCTS OF DEVIATIONS                CORRE  48
C         FROM TEMPORARY MEANS FOR M OBSERVATIONS                       CORRE  49
      L 0                                                               CORRE  50
      DO 180 I=1,KK                                                     CORREMO6
      JK 0                                                              CORRE  52
```

```
      DO 170 J 1,M                                                      CORRE 53
      L L61                                                             CORRE 54
  170 D J  RX L -T J                                                    CORRE 55
      DO 180 J 1,M                                                      CORRE 56
      R J  B J 6D J                                                     CORRE 57
      DO 180 K 1,J                                                      CORRE 58
      JK JK61                                                           CORRE 59
  180 R JK  R JK 6D J *D K                                              CORRE 60
      IF N-KK  205, 205, 185                                            CORRE 61
C        READ THE REST OF OBSERVATIONS ONE AT A TIME, SUM               CORRE 62
C        THE OBSERVATION, AND CALCULATE SUMS OF CROSS-                  CORRE 63
C        PRODUCTS OF DEVIATIONS FROM TEMPORARY MEANS                    CORRE 64
  185 KK N-KK                                                           CORRE 65
      DO 200 I 1,KK                                                     CORRE 66
      JK 0                                                              CORRE 67
      CALL DATA  M,D                                                    CORRE 68
      DO 190 J 1,M                                                      CORRE 69
      XBAR J  XBAR J 6D J                                               CORRE 70
      D J  D J -T J                                                     CORRE 71
  190 B J  B J 6D J                                                     CORRE 72
      DO 200 J 1,M                                                      CORRE 73
      DO 200 K 1,J                                                      CORRE 74
      JK JK61                                                           CORRE 75
  200 R JK  R JK 6D J *D K                                              CORRE 76
C        CALCULATE MEANS                                                CORRE 77
  205 JK 0                                                              CORRE 78
      DO 210 J 1,M                                                      CORRE 79
      XBAR J  XBAR J /FN                                                CORRE 80
C        ADJUST SUMS OF CROSS-PRODUCTS OF DEVIATIONS                    CORRE 81
C        FROM TEMPORARY MEANS                                           CORRE 82
      DO 210 K 1,J                                                      CORRE 83
      JK JK61                                                           CORRE 84
  210 R JK  R JK -B J *B K /FN                                          CORRE 85
C        CALCULATE CORRELATION COEFFICIENTS                             CORRE 86
      JK 0                                                              CORRE 87
      DO 220 J 1,M                                                      CORRE 88
      JK JK6J                                                           CORRE 89
  220 STD J   SQRT  ABS R JK                                            CORRE 90
      DO 230 J 1,M                                                      CORRE 91
      DO 230 K J,M                                                      CORRE 92
      JK J6 K*K-K /2                                                    CORRE 93
      L M* J-1 6K                                                       CORRE 94
      RX L  R JK                                                        CORRE 95
      L M* K-1 6J                                                       CORRE 96
      RX L  R JK                                                        CORRE 97
      IF(STD(J)*STD(K))225,222,225                                      CORREM01
  222 R(JK)=0.0                                                         CORREM02
      GO TO 230                                                         CORREM03
  225 R(JK)=R(JK)/(STD(J)*STD(K))                                       CORREM04
  230 CONTINUE                                                          CORREM05
C        CALCULATE STANDARD DEVIATIONS                                  CORRE 99
      FN SQRT FN-1.0                                                    CORRE100
      DO 240 J 1,M                                                      CORRE101
  240 STD J  STD J /FN                                                  CORRE102
C        COPY THE DIAGONAL OF THE MATRIX OF SUMS OF CROSS-PRODUCTS OF   CORRE103
C        DEVIATIONS FROM MEANS.                                         CORRE104
      L -M                                                              CORRE105
      DO 250 I 1,M                                                      CORRE106
      L L6M61                                                           CORRE107
  250 R I  RX L                                                         CORRE108
```

```
      RETURN                                                    CORRE109
      END                                                       CORRE110
// DUP
*STORE      WS  UA  CORRE
```

```
// DUP
*DELETE             ORDER
// FOR
*ONE WORD INTEGERS
      SUBROUTINE ORDER  M,R,NDEP,K,ISAVE,RX,RY
      DIMENSION R 1 ,ISAVE 1 ,RX 1 ,RY 1
C        COPY INTERCORRELATIONS OF INDEPENDENT VARIABLES
C        WITH DEPENDENT VARIABLE
      MM 0
      DO 130 J 1,K
      L2 ISAVE J
      IF NDEP-L2  122, 123, 123
  122 L NDEP& L2*L2-L2 /2
      GO TO 125
  123 L L2& NDEP*NDEP-NDEP /2
  125 RY J  R L
C        COPY A SUBSET MATRIX OF INTERCORRELATIONS AMONG
C        INDEPENDENT VARIABLES
      DO 130 I 1,K
      L1 ISAVE I
      IF L1-L2  127, 128, 128
  127 L L1& L2*L2-L2 /2
      GO TO 129
  128 L L2& L1*L1-L1 /2
  129 MM MM&1
  130 RX MM  R L
C        PLACE THE SUBSCRIPT NUMBER OF THE DEPENDENT
C        VARIABLE IN ISAVE K&1
      ISAVE K&1  NDEP
      RETURN
      END
// DUP
*STORE      WS  UA  ORDER
```

