NONLINEAR PROGRAMMING TECHNIQUES FOR THE MULTIPLE RESPONSE PROBLEM

A THESIS

Presented to

The Faculty of the Division of Graduate

Studies and Research

by

Timothy George Fields

In Partial Fulfillment

of the Requirements for the Degree

Master of Science

in the School of Industrial and Systems Engineering

Georgia Institute of Technology

February, 1974

NONLINEAR PROGRAMMING TECHNIQUES FOR

THE MULTIPLE RESPONSE PROBLEM

Approved:

Chairman

Date approved by Chairman: 2-4-74

ACKNOWLEDGMENTS

The author wishes to express his sincere thanks to his thesis advisor, Dr. Douglas C. Montgomery, whose invaluable advice, encouragement and guidance made the successful completion of this research possible.

The author is also indebted to Drs. Mokhtar S. Bazaraa and Russell G. Heikes for their advice and constructive criticism as members of the thesis committee.

A note of appreciation is extended to Dr. Terrence Connolly, whose advice and assistance proved especially helpful at critical times during the research.

These acknowledgments would be incomplete without an expression of gratitude to the United States Army for making two years of graduate study possible.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF TABLES (Continued)

LIST OF ILLUSTRATIONS

SUMMARY

This thesis presents a study in the application of certain nonlinear programming techniques to the multiple response problem, a typical problem that evolves through the use of response surface techniques. The research surveys the existing techniques and the utility of nonlinear programming models for the problem is investigated.

The Hooke and Jeeves Pattern Search Technique is used as the optimization algorithm. The technique is adapted for use with either constrained or unconstrained problems.

The multiple response problem is considered in three different configurations; 1) single objective function, with other responses treated as constraints and considered explicitly; 2) single objective function with implicit consideration of remaining responses as constraints; and, 3) a weighting function scheme wherein a composite function is made up of all responses which are individually weighted.

No single model can be considered the best for all algorithms, but for the Hooke and Jeeves approach, the weighted function is to be preferred when compared with currently existing techniques found in the response surface field.

CHAPTER I

INTRODUCTION

Problem Statement

Response surface methodology is generally characterized by the attempt, through designed experimentation, to approximate a complex and unknown function

$$\eta = f(\xi_1, \xi_2, \ldots, \xi_n)$$

by some low order polynomial

$$\beta = f(x_1, x_2, \ldots, x_n)$$

where the x_i, $i = 1,2,\ldots,n$, are coded from the natural variables, ξ_i, $i = 1,2,\ldots,n$, and f represents the approximating function. It is assumed that this function can only be derived through experimentation, where the effects of different levels of the decision variables are measured. The function is applicable only in the region of experimentation. The objective then is to optimize the function to determine the best operating levels on the variables for the process under analysis. Since the function, f, is a fitted surface, any optimal point found lying outside the region of experimentation cannot be considered valid and new experimentation must be undertaken to approximate a new function in that region.

If a situation exists where more than one function must be optimized, we have encountered the "multiple" response problem. For example, an experimenter may wish to maximize the yield of a process while simultaneously minimizing the percent of impurities in that yield, where both surfaces can be determined only through experimental means.

Nonlinear programming is generally defined as any collection of techniques used in optimizing some mathematical function

$$\begin{aligned} &\text{maximize } f(X) \\ &\text{subject to } g_i(X) \leq 0 \text{ for } i = 1,2,\ldots,m \\ &\qquad\qquad\quad h_i(X) = 0 \text{ for } i = 1,2,\ldots,k \end{aligned}$$

where the objective function or some of the constraints, or a combination of these, are nonlinear. A great deal of research has been done in nonlinear programming. We concern ourselves here only with the particular algorithm used in this research.

Applications of nonlinear programming techniques to the field of response surface methodology have not been widely attempted. The intent here is to extend to the statistical literature some possible nonlinear programming techniques with respect to both the formulation and the solution of the multiple response problem. It is assumed throughout that low order polynomials have been fitted to all surfaces considered and are well-defined within the region of experimentation. Solutions existing outside the region of experimentation for any fitted surface are assumed to be invalid and necessitate new experimental exploration before any nonlinear programming methods can be applied. A restatement of the multiple response problem into a workable nonlinear programming form will be illustrated and a typical nonlinear programming technique applied.

The response surface problem is characterized by relatively few independent variables, generally not more than seven, and few constraints. The fitted surfaces will generally not be higher than second order due to design difficulty and applicability, and seem to work well in most practical situations. The problem generally consists of a quadratic objective function and one or more constraints of no higher than second order. Range constraints on the variables are often present since an underlying assumption made throughout is that the objective function and possibly some of the constraints are derived as a result of performing designed experiments and therefore the surfaces are valid only over the specific region of interest in which the data were collected. In Chapter II an outline of the optimization method and development of the models is given. Three typical response surface problems are investigated and considered in three different model forms and a nonlinear optimization technique applied. The results of this investigation are discussed in Chapter III.

This research particularly considers the multiplicity of the response functions and some methods of handling them. The main thrust here is not to develop a new approach to optimization but rather to apply existing methods to a well-known problem, and particularly to contrast the methods investigated with the only methods presently used and reflected in the typical statistical literature. This represents a step in the direction of broadening the scope of solution approaches available to the statistician concerned with response surface methodology. In all discussion the problem addressed will be considered a maximization problem.

Literature Survey

Very little has been reported in the response surface literature with respect to multiple response problems. Most proposed solution procedures are graphical in nature. Early references, G.E.P. Box (1) and J. S. Hunter (11), only mention the multiple response problem and note that "it is interesting to look at" the superimposition of the two response surfaces, but acknowledge that such methods would be difficult for more than two variables and impossible for greater than three variables. In 1959 Umland and Smith (18) used Lagrange multipliers to solve two convex response surfaces which measured yield and purity. For their particular problem the purity function was considered a constraining relationship and successively set to acceptable values. The yield function was then optimized subject to the constraining relation through the use of Lagrange multipliers. The problem was in two variables and the results were favorably compared to graphical means of solution. In a comparable study, in 1960, Lind, et al., (12) used graphical means to optimize a yield-cost system for American Cyanimid where both relationships were response surfaces.

Not strictly in the multiple response area, but concerned with constrained optimization of response functions (into which form such multi-response problems can be placed) are three studies. Schrage (17), in 1958, used the method of steepest ascent and linear programming to optimize a catalytic cracking operation. Linear approximations were first applied to the nonlinear constraints and linear programming was applied sequentially. In 1959, Hoerl (9) introduced the constraint

$$\sum_{i=1}^{n} x_i^2 = X'X = C$$

where $X' = (x_1, x_2, \ldots, x_n)$, for use in ridge analysis but this still amounted to interpretation of the constrained problem through graphical means. Michaels and Pengilly (13) used Lagrangian multipliers applied to a response surface objective function and one algebraically derived cost constraint.

In 1971 Myers (15) mentions the multiple response example of Lind and indicates the graphical approach to a solution. In 1973 Heller and Staats (8) absorbed the cost constraint (or cost objective function) into the yield objective function to form a net profit objective function and used the cost per unit as the basis for the distance metric of their n-space. Their objective function was subject to both algebraic and response surface constraints and the problem solution was arrived at through a method based on Zoutendijk's (19) method of feasible directions. Myers and Carter (16) (1973) address the multiple response problem in much the same manner as Umland and Smith. One response was restated in constraint form and the method of Lagrange multipliers applied. Myers and Carter, however, chose not to fix the constant value of the constraint but rather they selected "directly values of the Lagrange multipliers, μ, in the region which gives rise to operating conditions on X, (a vector of independent or design variables)... that result in <u>absolute</u> <u>maxima</u> on y_p (the objective function), conditional on being on a surface of the constraint response". In the case of one constraint this evolves to a two-dimensional graphing of the Lagrange multipliers over the region in which feasible solution points exist. The difficulty of extension to a larger number of constraints, although done in the reference cited for a specialized problem, negates the attractiveness of this method.

Although the history of nonlinear programming is considerably richer than the more specific response surface area outlined previously, we will concern ourselves only with the literature that gives rise to the method actually used in solving the multi-response problem in this research.

As a transition from the response surface methodology to nonlinear programming let us mention the work of Carroll (3) in 1961 who introduced the Created Response Surface Technique (CRST) which restates the constrained problem into an unconstrained problem by means of incorporating the constraints into the objective function. A penalty constant is attached to each such constraint and has the effect of severely reducing (in a maximization problem) the optimum value of the objective function. Through the sequential application of gradually reduced penalty constants and unconstrained optimization techniques, this constrained problem reaches the same optimum value as the original objective function. This work serves as one of the forerunners of penalty and barrier function optimization techniques in the field of nonlinear programming.

Consideration of a large number of mathematical programming techniques is not necessary in order to introduce the basic methodology into the response surface area. Consideration of multiple responses and their model formulation is the main thrust of this thesis. With the assumption that we have well-defined functions within the area of interest for the response surface it remains only to apply any effective optimization technique to the models developed. Two methods of treating the multiple objective function have arisen in the literature.