```
// DUP
*DELETE             MINV
// FOR
*ONE WORD INTEGERS
      SUBROUTINE MINV A,N,D,L,M                                         MINV   1
      DIMENSION A 1 ,L 1 ,M 1                                           MINV   2
C        SEARCH FOR LARGEST ELEMENT                                     MINV   3
      D 1.0                                                             MINV   4
      NK -N                                                             MINV   5
      DO 80 K 1,N                                                       MINV   6
      NK NK&N                                                           MINV   7
      L K  K                                                            MINV   8
      M K  K                                                            MINV   9
      KK NK&K                                                           MINV  10
      BIGA A KK                                                         MINV  11
      DO 20 J K,N                                                       MINV  12
      IZ N* J-1                                                         MINV  13
      DO 20 I K,N                                                       MINV  14
      IJ IZ&I                                                           MINV  15
   10 IF  ABS BIGA - ABS A IJ    15,20,20                               MINV  16
   15 BIGA A IJ                                                         MINV  17
      L K  I                                                            MINV  18
      M K  J                                                            MINV  19
   20 CONTINUE                                                          MINV  20
C        INTERCHANGE ROWS                                               MINV  21
      J L K                                                             MINV  22
      IF J-K  35,35,25                                                  MINV  23
   25 KI K-N                                                            MINV  24
      DO 30 I 1,N                                                       MINV  25
      KI KI&N                                                           MINV  26
      HOLD -A KI                                                        MINV  27
      JI KI-K&J                                                         MINV  28
      A KI  A JI                                                        MINV  29
   30 A JI  HOLD                                                        MINV  30
C        INTERCHANGE COLUMNS                                            MINV  31
   35 I M K                                                             MINV  32
      IF I-K  45,45,38                                                  MINV  33
   38 JP N* I-1                                                         MINV  34
      DO 40 J 1,N                                                       MINV  35
      JK NK&J                                                           MINV  36
      JI JP&J                                                           MINV  37
      HOLD -A JK                                                        MINV  38
      A JK  A JI                                                        MINV  39
   40 A JI  HOLD                                                        MINV  40
C        DIVIDE COLUMN BY MINUS PIVOT  VALUE OF PIVOT ELEMENT IS        MINV  41
C        CONTAINED IN BIGA                                              MINV  42
   45 IF(ABS(BIGA)-1.E-20)46,46,48                                      MINV M03
   46 D 0.0                                                             MINV  44
      RETURN                                                            MINV  45
   48 DO 55 I 1,N                                                       MINV  46
      IF I-K  50,55,50                                                  MINV  47
   50 IK NK&I                                                           MINV  48
      A IK  A IK / -BIGA                                                MINV  49
   55 CONTINUE                                                          MINV  50
C        REDUCE MATRIX                                                  MINV  51
      DO 65 I 1,N                                                       MINV  52
      IK NK&I                                                           MINV  53
      HOLD=A(IK)                                                        MINV M01
      IJ I-N                                                            MINV  54
      DO 65 J 1,N                                                       MINV  55
```

```
      IJ IJ&N
      IF I-K  60,65,60
   60 IF J-K  62,65,62
   62 KJ IJ-I&K
      A(IJ)=HOLD*A(KJ)+A(IJ)
   65 CONTINUE
C        DIVIDE ROW BY PIVOT
      KJ K-N
      DO 75 J 1,N
      KJ KJ&N
      IF J-K  70,75,70
   70 A KJ  A KJ /BIGA
   75 CONTINUE
C        PRODUCT OF PIVOTS
      D D*BIGA
C        REPLACE PIVOT BY RECIPROCAL
      A KK  1.0/BIGA
   80 CONTINUE
C        FINAL ROW AND COLUMN INTERCHANGE
      K N
  100 K  K-1
      IF K  150,150,105
  105 I L K
      IF I-K  120,120,108
  108 JQ N* K-1
      JR N* I-1
      DO 110 J 1,N
      JK JQ&J
      HOLD A JK
      JI JR&J
      A JK  -A JI
  110 A JI   HOLD
  120 J M K
      IF J-K  100,100,125
  125 KI K-N
      DO 130 I 1,N
      KI KI&N
      HOLD A KI
      JI KI-K&J
      A KI  -A JI
  130 A JI   HOLD
      GO TO 100
  150 RETURN
      END
// DUP
*STORE      WS  UA  MINV
```

```
// DUP
*DELETE             MULTR
// FOR
*ONE WORD INTEGERS
      SUBROUTINE MULTR  N,K,XBAR,STD,D,RX,RY,ISAVE,B,SB,T,ANS
      DIMENSION XBAR 1 ,STD 1 ,D 1 ,RX 1 ,RY 1 ,ISAVE 1 ,B 1 ,SB 1 ,
     1          T 1 ,ANS 10
      MM K&1
C        BETA WEIGHTS
      DO 100 J 1,K
  100 B J  0.0
      DO 110 J 1,K
      L1 K* J-1
      DO 110 I 1,K
      L L1&I
  110 B J  B J &RY I *RX L
      RM 0.0
      BO 0.0
      L1 ISAVE MM
C        COEFFICIENT OF DETFRMINATION
      DO 120 I 1,K
      RM RM&B I *RY I
C        REGRESSION COEFFICIENTS
      L ISAVE I
      B I  B I * STD L1 /STD L
C        INTERCEPT
  120 BO BO&B I *XBAR L
      BO XBAR L1 -BO
C        SUM OF SQUARES ATTRIBUTABLE TO REGRESSION
      SSAR RM*D L1
C        MULTIPLE CORRELATION COEFFICIENT
  122 RM  SQRT  ABS RM
C        SUM OF SQUARES OF DEVIATIONS FROM REGRESSION
      SSDR D L1 -SSAR
C        VARIANCE OF ESTIMATE
      FN N-K-1
      SY SSDR/FN
C        STANDARD DEVIATIONS OF REGRESSION COEFFICIENTS
      DO 130 J 1,K
      L1 K* J-1 &J
      L ISAVE J
  125 SB J   SQRT  ABS  RX L1 /D L  *SY
C        COMPUTED T-VALUES
  130 T J  B J /SB J
C        STANDARD ERROR OF ESTIMATE
  135 SY  SQRT  ABS SY
C        F VALUE
      FK K
      SSARM SSAR/FK
      SSDRM SSDR/FN
      F SSARM/SSDRM
      ANS 1  BO
      ANS 2  RM
      ANS 3  SY
      ANS 4  SSAR
      ANS 5  FK
      ANS 6  SSARM
      ANS 7  SSDR
      ANS 8  FN
      ANS 9  SSDRM
```

```
      ANS 10  F                                                  MULTR 57
      RETURN                                                     MULTR 58
      END                                                        MULTR 59
// DUP
```

```
// FOR
*ONE WORD INTEGERS
      SUBROUTINE GMPRD A•B•R•N•M•L                                    GMPRD   1
      DIMENSION A 1 •B 1 •R 1                                         GMPRD   2
      IR 0                                                            GMPRD   3
      IK -M                                                           GMPRD   4
      DO 10 K 1•L                                                     GMPRD   5
      IK IK&M                                                         GMPRD   6
      DO 10 J 1•N                                                     GMPRD   7
      IR IR&1                                                         GMPRD   8
      JI J-N                                                          GMPRD   9
      IB IK                                                           GMPRD  10
      R IR  0                                                         GMPRD  11
      DO 10 I 1•M                                                     GMPRD  12
      JI JI&N                                                         GMPRD  13
      IB IB&1                                                         GMPRD  14
   10 R IR  R IR &A JI *B IB                                          GMPRD  15
      RETURN                                                          GMPRD  16
      END                                                             GMPRD  17
// DUP
*STORE      WS  UA  GMPRD
```

```
*DELFTE             EIGEN
// FOR
*LIST SOURCE PROGRAM
*ONE WORD INTEGERS
      SUBROUTINE EIGEN A,R,N,MV
      DIMENSION A 1 ,R 1
C        GENFRATE IDENTITY MATRIX
      IF MV-1  10,25,10
   10 IQ -N
      DO 20 J 1,N
      IQ IQ&N
      DO 20 I 1,N
      IJ IQ&I
      R IJ  0.0
      IF I-J  20,15,20
   15 R IJ  1.0
   20 CONTINUE
C        COMPUTE INITIAL AND FINAL NORMS  ANORM AND ANORMX
   25 ANORM 0.0
      DO 35 I 1,N
      DO 35 J I,N
      IF I-J  30,35,30
   30 IA I& J*J-J /2
      ANORM ANORM&A IA *A IA
   35 CONTINUE
      IF ANORM  165,165,40
   40 ANORM 1.414*SQRT ANORM
      ANRMX ANORM*1.0E-6/FLOAT N
C        INITIALIZE INDICATORS AND COMPUTE THRESHOLD, THR
      IND 0
      THR ANORM
   45 THR THR/FLOAT N
   50 L 1
   55 M L&1
C        COMPUTE SIN AND COS
   60 MQ  M*M-M /2
      LQ  L*L-L /2
      LM L&MQ
   62 IF  ABS A LM  -THR  130,65,65
   65 IND 1
      LL L&LQ
      MM M&MQ
      X 0.5* A LL -A MM
   68 Y -A LM / SQRT A LM *A LM &X*X
      IF X  70,75,75
   70 Y -Y
   75 SINX Y/ SQRT 2.0* 1.0&  SQRT 1.0-Y*Y
      SINX2 SINX*SINX
   78 COSX  SQRT 1.0-SINX2
      COSX2 COSX*COSX
      SINCS  SINX*COSX
C        ROTATF L AND M COLUMNS
      ILQ N* L-1
      IMQ N* M-1
      DO 125 I 1,N
      IQ  I*I-I /2
      IF I-L  80,115,80
   80 IF I-M  85,115,90
   85 IM I&MQ
      GO TO 95
```