Geoffrion, et al., (6) introduce a weighting function criterion in developing an approach to the multi-criterion optimization problem. The objectives are weighted according to different schemes, depending generally on their utility to the decision-maker. Dyer (4), in 1972, in a similar vein, applied the theory to a man-machine interaction algorithm for the solution of the multi-criterion problem. Geoffrion and Hogan (7) address the problem of coordination between different autonomous levels of organization. The Coordinator, or headquarters, requests the local optimums and the directions of function value improvement from each of the subordinate levels, based on a specific set of data. Based on the preference function of the Coordinator, and in consideration of the information received from the lower divisions, a direction and step size are decided upon, a new set of data generated, and the process continues, culminating in a best response for all functions. Such highly interactive algorithms are very dependent upon the type of optimization technique employed and are not investigated here.

Scope of the Thesis

For purposes of comparison of different models it is desirable that a programming technique that can consider both constrained and unconstrained formulations be used. Although not specifically designed for constrained optimization, the Hooke and Jeeves pattern search (10) technique was adapted for use in either the constrained or unconstrained case.

The approach is to first formulate the multiple response problem in two different configurations and then to apply a nonlinear programming algorithm, the modified Hooke and Jeeves procedure, to these restated problems. The intent is to compare the results of the formulations and solutions, primarily from a qualitative standpoint. The results are compared to the original treatment of the problem. The effort is to present alternative approaches to the multiple response problem, emphasizing problems previously treated in the literature. This represents an initial step in the direction of applying nonlinear programming techniques to the multiple response problem. Previous published efforts in this field have been confined primarily to graphical means of solution.

CHAPTER II

MODEL DEVELOPMENT AND APPLICATION OF A NONLINEAR PROGRAMMING TECHNIQUE

The Algorithm

A brief outline of the modified Hooke and Jeeves pattern search technique will now be presented. The algorithm was considered particularly well-suited for a number of reasons. (1) It is relatively simple when compared with gradient techniques. It requires no gradient computation and is simple from a programming standpoint. (2) The algorithm is adaptable to either constrained or unconstrained formulations and for this reason is particularly well-suited to the application intended here, i.e., the investigation of different multiple response models. Since some of the models consider constraints and others do not it becomes important to have an equal basis from which to compare results. (3) The pattern search technique also may be more amenable to work already reported in the response surface area. (4) Lastly, function evaluations, particularly in the weighting function approach, may prove more valuable than gradient techniques.

A simplified flow chart is shown in Figure 1 for the general Hooke and Jeeves pattern search technique. For simplicity we consider only three points. Let

X^k_{Base} - the base point at the k^{th} iteration,

X_B - the point around which explore moves are conducted, and

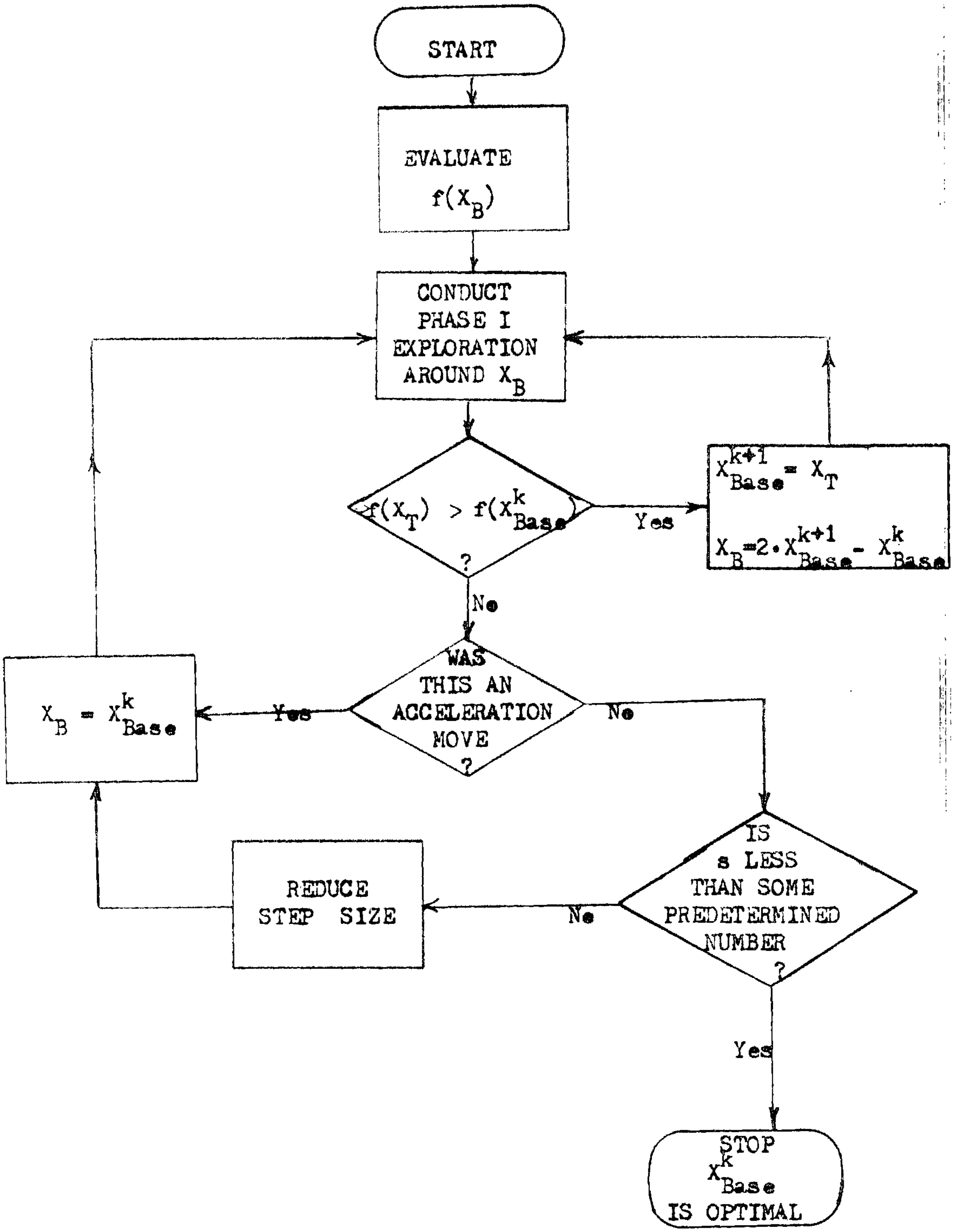

Figure 1 Hooke and Jeeves Pattern Search Technique Flow Chart

X_T — any evaluated point around X_B.

Other notation is as follows. The step size of the explore move is denoted by s; i, i = 1,2,...,n, represents the number of coordinate directions; k is an iteration index; β is an indicator function; and ϵ represents some predetermined small value greater than 0. The method follows basically the following steps:

Initially $X_B = X^k_{Base}$, $i = k = 1$, $\beta = 1$.

Phase I (Exploratory move)

1 If $i = n + 1$, go to Phase II.

2 Otherwise, let $X_T = X_B + \beta \cdot s \cdot d_i$ where

$d_i = (d'_1, d'_2, \ldots, d'_n)$, $d'_j = 0$ for $i \neq j$; $d'_j = 1$ for $i=j$.

3 If $f(X_T) > f(X_B)$, let $X_B = X_T$, $i=i+1$, $\beta = 1$, Return to Step 1.

4 Otherwise, check the value of β. If $\beta = 1$, set $\beta = -1$ and repeat Step 2. If $\beta = -1$, X_B remains the same, $i=i+1$, $\beta = 1$, Return to Step 1.

Phase II (Acceleration move)

1 If $f(X_T) > f(X^k_{Base})$, let $X^{k+1}_{Base} = X_T$, $X_B = 2 \cdot X^{k+1}_{Base} - X^k_{Base}$, Set $i = 1$, and return to Phase I.

2 Otherwise check the step size, s

If $s \leq \epsilon$, Stop, X^k_{Base} is optimal,

If $s > \epsilon$, let $s = \frac{1}{2}s$, $i=1$, $X_B = X^k_{Base}$, Return to Phase I.

Constraints

A variation has been made to the basic algorithm in order to adapt it for use with the constrained problems. Two categories of constraints are considered: (1) range or boundary constraints on the individual variables, and (2) general constraints. The development of a modified pattern search to accomodate constraints demands that we consider both types.

The first type, range constraints, are handled the same way for all models. If a constraint violation occurs during either an explore move or an acceleration move, the variable in question is simply retained at the boundary before the evaluation of the function. If the move is a success, the variable is retained at the bound and the algorithm continues in the remaining coordinate directions. If the move is a failure there is no problem since the next move in that variable direction will be away from the bound.

General constraints may be treated differently by the different models. Generally, if any constraints of this type are violated, the point under consideration at the time that the violation occurs is rejected as a failure to improve the objective function value.

The Models

Two different approaches were taken to develop the models used in this investigation. One of these is subdivided into two considerations. The Type I model is the kind of formulation encountered in all of the response surface literature to this point. This approach restructures the problem from a multiple objective function type problem into one which has only one objective function and some number of constraints. To do this, a decision must be made to treat one response as "most important", while the remaining r-1 of the responses are set at a particular level or a ceiling is placed upon their possible values. The original problem

$$\text{Max } (f(X), y_i(X)) \qquad i = 1,2,\ldots,r-1$$

$$\text{st. } g_k(X) \leq 0 \qquad k = 1,2,\ldots,m$$

becomes

$$\text{Max } f(X)$$

$$\text{st: } y_i(X) - \alpha_i \leq 0 \qquad i = 1,2,\ldots,r-1$$

$$g_k(X) \leq 0 \qquad k = 1,2,\ldots,m$$

where α_i represent the maximum acceptable levels of the secondary objective functions.