```
 90 IM M&IQ                                                EIGEN 57
 95 IF I-L   100,105,105                                   EIGEN 58
100 IL I&LQ                                                EIGEN 59
    GO TO 110                                              EIGEN 60
105 IL L&IQ                                                EIGEN 61
110 X A IL *COSX-A IM *SINX                                EIGEN 62
    A IM   A IL *SINX&A IM *COSX                           EIGEN 63
    A IL   X                                               EIGEN 64
115 IF MV-1   120,125,120                                  EIGEN 65
120 ILR ILQ&I                                              EIGEN 66
    IMR IMQ&I                                              EIGEN 67
    X R ILR *COSX-R IMR *SINX                              EIGEN 68
    R IMR   R ILR *SINX&R IMR *COSX                        EIGEN 69
    R ILR   X                                              EIGEN 70
125 CONTINUE                                               EIGEN 71
    X 2.0*A LM *SINCS                                      EIGEN 72
    Y A LL *COSX2&A MM *SINX2-X                            EIGEN 73
    X A LL *SINX2&A MM *COSX2&X                            EIGEN 74
    A LM   A LL -A MM   *SINCS&A LM * COSX2-SINX2          EIGEN 75
    A LL   Y                                               EIGEN 76
    A MM   X                                               EIGEN 77
C      TESTS FOR COMPLETION                                EIGEN 78
C      TEST FOR M   LAST COLUMN                            EIGEN 79
130 IF M-N   135,140,135                                   EIGEN 80
135 M M&1                                                  EIGEN 81
    GO TO 60                                               EIGEN 82
C      TEST FOR L   SECOND FROM LAST COLUMN                EIGEN 83
140 IF L- N-1    145,150,145                               EIGEN 84
145 L L&1                                                  EIGEN 85
    GO TO 55                                               EIGEN 86
150 IF IND-1   160,155,160                                 EIGEN 87
155 IND 0                                                  EIGEN 88
    GO TO 50                                               EIGEN 89
C      COMPARE THRESHOLD WITH FINAL NORM                   EIGEN 90
160 IF THR-ANRMX   165,165,45                              EIGEN 91
C      SORT EIGENVALUES AND EIGENVECTORS                   EIGEN 92
165 IQ -N                                                  EIGEN 93
    DO 185 I 1,N                                           EIGEN 94
    IQ IQ&N                                                EIGEN 95
    LL I& I*I-I /2                                         EIGEN 96
    JQ N* I-2                                              EIGEN 97
    DO 185 J I,N                                           EIGEN 98
    JQ JQ&N                                                EIGEN 99
    MM J& J*J-J /2                                         EIGEN100
    IF A LL -A MM   170,185,185                            EIGEN101
170 X A LL                                                 EIGEN102
    A LL   A MM                                            EIGEN103
    A MM   X                                               EIGEN104
    IF MV-1   175,185,175                                  EIGEN105
175 DO 180 K 1,N                                           EIGEN106
    ILR IQ&K                                               EIGEN107
    IMR JQ&K                                               EIGEN108
    X R ILR                                                EIGEN109
    R ILR   R IMR                                          EIGEN110
180 R IMR   X                                              EIGEN111
185 CONTINUE                                               EIGEN112
    RETURN                                                 EIGEN113
    END                                                    EIGEN114
// DUP
*STORE       WS  UA  EIGEN
```

```
// FOR
*ONE WORD INTEGERS
      SUBROUTINE MSTR A,R,N,MSA,MSR
      DIMENSION A 1 ,R 1
      DO 20 I 1,N
      DO 20 J 1,N
C        IF R IS GENERAL, FORM ELEMENT
      IF MSR  5,10,5
C        IF IN LOWER TRIANGLE OF SYMMETRIC OR DIAGONAL R, BYPASS
    5 IF I-J  10,10,20
   10 CALL LOC I,J,IR,N,N,MSR
C        IF IN UPPER AND OFF DIAGONAL  OF DIAGONAL R, BYPASS
      IF IR  20,20,15
C        OTHERWISE, FORM R I,J
   15 R IR  0.0
      CALL LOC I,J,IA,N,N,MSA
C        IF THERE IS NO A I,J , LEAVE R I,J  AT 0.0
      IF IA  20,20,18
   18 R IR  A IA
   20 CONTINUE
      RETURN
      END
// DUP
*STORE      WS  UA  MSTR
```

```
// FOR
*ONE WORD INTEGERS
      SUBROUTINE MPRD A,B,R,N,M,MSA,MSB,L
      DIMENSION A 1 ,B 1 ,R 1
C         SPECIAL CASE FOR DIAGONAL BY DIAGONAL
      MS MSA*10&MSB
      IF MS-22  30,10,30
   10 DO 20 I 1,N
   20 R I  A I *B I
      RETURN
C         ALL OTHER CASES
   30 IR 1
      DO 90 K 1,L
      DO 90 J 1,N
      R IR  0
      DO 80 I 1,M
      IF MS  40,60,40
   40 CALL LOC J,I,IA,N,M,MSA
      CALL LOC I,K,IB,M,L,MSB
      IF IA  50,80,50
   50 IF IB  70,80,70
   60 IA N* I-1 &J
      IB M* K-1 &I
   70 R IR  R IR &A IA *B IB
   80 CONTINUE
   90 IR IR&1
      RETURN
      END
// DUP
*STORE      WS  UA  MPRD
```

```
// FOR
*ONE WORD INTEGERS
      SUBROUTINE TPRD A,B,R,N,M,MSA,MSB,L
      DIMENSION A 1 ,B 1 ,R 1
C        SPECIAL CASE FOR DIAGONAL BY DIAGONAL
      MS MSA*10&MSB
      IF MS-22  30,10,30
   10 DO 20 I 1,N
   20 R I  A I *B I
      RETURN
C        MULTIPLY TRANSPOSE OF A BY B
   30 IR 1
      DO 90 K 1,L
      DO 90 J 1,M
      R IR  0.0
      DO 80 I 1,N
      IF MS  40,60,40
   40 CALL LOC I,J,IA,N,M,MSA
      CALL LOC I,K,IB,N,L,MSB
      IF IA  50,80,50
   50 IF IB  70,80,70
   60 IA N* J-1 &I
      IB N* K-1 &I
   70 R IR  R IR &A IA *B IB
   80 CONTINUE
   90 IR IR&1
      RETURN
      END
// DUP
*STORE      WS  UA  TPRD
```

```
// DUP
*DELETE             LINEQ
// FOR
*ARITHMETIC TRACE
*TRANSFER TRACE
*LIST SOURCE PROGRAM
*ONE WORD INTEGERS
      SUBROUTINE LINEQ(N,MD,D,SX,RY,ISAVE,SSAR,M)
C     THIS SUBROUTINE CALCULATES THE LINEAR PORTION OF THE REGRESSION
C     SUM OF SQUARES
C                    THE FOLLOWING DIMENSIONS MUST BE GREATER THAN MD * MD
C                    WHERE MD IS THE NUMBER OF LINEAR X TERMS
      DIMENSION SX(36)
C                    THE FOLLOWING DIMENSIONS MUST BE GREATER THAN THE TOTAL
C                    NUMBER OF VARIABLES
      DIMENSION ISAVE(29),RY(29)
C                    THE FOLLOWING DIMENSIONS MUST BE GREATER THAN MD
      DIMENSION D(10),U(10),V(10)
C                BETA WEIGHTS
      DO 101 J=1,MD
  101 B(J) = 0.0
      CALL MINV (SX,MD,DET,U,V)
      DO 111 J=1,MD
      LI = MD * (J-1)
      DO 111 I=1,MD
      L=LI+I
  111 B(J) = B(J) + RY(I) * SX(L)
      RM = 0.0
      LI = ISAVE(M)
C                COEFFICIENT OF DETERMINATION
      DO 121 I=1,MD
  121 RM = RM + B(I) * RY(I)
C                LINEAR REGRESSION SUM OF SQUARES
      SSAR = RM * D(LI)
      RETURN
      END
// DUP
*STORE      WS  UA  LINEQ
```