Two applications of optimization with constraints are considered.

Type IA - explicit consideration

Type IB - implicit consideration by means of a penalty function.

Application of the modified Hooke and Jeeves algorithm to a constrained problem was one of the investigative goals.

For the Type IA model the formulation is simply

$$\text{Max } f(X)$$

$$\text{st. } y_i(X) - \alpha_i \leq 0 \quad , \quad i = 1,2,\ldots,r-1$$

$$g_k(X) \leq 0 \quad , \quad k = 1,2,\ldots,m$$

Any point which violates a constraint is treated as a failure and the search returns to the last best point.

The form for the Type IB becomes:

$$\text{Max } f(X) - P(\max((y_i(X)-\alpha_i),0))^2 \ , \ i = 1,2,\ldots,r-1$$

$$\text{st: } g_k(X) \leq 0 \qquad , \ k = 1,2,\ldots,m$$

where P represents a large penalty constant. The objective function therefore is reduced by the amount of the penalty function only if a restructured constraint, $y_i(X)-\alpha_i$, is violated. Although the same approach can be made to all constraints, this investigation treats true constraints explicitly and considers only the restated objective functions in the penalty context. The degree to which any constraint is violated is a function of the penalty size.

The second model intuitively appeals in instances where minor constraint violations can be permitted and in fact the previous work done in the area (for example, see Umland and Smith) seems to indicate that the constraint value is not inflexible. Explicit consideration on the other hand, permits no violation of the fixed level of the constraint value.

The second method of approach is a weighting factor scheme. The multiple responses are treated as objective functions and given weights as follows:

$$\text{Max } w_1 \cdot f(X) + w_2 \cdot y_i(X) \ \ldots + w_r \cdot y_{r-1}$$

$$\text{st.} \quad g_k(X) \qquad\qquad k = 1,2,\ldots,m$$

In the treatment of the dual response problem the $\Sigma w_i = 1$ in all cases. The nonlinear programming literature assigns the weights based on some subjective criteria and generally with some knowledge of the problem and its interactions. Although such knowledge might be available for our purposes, for the example problems dealing only with two responses the assumption that no knowledge is available is made. Rather, the objective is to give the decision-maker a series of results from which to make a decision. The weights are assigned on an incremental basis, successively varied over a suitably chosen range. The result is a list of responses for each objective function at each level of weighting. As shown in the example problems, an initial coarse increment can be assigned in order to determine the weights that yield the values desired. When those weights have been determined, a finer incrementing can take place and so forth to whatever degree required.

Weighting Function Extension to a Three-Response Problem

In extending the weighting function approach to larger problems, namely more than two objective functions, certain factors become more important. It would appear that the attractive feature of enumerating the weights assigned over the unit interval is diminished since the number of different combinations required grows larger very quickly as the number of functions increase. Also, scaling might be required if, for example, one function, say f_1, measures cost in thousands of dollars while a second response, f_2, measures percent yield, on the scale of

0-100%. Since the composite objective function is the vehicle upon which the optimization technique works, the tendency would be, without scaling, to favor an optimal solution which maximized f_1 alone. In effect, we implicitly weight f_1 by 10^2, the factor by which the average value of f_1 is greater than that of f_2. If we fail to take such scale difference into account, a great deal of time and effort is spent refining our weights over the unit interval.

We can, by careful scaling measures reduce the problem involved in the larger response case. Throughout the literature that deals with the weighted objective function some "marginal" value is assigned to the weights based on their worth to the decision-maker relative to the other objectives. No such steps were taken in the dual response case, but in the example that follows we are able to reduce the problem to a simple requirement for a preference order from the decision-maker. We assume, as in the two-response situation, that no specific value for any objective is required, but rather a choice of alternatives is the desired goal. In fact, for the three objective function case, as in the example, 11 different levels for each function can be evaluated in 66 iterations of the optimization technique. For four objectives, six levels can be evaluated in 56 iterations with the necessary reduction in refinement of the interval. In either case, a sufficient number of alternatives exist in tabular form for the decision-maker to made a choice.

Scaling

A scaling approach is presented which complements the basic approach of evaluating over some preselected interval rather than presetting an expected function value. As an example of the latter, let us say that a composite function F is made up of f_i as follows:

$$F = w_1f_1 + w_2f_2 + w_3f_3$$

where the values of the individual functions f_i, i=1,2,3 vary as follows:

$$10,000 \leq f_1 \leq 20,000$$

$$10 \leq f_2 \leq 50$$

$$50 \leq f_3 \leq 1000$$

It is important to note that these values are the extrema of the function values and do not represent any preference on the part of the decision-maker. Any preference is indicated by the weights, w_i, i=1,2,3. For scaling purposes we introduce a scaling factor s_i, i=1,2,3 as follows:

$$F = w_1s_1f_1 + w_2s_2f_2 + w_3s_3f_3.$$

The scaling factors serve to more equitably distribute the absolute magnitude of the individual function contributions to the composite function F. If we were to scale, for instance, by average f_i values, $\bar{f}_i$, so that all functions are expressed in terms of f_1, we could proceed as follows:

$$F = w_1s_1 + w_2s_2\,\frac{\bar{f}_2(10)}{\bar{f}_1(10^3)} + w_3s_3\,\frac{\bar{f}_3(10^2)}{\bar{f}_1(10^3)}$$

Then, in order for each of the functions to be of the same order of magnitude and therefore of equal importance in contributing to the composite function F, we set

$$s_1 = 1, \qquad s_2 = 10^{-2}, \qquad \text{and } s_3 = 10^{-1}$$

which will reduce each contributing function to the same relative size.

A variation of this approach has been used here in keeping with the value range concept of the weighting function. Let

$$F = w_1 s_1 \ (\underline{f}_1, \bar{f}_1) + w_2 s_2 \frac{f_2(\underline{f}_2, \bar{f}_2)}{f_1(\underline{f}_1, \bar{f}_1)} + w_3 s_3 \frac{f_3(\underline{f}_3, \bar{f}_3)}{f_1(\underline{f}_1, \bar{f}_1)}$$

where $(\underline{f}_1, \bar{f}_1)$ is the scaled range on f_1, and $(\underline{f}_i, \bar{f}_i)$ represent the minimum and maximum, respectively of the f_1, i=1,2,3. The problem then is to determine a range on the s_i, i=1,2,3 such that all functions contribute equitably (in an absolute magnitude sense) to F. The absolute extrema on s_i obviously occur at the opposite extrema of the functions compared:

$$\bar{s}_i = \frac{\bar{f}_1}{\underline{f}_i} \quad \text{and} \quad \underline{s}_i = \frac{\underline{f}_1}{\bar{f}_i}$$

The range on s_i is then between $\underline{s}_i$ and $\overline{s}_i$, i.e.,

$$\underline{s}_i \leq s_i \leq \overline{s}_i$$

Although this is the most conservative range, it precludes an eventual optimal solution in the vicinity of the extrema which would then require more refinement.

From the example:

$$10{,}000 \leq f_1 \leq 20{,}000$$

$$10 \leq f_2 \leq 50$$

$$50 \leq f_3 \leq 1000$$

we find

$$\overline{s}_2 = \frac{20{,}000}{10} = 2000 \qquad \underline{s}_2 = \frac{10{,}000}{50} = 200$$

$$\overline{s}_3 = \frac{20{,}000}{50} = 400 \qquad \underline{s}_3 = \frac{10{,}000}{1{,}000} = 10$$

Then

$$0 \leq s_i \leq 1$$

$$200 \leq s_2 \leq 2000$$

$$10 \leq s_3 \leq 400$$

At this point each value for the s_i, $i=1,2,3$ is multiplied by the preference weight assigned by the decision-maker, the interval determined based on the number of observations desired, and the optimization technique applied.

Application - Examples

The models indicated were applied to three response surface problems which are typical of those discussed in the literature.

The first problem is due to Umland and Smith (18), and consists of two response surface. The primary response, yield (y_P), and a secondary response, purity (y_S), is given in the equations below.

$$y_P = 55.84 + 7.31x_1 + 26.65x_2 - 3.03x_1^2 - 6.96x_2^2 + 2.69x_1x_2$$

y_P - predicted yield

$$y_S = 85.72 + 21.85x_1 + 8.59x_2 - 9.20x_1^2 - 5.18x_2^2 - 6.26x_1x_2$$

y_S - predicted purity

It is assumed that x_1, x_2 are independent factors, continuous and controllable by the experimenter.

A graph of the fitted response surfaces is shown in Figure 2. Both functions are concave in the region of interest and the objective is to maximize both. There are no other explicit constraints. The approach that the authors used was to fix the secondary response at three different values - 95%, 92.5%, and 90% - below which the purity level should not move. They then proceeded to choose x_1 and x_2 to maximize yield using the method of Lagrange multipliers. Their results are shown below:

Purity	94.87	92.47	89.995
Yield	83.66	86.73	88.68
x_1	0.965	1.005	1.075
x_2	1.088	1.316	1.479

It appears from the results that small violations of the imposed

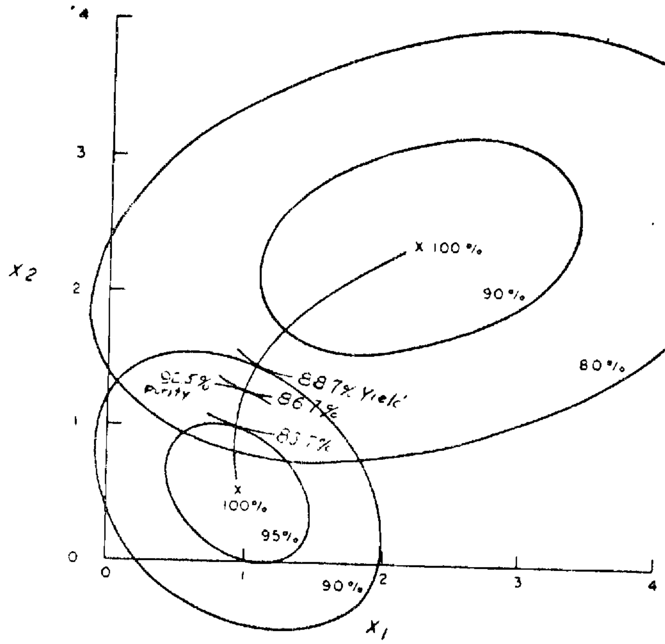

Figure 2. Umland and Smith Response Surfaces (after Umland and Smith (18))

purity constraint are not important in view of the nature of the problem.

The next two problems are taken from an article by R. H. Myers and W. H. Carter (16).

The authors first consider a dual response problem in three variables. The responses:

$$y_P = 65.39 + 9.24x_1 + 6.36x_2 + 5.22x_3 - 7.23x_1^2 - 7.76x_2^2 - 13.11x_3^2$$
$$-13.68x_1x_2 - 18.92x_1x_3 - 14.68x_2x_3 \qquad (1)$$

$$y_S = 56.42 + 4.65x_1 + 8.39x_2 + 2.56x_3 + 5.25x_1^2 + 5.62x_2^2 + 4.22x_3^2$$
$$+ 8.74x_1x_2 + 2.32x_1x_3 + 3.78x_2x_3 \qquad (2)$$

Range constraints are imposed on all x_i as follows:

$$-2.5 \leq x_i \leq 2.5 \quad i = 1,2,3$$

The solution method of Myers and Carter for both problems is basically a combination of the method of Lagrangian multipliers and graphical analysis. The solution method is as follows. As before, two responses are defined,

$$y_P = b_0 + \bar{X}'b + \bar{X}'B\bar{X} \qquad (3)$$

and

$$y_S = c_0 + \bar{X}'c + \bar{X}'C\bar{X} \qquad (4)$$

where $\bar{X}$ is a vector of independent or design variables, b and c are vectors of first order regression coefficients, and B and C are matrices containing the second order regression coefficients. For example,

$$B = \begin{bmatrix} b_{11} & b_{12}/2 & \cdots & b_{1n}/2 \\ & b_{22} & \cdots & b_{2n}/2 \\ & & & \vdots \\ \text{sym} & & & b_{nn} \end{bmatrix},$$

where the b_{ij} are second order coefficients. The Lagrange function is

$$L = b_0 + \bar{X}'b + \bar{X}'B\bar{X} - \mu(c_0 + \bar{X}'c + \bar{X}'C\bar{X} - k),$$

where k is an acceptable level for y_S. Setting $\frac{\partial L}{\partial X} = 0$ results in

$$(B-\mu C)\bar{X} = \tfrac{1}{2}(\mu c - b) \tag{5}$$

The matrix of second partials is then found to be

$$M(\bar{X}) = 2(B - \mu C) \tag{6}$$

The above equations hold irrespective of the value for k. It is in this respect that the Myers and Carter method differs from previous approaches, notably Umland and Smith. Rather than fix y_S at a particular value, k, the approach is to select a range of values for μ to insure that the matrix M(X), in eq. (6), is positive definite (for minimization) or negative definite (for maximization).

For the case where C is definite, consider the quadratic form with matrix given by M(X), say,

$$q = w'(B - \mu C)w$$

Since C is symmetric definite there exists a non-singular matrix S such that

$$S'BS = \text{diag}\ (\lambda_1, \lambda_2, \ldots, \lambda_n)$$

and

$$S'CS = I_n$$

Letting $W' = V'S'$, we have

$$q = V'\ \text{diag}\ (\lambda_1 - \mu, \lambda_2 - \mu, \ldots, \lambda_n - \mu)V. \tag{7}$$

where the λ_i's are the eigenvalues of the real, symmetric matrix T given by

$$T = D_2^{(-\frac{1}{2})} Q'BQD_2^{(-\frac{1}{2})}, \tag{8}$$

where D_2 - diagonal matrix containing the eigenvalues of C, $D_2^{(-\frac{1}{2})}$ - diagonal matrix containing the reciprocals of the square roots of the eigenvalues of C, and Q is the orthogonal matrix for which

$$Q'CQ = D_2$$

The eigenvalues of T are arranged in ascending order, λ_n being the largest. From equation (7) we can see that for a negative definite M(X) it requires that μ be greater than λ_n and for a positive definite M(X), μ must be less than λ_1. The values for μ thus determined are used in equation (5) to generate values of x representing points of constrained primary response. The authors then graph the results and chose the operating conditions for X which satisfy the desired constraint value.

In an instance where C is indefinite solutions still exist if the matrix B is definite. Such conditions make computations only slightly more difficult. In situations where both matrices are indefinite, it is impossible to obtain a solution using this method.

The approach can best be illustrated by an example. The problem considered here is as shown in equations (1) and (2). The problem is interpreted as one of maximizing y_p without allowing y_s to become larger than 65. C in this case was found to be positive definite and so values of μ greater than λ_n are desired in order to maximize y_p. The eigenvalues of T in equation (8) were found to be

$$\lambda_1 = -4.0617 \qquad \lambda_2 = -0.9945 \qquad \lambda_3 = 0.08017$$

Therefore substitutions into equation (5) were made with values of μ greater than 0.08017 to generate values of x representing points of constrained primary maximum response. Values of y_p and y_s were then computed using equations (1) and (2) and the graphs of Figures (3) and (4) are the results. Figure (3) indicates operating conditions to insure constrained maximima of y_p for a given level of y_s. Figure (4) plots maximum levels of y_p against fixed levels of y_s. The results are shown below.

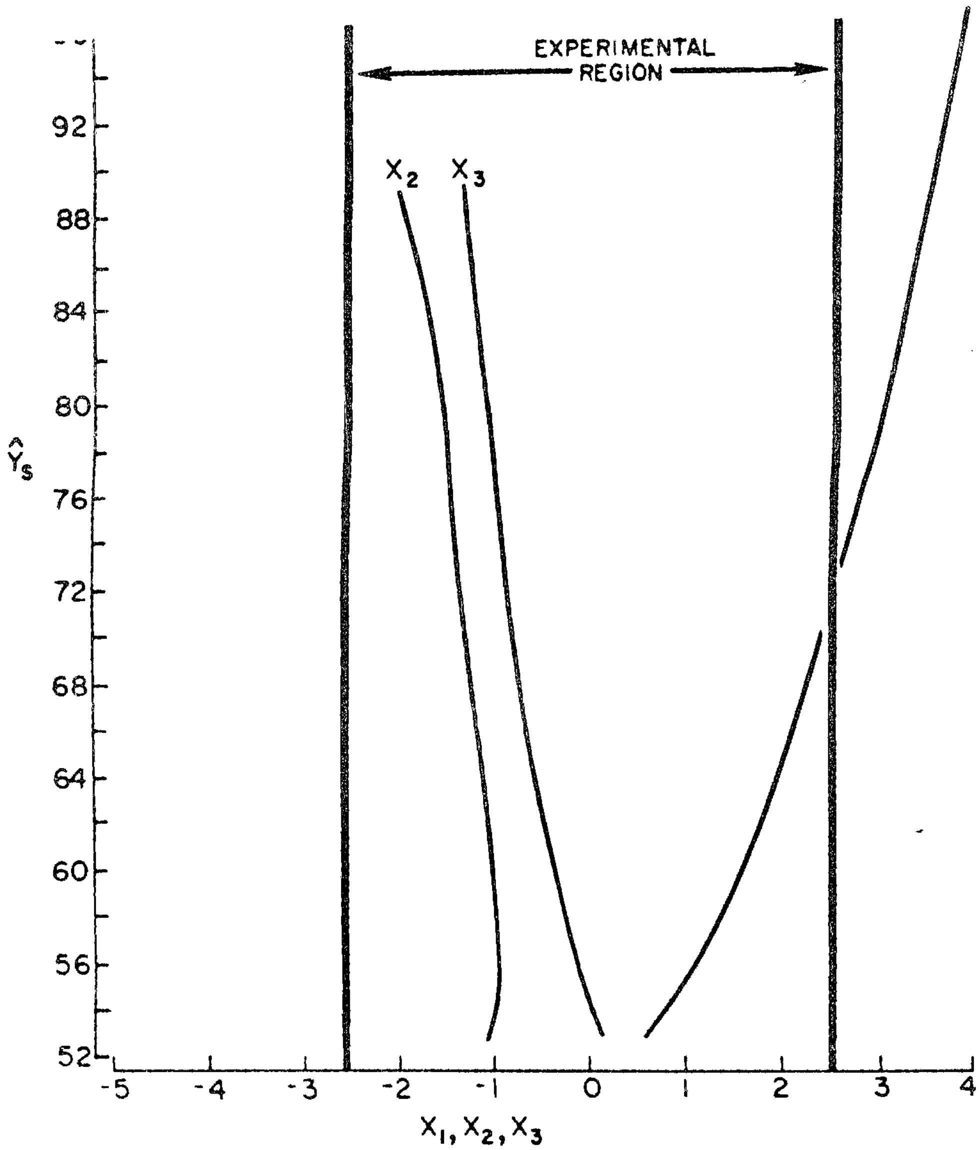

Figure 3. Conditions of Constrained Maxima on Primary Response for Fixed Values of $\hat{y}_s$. (after Myers and Carter (16))