```
// DUP
*DELETE              OBSER
// FOR
*ONE WORD INTEGERS
*ARITHMETIC TRACE
*TRANSFER TRACE
*LIST SOURCE PROGRAM
      SUBROUTINE OBSER (M,ISAVE,MNDEP,MD,N)
C     THIS SUBROUTINE READS THE INPUT DATA AND GENERATES THE OTHER DATA
C     TO BE USED
C                    THE FOLLOWING DIMENSION MUST BE GREATER THAN THE NUMBER OF
C                    LINEAR X TERMS  +  2
      DIMENSION  OB(10)
C                    THE FOLLOWING DIMENSION MUST BE GREATER THAN THE
C                    TOTAL NUMBER OF VARIABLES
      DIMENSION D(29),ISAVE(29)
      COMMON MY,IN
    1 FORMAT(12F6.0)
      ML=MD+MNDEP
      MM = M*N
      MO=MD + MNDEP
      J = ISAVE(1)
      JA = ISAVE(2)
      L = MNDEP +MD
      DO 36 JJ = 1,N
      KK=0
      READ(MY,1) (OB(I),I=1,MO)
      DO 35 I=1,MNDEP
      KK =KK+1
   35 D(KK) = OB(I)
      DO 31 I=J,L
      KK=KK+1
   31 D(KK) = OB(I)
      DO 32 I = J,L
      KK=KK+1
   32 D(KK) = OB(I) * OB(I)
      DO 33 I=J,L
      DO 33 II = JA,L
      IF (I-II) 41,33,33
   41 KK=KK+1
      D(KK) = OB(I) * OB(II)
   33 CONTINUE
      WRITE(1'IN) (D(KK),KK=1,M)
   36 CONTINUE
      RETURN
      END
// DUP
*STORE      WS  UA  OBSER
```

```
// DUP
*DELETE             DATA
// FOR
*LIST SOURCE PROGRAM
*ONE WORD INTEGERS
      SUBROUTINE DATA(M,D)
C                   THE FOLLOWING DIMENSION MUST BE GREATER THAN
C                   THE TOTAL NUMBER OF VARIABLES
      DIMENSION D(29)
      COMMON MY,IN
      READ(1'IN) D
      RETURN
      END
// DUP
*STORE      WS  UA  DATA
```

```
// DUP
*DELETE             PUREE
// FOR
*LIST SOURCE PROGRAM
*ONE WORD INTEGERS
*ARITHMETIC TRACE
*TRANSFER TRACE
      SUBROUTINE PUREE (IHRX,PE,ML,N,ISAVE,NDEP)
C     THIS SUBROUTINE CALCULATES THE PURE ERROR PORTION OF THE RESIDUAL
C     SUM OF SQUARES
C                  THE FOLLOWING DIMENSION MUST BE GREATER THAN THE
C                  TOTAL NUMBER OF VARIABLES
      DIMENSION D(29),ISAVE(29),BRX(29),FRX(29),DRX(29),DFRX(29)
C                  THE FOLLOWING DIMENSION MUST BE GREATER THAN THE TOTAL
C                  NUMBER OF VARIABLES BY THE NUMBER OF LINEAR X TERMS + 1
      DIMENSION ARX(29,10)
      COMMON  MY,IN
      MD=ML-1
      IN=1
      DO 64 IJ =1,N
      READ(1'IN) D
      LL=1
      ARX(IJ,LL) = D(NDEP)
      K = ISAVE(1)
      DO 65 LL=2,ML
      ARX(IJ,LL) = D(K)
   65 K=K+1
   64 CONTINUE
      IHRX = 0
      IG=0
      PE =0.
      DO 99 JA=1,N
      BRX(JA) =0.
      FRX(JA) = 0.
      DRX(JA)=0.
      DFRX(JA) =0.
   99 CONTINUE
      NN=N-1
      JA =1
      DO 66 IJ=2,N
      DO 63 LL=2,ML
      IL=IJ+1
      CRX= ARX(IJ,LL) - ARX(IL,LL)
      IF (CRX) 82,62,82
   62 IF(LL-ML) 63,67,63
   63 CONTINUE
   67 DO 76 LL=2,ML
      II=IJ-1
      ERX = ARX(II,LL) - ARX(IJ,LL)
      IF(ERX) 68,81,68
   81 IF(LL-ML) 76,88,76
   76 CONTINUE
   82 DO 84 LL=2,ML
      II=IJ-1
      ERX= ARX(II,LL) - ARX(IJ,LL)
      IF(ERX) 66,86,66
   86 IF(LL-ML) 84,87,84
   84 CONTINUE
   68 IG=0
   88 IG =IG+1
```