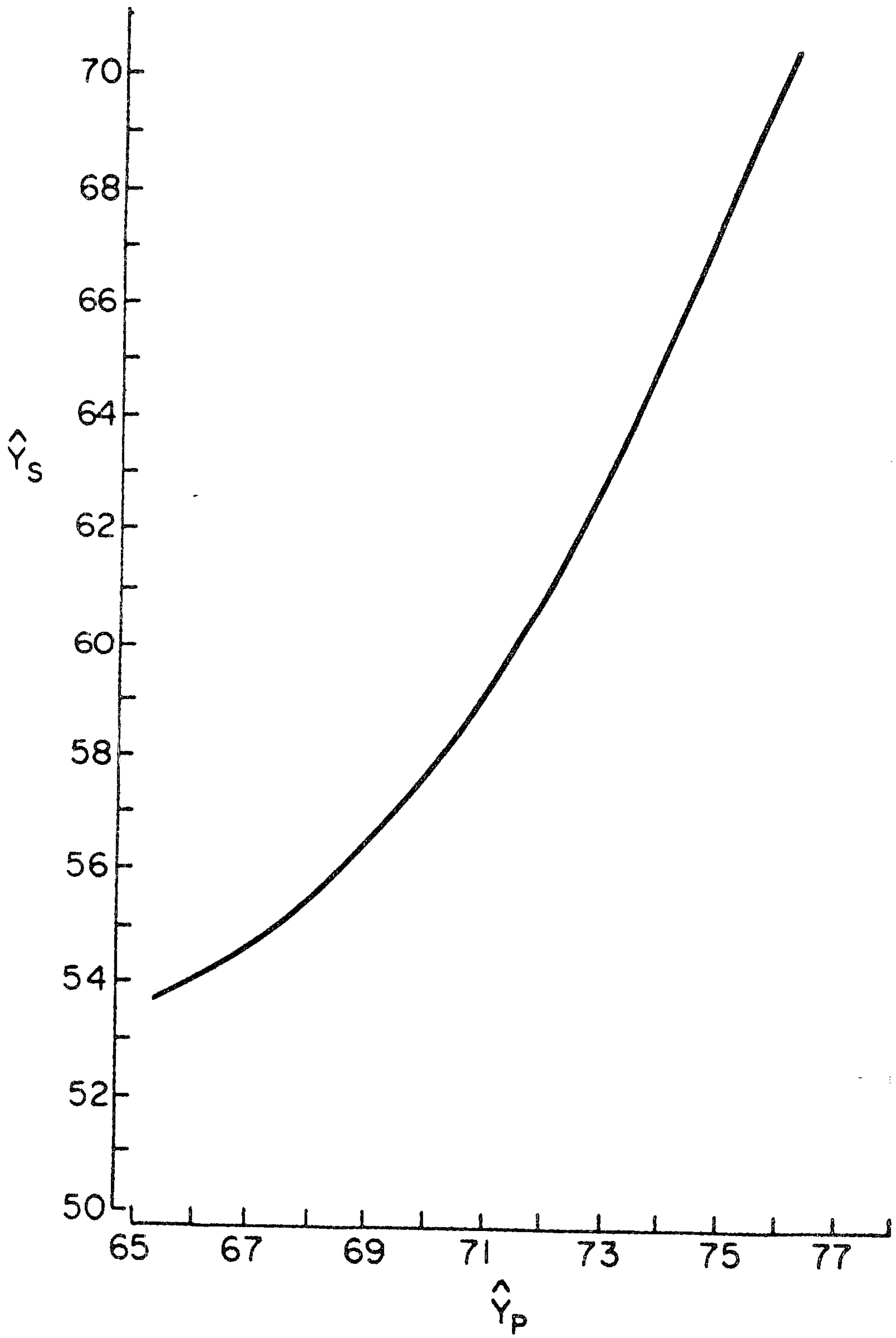

Figure 4. Maximum Estimated Primary Response at Specific Values of the Constraint Response. (after Myers and Carter (16))

y_P	y_S	x_1	x_2	x_3
74.04	65.23	2.07	-1.15	-0.6

Again, violation of the bound on the secondary response does not seem to be deemed important.

The third problem, also from Myers and Carter, extends the same solution method to a two variable problem with more than one constraint. The responses are as follows:

$$y_P = 53.69 + 7.26x_1 - 10.33x_2 + 7.22x_1^2 + 6.43x_2^2 + 11.36x_1x_2$$

$$y_S = 82.17 - 1.01x_1 - 8.61x_2 + 1.40x_1^2 - 8.76x_2^2 - 7.20x_1x_2$$

the fitted surfaces are shown in Figure (5). The authors also impose a constraint on the secondary response as follows:

$$84 < y_S < 88$$

It is apparent from the Figure (5) that the constraint response can be retained within the limit imposed, between 84 and 88, while the primary response increases indefinitely. Because of this, an added constraint is introduced:

$$x_1^2 + x_2^2 \leq 1$$

The results are:

y_P	y_S	x_1	x_2
67.79	87.80	0.85	-0.6

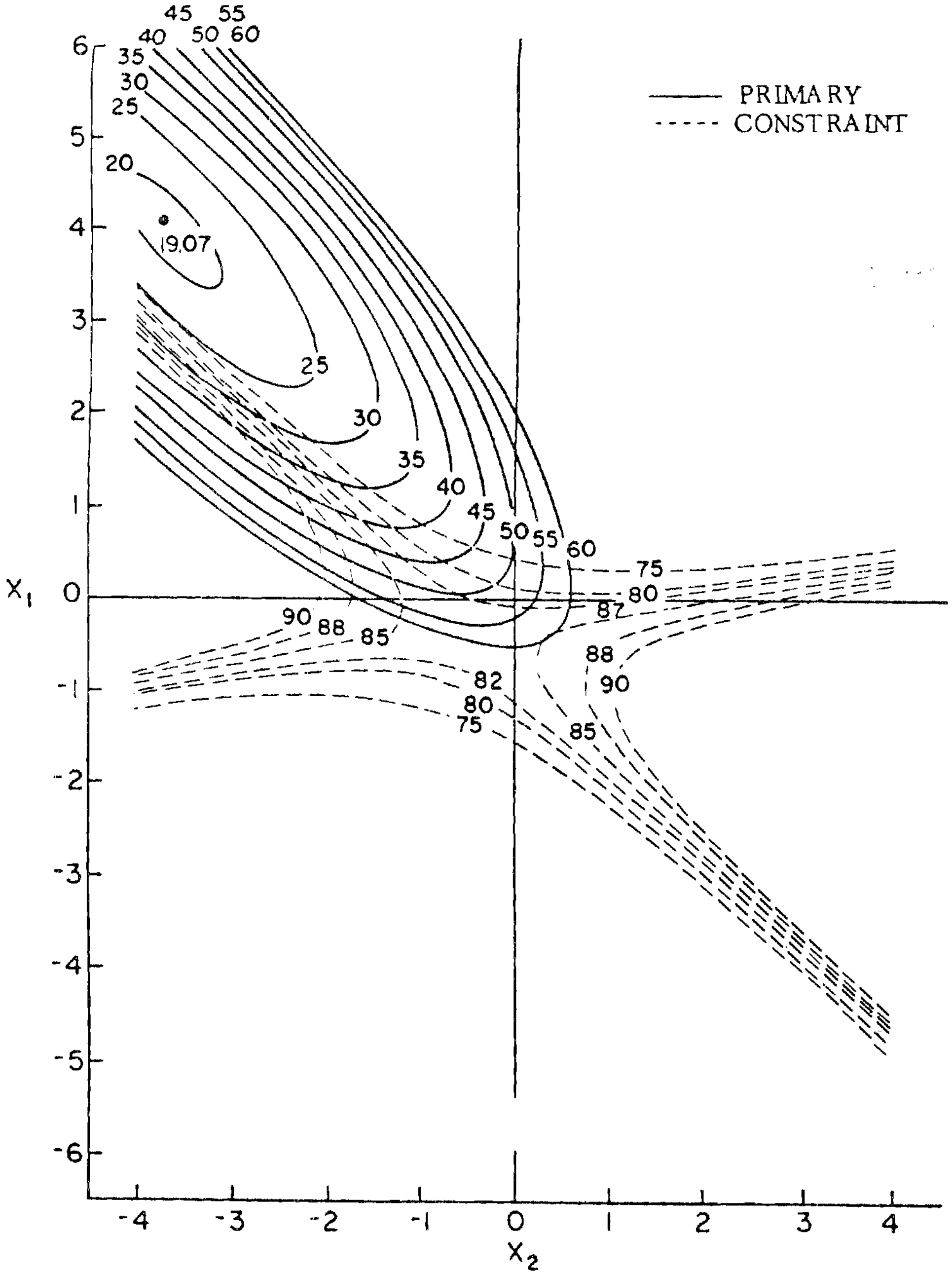

Figure 5. Myers and Carter Response Surfaces. (after Myers and Carter(16))

A Three - Response Example

The three response example illustrated is a modified combination of the Umland and Smith and Myers and Carter problems:

f_1 represents the process yield (in pounds)

$$\text{Yield} = f_1 = 558.4 + 73.1x_1 + 266.5x_2 - 30.3x_1^2 - 69.6x_2^2 + 26.9x_1x_2$$

f_2 is a product purity (in percent)

$$\text{Purity} = f_2 = 85.72 + 21.85x_1 + 8.59x_2 - 9.2x_1^2 - 5.18x_2^2 - 6.26x_1x_2$$

f_3 is a cost relationship (in dollars)

$$\text{Cost} = f_3 = 49{,}324 + 7143x_1 - 10{,}366x_2 + 7{,}300x_1^2 + 6{,}450x_2^2 + 12{,}109x_1x_2$$

The ranges on the responses are as follows:

$$1 \leq f_1 \leq 953$$

$$1 \leq f_2 \leq 98.77$$

$$25{,}000 \leq f_3 \leq 150{,}333$$

These values represent the absolute extrema for the function values with truncation at some points which are obviously infeasible. This range can be considerably reduced and refined by considering only feasible points within the design ranges, but have been left in this form for illustrative purposes. Using f_1 as the base interval we get:

$$\overline{s_2} = \frac{953}{1} \qquad \underline{s_2} = \frac{1}{98.77} \qquad \overline{s_3} = \frac{953}{25{,}000} \qquad \underline{s_3} = \frac{1}{150{,}333}$$

yielding

$$0 \leq s_1 \leq 1$$

$$0 \leq s_2 \leq 953$$

$$0 \leq s_3 \leq 0.04$$

Let us assume that the decision-maker assigns weights of 0.6 to f_1, 0.03 to f_2, and 1.0 to f_3. In multiplying the s_i's by the respective weights, we derive composite weights, W_i, with $W_i = w_i s_i$ with values

$$0 \leq W_1 \leq 0.6$$

$$0 \leq W_2 \leq 28.6$$

$$0 \leq W_3 \leq 0.04$$

The composite form of the objective function becomes:

$$F = W_1 f_1 + W_2 f_2 - W_3 f_3$$

where our interest is in maximizing the yield and percent and minimizing cost.

If we take 11 observations in each interval our increments become 0.06 from 0.0 to 0.60 on W_1, 2.86 from 0.0 to 20.3 on W_2, and 0.004 from 0.0 to 0.04 on W_3. The results of applying the Hooke and Jeeves algorithm to the composite function as now formulated are shown in Chapter III.

CHAPTER III

RESULTS AND DISCUSSION OF RESULTS

The Umland and Smith Problem

Explicit Constraint Consideration

The results of applying the Hooke and Jeeves algorithm when the secondary response is preset to a specific value (a lower limit, in this case) is shown in Table 9, Appendix B. Although the results for all starting points and initial step sizes appear relatively consistent, some variation does occur. Based upon accepting the best value for the runs made we arrive at the following findings:

For the secondary response value (y_S) equal to 90.0%:

y_P = 88.6621 y_S = 90.0011 x_1 = 1.07266 x_2 = 1.480

For y_S set at 92.5%:

y_P = 86.5857 y_S = 92.5008 x_1 = 1.07603 x_2 = 1.280

For y_S set to 95.0%:

y_P = 83.4485 y_S = 95.0001 x_1 = 0.94438 x_2 = 1.080

All values lie on or near the locus of points forming the intersection of the response surfaces at the fixed level value. However, because of the nature of the algorithm, the point on the constraint at which the search technique first crosses lies very close to the final optimum point. Basically, a starting point that is very close to the constraint will cause the search to find as an optimum a nearby point on or near the constraint. Similarly, a point that is evaluated at or near the constraint will be found to be optimum also, although actually at some distance from the true optimum.

It may be noted that a large number of values for x_2 in the explicit constraint consideration, Table 9, Appendix B, seem somewhat regular and appear rounded to the size of the initial step. Three contributing factors and their interaction are responsible; (1) the nature of the search technique, (2) the nature of the constraint, and (3) the starting point. The search technique is such that the first direction explored is always the x_1 direction. If an improvement occurs, that point becomes the new base point and subsequent directions explored. Because of the nature of the constraint, as seen in Figure 2, subsequent exploration moves in the x_2 direction will result in failures once the base point is sufficiently close to the constraint. Both functions are concave in the region of interest and the feasible region lies beneath them. Therefore, for all feasible starting points, the same problem exists, since the constraint is approached from generally the same direction. The total effect is seen to be one of approaching the constraint only in the x_1 direction once the search is within an initial step size distance from the constraint. The approach then must be one of a number of different starting points and starting step sizes, although, for the small range considered here, a tendency toward smaller initial step sizes might prove more efficient. The same difficulty occurs with other search algorithms also. In particular, the cyclic coordinate method, wherein the optimum point found in the x_1 direction would be the initial x_1 point since the moves would continue in the x_1 direction until failure, which, for this case would be the constraint itself. Any algorithms not having this difficulty would have to evaluate in all coordinate directions before any moves are made. The method of treating as failures points which violate constraints may prove inadequate for problems with more complicated constraints. For these problems, it may be necessary to use some algorithm designed to better handle constrained problems. For the response surface problem, the range of values on starting points is not generally too extensive and some enumeration scheme may be developed. The results for this problem, although depending somewhat on the starting point and the step size, are not unsatisfactory. Similar approaches are the only recourse in any non-convex optimizing attempts.

Two features of this method of considering the multiple response problem are readily apparent. A feasible starting point must be available or the algorithm never leaves the starting point. Also, no violation of the fixed level of the secondary response occurs. By treating violations as failures in the search this property is assured.

The main advantage of this approach is that the decision-maker has an opportunity to strictly fix a bound on the response. Although such restrictions will cause lower values in the responses, as compared with the original results of Umland and Smith, shown below, for instance, no violations of the imposed constraints will occur.

Purity (y_S)	94.87	92.47	89.995
Yield (y_P)	83.66	86.73	88.68
x_1	0.965	1.005	1.075
x_2	1.088	1.316	1.479

Implicit Constraint Consideration

Implicit treatment of the imposed constraints yields much more consistent results as shown in Table 10, Appendix B. The penalty assigned in this case was 1000. Varying the penalty value only varies the closeness of the secondary response value to the limit imposed. As is readily apparent, in no case is the value found further away than .001. Based on choosing the best value for the global optimum the following values are assigned:

For $y_S \geq 90.0\%$:

$y_P = 88.6623$ $y_S = 89.9997$ $x_1 = 1.08223$ $x_2 = 1.47497$

For $y_S \geq 92.5\%$:

$y_P = 88.6441$ $y_S = 92.4998$ $x_1 = 1.00562$ $x_2 = 1.31055$

For $y_S \geq 95.0\%$:

$y_P = 83.4562$ $y_S = 94.9992$ $x_2 = .96643$ $x_2 = 1.07373$

Although the primary response values are slightly lower than those found by Umland and Smith, and constraints in each case violated, the secondary response values are very close to their limit, whereas Umland and Smith's values are further away. A feasible starting point is not required for this formulation.

The advantage of this approach seems to lie in its consistency. The approach might be useful if the limit values are known, but are not required to be strictly adhered to. Additionally, by varying the penalty size, a point may be reached where the amount of constraint violation can be considered insignificant.

Weighting Factors

Results of the weighting factor method are shown in Tables 1 and 2. The results are included here because the advantage of this approach lies in the actual tabulation of the results. The results are most consistent and compare favorably with the Umland and Smith results. The weighted objective function value is not given here as it has no comparison value. The weights in Table 1 were incremented by a value of .1 and those in Table 2 were incremented by .01. The starting point in this case was X = (0.0,0.0) and the initial step size was 0.5. The same results occur irrespective of step size or starting point since we have no constraints per se in the problem.

This approach seems particularly valuable if the expected level of a response process is not known, or little knowledge is available about expected responses. Once a broad, coarse listing of response expectations is made available, as in Table 1, a subjective determination can be made as to what levels are desired, and a finer set of runs can be made, as in Table 2. This particular example is used to illustrate the range of values that include the acceptable levels of 90.0%, 92.5%, and 95% for the purity response in this problem. The weighting function approach has the effect of taking the decision-making problem out of a subjective area and places it in a readily available tabular form. By looking at such a tabular display, a decision maker can see the marginal trade-off values he can expect for a change in any objective function value and determine the operating level accordingly.