```
      IF (IJ-N) 66,98,66
   87 IG =IG +1
      IF(IJ-IG-1) 98,71,98
   71 IG=IG+1
   98 IE=IJ-IG+1
      DO 75 K= IE,IJ
      BRX(JA) = ARX(K,1) + BRX(JA)
      FRX(JA) = ARX(K,1) * ARX(K,1) + FRX(JA)
      DRX(JA) = IG
   75 CONTINUE
      DFRX(JA) = IG-1
      JA =JA+1
   66 CONTINUE
      JD=JA-1
      DO 92 JA=1,JD
   92 IHRX = DFRX(JA) + IHRX
      DO 94 JA=1,JD
   94 PE=FRX(JA) - (BRX(JA) * BRX(JA) / DRX(JA)) + PE
      RETURN
      END
// DUP
*STORE      WS  UA  PUREE
```

```
// DUP
*DELETE              OPTUM
// FOR
*LIST SOURCE PROGRAM
*ONE WORD INTEGERS
*TRANSFER TRACE
*ARITHMETIC TRACE
      SUBROUTINE OPTUM(B2,D,MD,B,T,MX,BO)
C                 THIS SUBROUTINE READS THE VARIOUS INCREMENTS AND STOPPING
C                 VALUES AND GENERATES THE CORRESPONDING X'S AND Y'S
C                 THE FOLLOWING DIMENSIONS MUST BE GREATER THAN THE NUMBER
C                 OF LINEAR X TERMS , MD IN THE PROGRAM
      DIMENSION X(10),B4(10),B3(10)
C                 THE FOLLOWING DIMENSIONS MUST BE GREATER THAN MD*MD
      DIMENSION T(36),D(36)
C                 THE FOLLOWING DIMENSIONS MUST BE GREATER THAN TWICE MD*MD
      DIMENSION B(2,36)
C                 THE FOLLOWING DIMENSION MUST BE GREATER THAN TWICE
C                 (MD+1) * MD/2
      DIMENSION B2(2,21)
      DIMENSION BO(6)
      COMMON MY,IN
    1 FORMAT('0','X',1X,I2,'=',E15.6)
    2 FORMAT('0','Y1=',E15.6)
    3 FORMAT('0','U=',3X,F10.5)
    4 FORMAT(2F5.0)
    5 FORMAT('0','Y2=',E15.6)
   33 READ(MY,4) ADDON,TOP
      IF(ADDON)34,35,34
   34 U=T(1)
      DO 11 J=2,MD
   11 U=(T(J)+U+ABS(T(J)-U))*.5
      DO 15 I=1,500
      U=U+ADDON
      W=U
      IF(BO(3))24,24,25
   25 W=-U
   24 MDMD=MD*(MD+1)/2
      DO 16 J=1,MDMD
   16 T(J)=B2(1,J)-(B2(2,J)*W)
      CALL MSTR(T,D,MD,1,0)
      CALL MINV(D,MD,DET,T,B3)
      DO 14 J=1,MD
   14 B4(J)=(B(2,J)*W-B(1,J))*.5
      DO 20 J=1,MD
   20 X(J)=0.
      KK=1
      DO 23 J=1,MD
      DO 17 K=1,MD
      X(J)=D(KK)*B4(K)+X(J)
      KK=KK+1
   17 CONTINUE
   23 CONTINUE
      YP=BO(1)
      YS=BO(2)
      DO 18 J=1,MD
      K=MD+J
      YP=YP+B(1,J)*X(J)+B(1,K)*X(J)*X(J)
   18 YS=YS+B(2,J)*X(J)+B(2,K)*X(J)*X(J)
      L=2*MD+1
```

```
      DO 19 J=1,MD
      DO 19 JJ=J,MD
      IF(J-JJ)21,19,19
   21 YP=YP+B(1,L)*X(J)*X(JJ)
      YS=YS+B(2,L)*X(J)*X(JJ)
      L=L+1
   19 CONTINUE
      WRITE(MX,3)W
      DO 22 J=1,MD
   22 WRITE(MX,1)J,X(J)
      WRITE(MX,2)YP
      WRITE(MX,5) YS
      IF (ABS(U)-TOP)15,33,33
   15 CONTINUE
   35 RETURN
      END
// DUP
*STORE      WS  UA  OPTUM
```

```
// DUP
*DELETE             DATA
// FOR
*LIST SOURCE PROGRAM
*ONE WORD INTEGERS
      SUBROUTINE DATA(M,D)
C                   THE FOLLOWING DIMENSION MUST BE GREATER THAN
C                   THE TOTAL NUMBER OF VARIABLES
      DIMENSION D(29)
      COMMON MY,IN
      READ(1'IN) D
      RETURN
      END
// DUP
*STORE      WS  UA  DATA
```