Table 1. Weighting Function Results for the Umland and Smith Problem - Increment = 0.1

WEIGHTS		YP	YS	OPTIMAL X	
.00	1.00	64.2766	98.7747	1.13965	.14063
.10	.90	71.9067	98.3920	1.04907	.44482
.20	.80	77.2554	97.4614	.99219	.70166
.30	.70	81.1500	96.1723	.96484	.92383
.40	.60	84.1357	94.5697	.96729	1.12207
.50	.50	86.5505	92.5942	1.00195	1.30371
.60	.40	88.6508	90.0182	1.07397	1.47803
.70	.30	90.5984	86.3697	1.19629	1.65234
.80	.20	92.5010	80.5650	1.39185	1.83899
.90	.10	94.3086	69.9418	1.70813	2.05762
1.00	.00	95.3624	46.8619	2.24902	2.34863

Table 2. Weighting Function Results for the Umland and Smith Problem - Increment = 0.01

WEIGHTS		YP	YS	OPTIMAL X	
.30	.70	81.1500	96.1723	.96484	.92383
.31	.69	81.4870	96.0243	.96387	.94482
.32	.68	81.8029	95.8791	.96301	.96484
.33	.67	82.1237	95.7247	.96289	.98535
.34	.66	82.4297	95.5706	.96240	1.00537
.35	.65	82.7341	95.4103	.96289	1.02539
.36	.64	83.0238	95.2509	.96289	1.04492
.37	.63	83.3124	95.0850	.96387	1.06445
.38	.62	83.5957	94.9150	.96484	1.08398
.39	.61	83.8671	94.7450	.96582	1.10303
.40	.60	84.1346	94.5704	.96777	1.12183
.41	.59	84.3973	94.3916	.96973	1.14062
.42	.58	84.6537	94.2098	.97168	1.15930
.43	.57	84.9067	94.0228	.97461	1.17773
.44	.56	85.1556	93.8312	.97729	1.19629
.45	.55	85.4022	93.6333	.98047	1.21484
.46	.54	85.6359	93.4382	.98438	1.23242
.47	.53	85.8749	93.2305	.98779	1.25098
.48	.52	86.1025	93.0244	.99219	1.26855
.49	.51	86.3307	92.8095	.99695	1.28638
.50	.50	86.5519	92.5928	1.00195	1.30383
.51	.49	86.7762	92.3640	1.00732	1.32178
.52	.48	86.9925	92.1343	1.01270	1.33936
.53	.47	87.2094	91.8945	1.01904	1.35693
.54	.46	87.4186	91.6538	1.02563	1.37402
.55	.45	87.6336	91.3962	1.03320	1.39160
.56	.44	87.8412	91.1372	1.04004	1.40918
.57	.43	88.0460	90.8710	1.04785	1.42639
.58	.42	88.2471	90.5990	1.05615	1.44336
.59	.41	88.4514	90.3111	1.06470	1.46094
.60	.40	88.6529	90.0149	1.07397	1.47827
.61	.39	88.8509	89.7117	1.08374	1.49536
.62	.38	89.0506	89.3925	1.09424	1.51270

Myers and Carter - Problem No. 1

Weighting Factors

The tabular output for this problem is shown in Table 3-5. The interval on the weights is progressively reduced from 0.1 to 0.001 as the region of interest is refined. The last tabulation is shown in Table 5. Finer incrementing can be easily accomplished to any degree and an appropriate operating level determined.

In generating the actual data, different starting points and initial step sizes were used with virtually the same results found in all cases. In the table illustrated the starting point was 0.,0.,0., and the initial step size was 0.01. Large variations in starting points, from feasible to infeasible, and variation of starting step sizes from 0.1 to 0.001 made a variation of less than 0.2 seconds of computer time. This is used to indicate only the small, absolute times involved. Comparisons between computer times for different runs has not been attempted due to the relative shortness of time for any run-two seconds being an upper limit-and the wide variation in times not necessarily due to the program or the problem. It appears that the implicit weight factor from the original work were w_1 between .687 and .688 and w_2 between .313 and .312.

Explicit Constraint Consideration

Some results of maximizing y_P while treating y_S as an explicit constraint and not allowing y_S to be larger than 65.0 are shown in Table 11 in Appendix B. The value of y_P = 73.9145 compares favorably with the optimum value found by Myers and Carter of 74.04, while their value for y_S is 65.23, a violation of the constraint. The y_S value found with the

Table 3. Weighting Function Results for the Myers and Carter Problem No. 1 - Increment = 0.1

WEIGHTS		YP	YS	OPTIMAL X		
.00	1.00	59.2991	52.7913	.5199	-1.1781	.0813
.10	.90	61.7870	52.9141	.6117	-1.1293	.1258
.20	.80	63.5690	53.2266	.6926	-1.0658	.1201
.30	.70	65.1017	53.7388	.7857	-1.0035	.0809
.40	.60	66.6197	54.5621	.9162	-.9549	.0074
.50	.50	68.3334	55.9824	1.1227	-.9406	-.1102
.60	.40	70.6326	58.8522	1.4770	-.9920	-.3031
.70	.30	74.6132	66.5180	2.1889	-1.2086	-.6625
.80	.20	77.2015	73.6279	2.5000	-1.1365	-.9324
.90	.10	78.0257	78.3282	2.5000	-.8701	-1.1000
1.00	.00	78.3239	84.0932	2.5000	-.5863	-1.2766

Table 4. Weighting Function Results for the Myers and Carter Problem No. 1 - Increment = 0.01

WEIGHTS		YP	YS	OPTIMAL X		
.60	.40	70.6330	58.8529	1.4773	-.9924	-.3031
.61	.39	70.9219	59.2955	1.5254	-1.0027	-.3289
.62	.38	71.2345	59.7950	1.5797	-1.0168	-.3566
.63	.37	71.5594	60.3369	1.6365	-1.0320	-.3859
.64	.36	71.9091	60.9458	1.6988	-1.0500	-.4174
.65	.35	72.2690	61.5997	1.7617	-1.0672	-.4500
.66	.34	72.6761	62.3726	1.8357	-1.0906	-.4873
.67	.33	73.0924	63.1990	1.9096	-1.1125	-.5250
.68	.32	73.5745	64.2009	1.9992	-1.1438	-.5688
.69	.31	74.0637	65.2655	2.0879	-1.1730	-.6129
.70	.30	74.6131	66.5178	2.1883	-1.2078	-.6625

Table 5. Weighting Function Results for the Myers and Carter Problem No. 1 - Increment = 0.001

WEIGHTS		YP	YS	OPTIMAL X		
.680	.320	73.5745	64.2009	1.9992	-1.1438	-.5688
.681	.319	73.6128	64.2824	2.0057	-1.1453	-.5719
.682	.318	73.6606	64.3848	2.0146	-1.1486	-.5766
.683	.317	73.7074	64.4852	2.0227	-1.1508	-.5807
.684	.316	73.7627	64.6048	2.0328	-1.1543	-.5859
.685	.315	73.8070	64.7008	2.0406	-1.1566	-.5898
.686	.314	73.8619	64.8204	2.0514	-1.1609	-.5945
.687	.313	73.9122	64.9307	2.0605	-1.1641	-.5992
.688	.312	73.9559	65.0268	2.0680	-1.1660	-.6031
.689	.311	74.0146	65.1565	2.0793	-1.1705	-.6086
.690	.310	74.0637	65.2655	2.0879	-1.1730	-.6129

modified algorithm is 64.9997, within the constraint value imposed. The data in Table 11 seems to indicate a local optimum in the vicinity of 1.5,-0.5,-0.6. This is to be expected since the primary response is not concave.

It appears that the problem encountered in the Umland and Smith problem is not found here. The constraints apparently do not tend to cause a one-directional improvement.

A feasible starting point must be available and Table 11 indicates the majority of feasible starting positions to the nearest whole number. The constraint in no case is violated. In instances where the secondary response level is absolute, this becomes an important feature.

Implicit Constraint Consideration

Example results of implicit treatment of the constraints are shown in Table 12, Appendix B. The different penalty values are used to illustrate that the variation in the penalty value only serves to alter the degree to which a violation of a constraint occurs. For the penalty set equal to 100, for example, constraint violations are only as large as 0.0039, while for the penalty equal to 1000, the largest violation is 0.0007. The best values achieved using this method is $y_P = 73.9442$ and $y_S = 65.0022$. The values again are comparable to those found in the original work. The primary response value is slightly lower but the constraint is not violated to the same degree, 0.0022 in this case compared with 0.23 in the original work. A feasible starting point is not required for this method and it generally appears to yield quite good results.

Myers and Carter - Problem No. 2

Weighting Factors

The weighting function tabulation, Tables 13-16, Appendix B, appears somewhat inconclusive, since only four different points evolve. The answer is apparent when the response surfaces, shown in Figure 5, are inspected. The responses are such that, for maximizing the primary function, the secondary response, a hyperbolic function, can be unbounded for either maximization or minimization. The imposition of a constraining relation on the y_S e.g., $84 < y_S < 88$, does not affect the unboundedness of the response. The only effective constraint is the one artificially imposed,

$$x_1^2 + x_2^2 \leq 1$$

The situation is further complicated by the fact that the contour of the imposed constraint closely parallels the primary response function contour in the 4th quadrant as illustrated in Figure 5. The result is as shown in Tables 13 and 14, where the optimum is achieved at only four points when the weights are incremented by 0.1. The point indicated in the table for values of w_1 between 0.1 and 0.6 closely corresponds to that found in the original work. A finer weighting scheme must be undertaken between $w_1 = 0.7$, $w_2 = 0.3$ and $w_1 = 0.8$, $w_2 = 0.2$, as shown in Tables 15 and 16.