```
// DUP
*DELETE              INDEF
// FOR
*IOCS(CARD,1132 PRINTER)
*LIST SOURCE PROGRAM
*ONE WORD INTEGERS
C                    THIS PROGRAM IS TO BE USED FOLLOWING MRSA WHEN B2
C                    IS INDEFINITE
C                    THE FOLLOWING DIMENSIONS MUST BE GREATER THAN (MD+1)*MD/2
C                    WHERE MD IS THE NUMBER OF LINEAR X TERMS
      DIMENSION BMATM(2,21),E(21),A(21),F(21),T(21),C(21),D(21)
C                    THE FOLLOWING DIMENSIONS MUST BE GREATER THAN MD*MD
      DIMENSION B1(6,6)
C                    THE FOLLOWING DIMENSION MUST BE GREATER THAN TWO TIMES THE
C                    NUMBER OF INDEPENDENT VARIABLES
      DIMENSION B(2,27)
C                    THE FOLLOWING DIMENSIONS MUST BE GREATER THAN
C                    THE NUMBER OF LINEAR X TERMS
      DIMENSION X(10)
      DIMENSION BO(6)
      COMMON MY,IN
    1 FORMAT(3F5.0)
    2 FORMAT('0',30X,'U=',F10.5)
    3 FORMAT('0','X',I2,'=',E15.6)
    4 FORMAT('0','Y1=',1X,E15.6)
    5 FORMAT('0','Y2=',1X,E15.6)
    6 FORMAT('0','GAMMA=',3X,F10.5)
    7 FORMAT('0','THE EIGENVALUES OF (B1-MUB2)')
    8 FORMAT(1X,'LAMDA',1X,I2,'=',F10.5)
    9 FORMAT(I5)
   30 FORMAT(8F10.5)
   31 FORMAT('1')
      WRITE(3,31)
      MX=3
      MY=2
      READ(MY,9) K
      XM=K+1
      MD=(-.5+SQRT(.25+2.*XM))-1
      L1=MD+1
      DO 10 I=1,2
   10 READ(MY,30) BO(I), (B(I,J),J=1,K)
      DO 71 I=1,2
      IB=1
      IC=1
      ID=2
      DO 61 J=L1,K
      B1(IB,IB)=B(I,J)
      IB=IB+1
      IF(J-L1-MD) 61,62,62
   62 B1(IC,ID)=B(I,J)/2.
      ID=ID+1
      IF(ID-L1)61,63,63
   63 IC=IC+1
      ID=IC
      IF(IC-ID)61,66,61
   66 ID=ID+1
   61 CONTINUE
      LLL=1
      DO 72 JJ=1,MD
      DO 72 II=1,MD
```

```
      IF(II-JJ)68,68,72
   68 BMATM(I,LLL)=B1(II,JJ)
      LLL=LLL+1
   72 CONTINUE
   71 CONTINUE
   33 READ(MY,1)U,ADD,TOP
      IF(U-50)34,35,35
   34 WRITE(MX,2) U
      MDMD=MD*(MD+1)/2
      DO 12 I=1,MDMD
      E(I)=BMATM(1,I)-U*BMATM(2,I)
   12 A(I)=E(I)
      CALL EIGEN(E,F,MD,0)
      CALL MSTR(E,T,MD,1,2)
      WRITE(3,7)
      DO 26 I=1,MD
   26 WRITE(3,8) I,T(I)
      G=T(1)
      DO 13 J=2,MD
   13 G=(T(J)+G+ABS(T(J)-G))*.5
      DO 15 I=1,500
      G=G+ADD
      K=1
      DO 32 J=1,MDMD
   32 C(J)=A(J)
      DO 25 L=1,MDMD,K
      C(L)=A(L)-G
      K=K+1
   25 CONTINUE
      CALL MSTR(C,D,MD,1,0)
      CALL MINV(D,MD,DET,T,F)
      DO 14 J=1,MD
   14 F(J)=(B(2,J)*U-B(1,J))*.5
      DO 20 J=1,MD
   20 X(J)=0.
      KK=1
      DO 23 J=1,MD
      DO 17 K=1,MD
      X(J)=D(KK)*F(K)+X(J)
      KK=KK+1
   17 CONTINUE
   23 CONTINUE
      YP=BO(1)
      YS=BO(2)
      DO 18 J=1,MD
      K=MD+J
      YP=YP+B(1,J)*X(J)+B(1,K)*X(J)*X(J)
   18 YS=YS+B(2,J)*X(J)+B(2,K)*X(J)*X(J)
      DO 19 J=1,MD
      DO 19 JJ=J,MD
      L=2*MD+J
      IF(J-JJ)21,19,19
   21 YP=YP+B(1,L)*X(J)*X(JJ)
      YS=YS+B(2,L)*X(J)*X(JJ)
   19 CONTINUE
      WRITE(MX,6)G
      DO 22 J=1,MD
   22 WRITE(MX,3)J,X(J)
      WRITE(MX,4)YP
      WRITE(MX,5)YS
```

```
      IF(G-TOP)15,33,33
   15 CONTINUE
   35 CALL EXIT
      END
// DUP
*STORE      WS  UA  INDEF
```