Explicit Constraint Consideration

The results of treating the secondary response and artificial constraint explicitly are shown in Table 17 in Appendix B. A situation similar to that which occurred in the explicit constraint consideration of the Umland and Smith problem, namely, a rounding effect of the second variable. The best point found is $y_P = 67.5716$ and $y_S = 86.8056$, both comparable to the Myers and Carter results.

Implicit Constraint Consideration

For this case, both the secondary response and the artificial constraint were treated as penalty functions. The results are shown in Table 18, Appendix B. The values for y_P are improved over other methods. The tendency appears for y_S to move to its lower limit, 84.0. In some instances either of the constraints are violated, but only marginally. Going along with what has been previously stated about this model, it seems that a rather larger increase in the primary response can be realized at marginal violation of constraint. Again, it becomes a function of the judgement rendered by the decision-maker.

Comparison of the Myers and Carter approach with the weighting function method suggests an important aspect of the problem which deserves closer analysis, namely, marginal analysis. It is generally of importance to the decision-maker to be able to know what trade-offs can be made between the objective function and the constraint(s). For example, he may wish to study the increase in yield that can be realized at the expense of purity. Both of the approaches allow for such marginal analysis. In discussing this analysis emphasis will be on the Myers and Carter problem #1, although similar type analyses are equally applicable to any of the other problems.

In the Myers and Carter approach determining trade-offs and operating conditions evolve basically again to a graphical analysis.

From Figure (4) it is apparent that measuring the relationship between the two responses is a simple matter of selecting one or the other of the responses to be of an acceptable level and reading the other response from the plot shown. Similarly, for the operating conditions, the decision-maker enters the graph (Figure (3)) with an acceptable operating level for one response and reads the required operating values on the variables. Example values for the Myers and Carter problem #1 are shown in Table 6. The results are very close to those obtained through the use of the weighting function as shown in Tables (3), (4), and (5). Extension to more than two responses would be impossible from a marginal analysis standpoint. The analysis using this approach is dependent upon the accuracy of the graphs generated and the accuracy to which they can be read. The weighting function approach, on the other hand, yields a tabulation directly of the values for all responses and the operating conditions on the independent variables as indicated in the Tables (3), (4), and (5).

Three Response Function

The results of the use of the weighting function to the three response case are shown in Table 7. In Table 8 we can see the results of a small programming change which excludes points not found in the interval -1.5 to 1.5, the assumed design range constraints. The result is a reduction of listed solutions and a corresponding reduction of computer usage. The inclusion of the infeasible points in Table 7 is a result of computing at the extremes of the weight distribution. Based on the tabular form of the output, the decision-maker can decide what

Table 6. Response Values and Operating Conditions for Myers and Carter Problem No. 1 obtained Graphically through the Myers and Carter Method

y_P	y_S	x_1	x_2	x_3
70.20	58.00	1.35	-1.00	-0.25
70.90	59.00	1.45	-1.00	-0.30
71.40	60.00	1.60	-1.00	-0.35
72.10	61.00	1.70	-1.05	-0.40
72.60	62.00	1.75	-1.10	-0.45
73.00	63.00	1.85	-1.15	-0.50
73.50	64.00	1.90	-1.15	-0.60
74.00	65.00	2.00	-1.20	-0.60
74.30	66.00	2.10	-1.20	-0.65
74.60	66.50	2.15	-1.20	-0.65

what weight range to further investigate, or simply choose the most preferred result from those listed.

Table 7. Weighting Function Results for the Three-Response Problem - All Points

WEIGHTS			YIELD	PURITY	COST	OPTIMAL X	
.00	.00	.040	-2191.390	-211.96	17100.9	-5.2150	5.7010
.00	2.86	.036	-479.405	-62.53	22097.1	-3.4715	3.9941
.00	5.72	.032	240.701	9.72	30339.6	-2.3074	2.3758
.00	8.58	.028	554.433	43.09	39340.2	-1.4746	2.0953
.00	11.44	.024	684.801	69.79	43073.3	-.8457	1.5262
.00	14.30	.020	727.487	82.50	55434.2	-.3516	1.1000
.00	17.16	.016	728.041	90.06	61969.3	.0477	.7731
.00	20.02	.012	709.630	94.55	67833.3	.3310	.5330
.00	22.88	.008	684.365	97.11	73314.1	.6064	.3508
.00	25.74	.004	661.107	98.39	78471.0	.9100	.2219
.00	28.60	.000	642.786	98.77	83556.2	1.1396	.1406
.06	.00	.036	-1559.553	-160.42	17027.5	-4.6359	5.1231
.06	2.86	.032	-177.751	-34.25	24739.4	-3.0064	3.5872
.06	5.72	.028	389.493	26.66	34267.1	-1.9703	2.5430
.06	8.58	.024	625.299	58.32	43469.4	-1.1359	1.8313
.06	11.44	.020	713.846	76.81	51769.3	-.5906	1.3148
.06	14.30	.016	734.233	87.17	59154.2	-.1203	.9332
.06	17.16	.012	724.012	93.17	65781.2	.2639	.6500
.06	20.02	.008	702.340	96.54	71353.9	.5569	.4434
.06	22.88	.004	679.690	98.23	77629.0	.8072	.3000
.06	25.74	.000	662.731	98.75	83351.6	1.1156	.2140
.12	.00	.032	-1027.321	-115.29	19029.9	-4.1723	4.5797
.12	2.86	.028	71.603	-9.35	27357.7	-2.6532	3.1502
.12	5.72	.024	503.114	41.61	37906.0	-1.6357	2.2266
.12	8.58	.020	677.845	68.25	47362.6	-.8961	1.5820
.12	11.44	.016	732.133	82.93	55759.3	-.3305	1.1203
.12	14.30	.012	735.835	91.17	63261.4	.1197	.7307
.12	17.16	.008	719.626	95.70	70113.3	.4912	.5492
.12	20.02	.004	699.421	97.96	76041.0	.8092	.3395
.12	22.88	.000	684.367	98.67	83214.4	1.0902	.2992
.18	.00	.028	-532.335	-75.75	21245.9	-3.6730	4.0539
.18	2.86	.024	274.242	12.53	31431.5	-2.2615	2.7874
.18	5.72	.020	599.434	54.70	41992.7	-1.3020	1.9231
.18	8.58	.016	714.795	76.49	51601.0	-.6012	1.3531
.18	11.44	.012	742.663	88.20	60133.5	-.0009	.9502
.18	14.30	.008	735.965	94.48	68027.1	.3750	.6719
.18	17.16	.004	719.309	97.55	75505.9	.7414	.4910
.18	20.02	.000	707.729	95.51	83153.6	1.0625	.3957
.24	.00	.024	-219.172	-41.42	24178.1	-3.1833	3.5531
.24	2.86	.020	434.699	31.68	35450.3	-1.8676	2.3969
.24	5.72	.016	667.629	66.20	46447.3	-.9617	1.6502
.24	8.58	.012	739.654	83.65	56374.3	-.2937	1.1500
.24	11.44	.008	749.647	92.63	65442.4	.2291	.8156
.24	14.30	.004	740.360	96.93	74139.9	.6594	.6072
.24	17.16	.000	732.370	90.22	83252.1	1.0336	.5008
.30	.00	.020	74.438	-11.52	27776.2	-2.7111	3.0750
.30	2.86	.016	553.465	45.40	39974.3	-1.4639	2.0500
.30	5.72	.012	716.741	76.25	51514.3	-.6072	1.4010
.30	8.58	.008	757.533	89.76	62142.3	.0395	.9375
.30	11.44	.004	760.304	95.95	72464.3	.5504	.7413
.30	14.30	.000	760.072	97.75	83614.7	1.0039	.6375
.36	.00	.016	305.500	14.47	32010.4	-2.2259	2.6250
.36	2.86	.012	651.314	63.22	45139.1	-1.0543	1.7342
.36	5.72	.008	753.401	84.99	57779.1	-.2137	1.1992
.36	8.58	.004	777.965	94.51	70284.5	.4233	.8995
.36	11.44	.000	739.287	96.99	84313.1	.9731	.7920
.42	.00	.012	483.500	57.31	38978.1	-1.7477	2.2008
.42	2.86	.008	721.981	76.88	51766.5	-.5949	1.4083
.42	5.72	.004	739.791	92.15	67276.2	.2527	1.0371
.42	8.58	.000	820.796	95.75	86450.1	.9025	.9520
.48	.00	.008	620.843	58.09	43193.5	-1.2052	1.8807
.48	2.86	.004	737.455	87.95	62046.3	-.0032	1.3153
.48	5.72	.000	855.463	93.51	90961.2	.9820	1.2258
.54	.00	.004	744.734	73.04	54321.3	-.4713	1.5553
.54	2.86	.000	897.101	83.23	103909.4	1.1323	1.5711
.60	.00	.000	953.524	46.34	193543.9	2.2490	2.3494

Table 8. Weighting Function Results for the Three-Response Problem - Infeasible Points Excluded

WEIGHTS			YIELD	PURITY	COST	OPTIMAL X	
.00	14.30	.020	727.437	82.50	55434.2	-.3516	1.1000
.00	17.16	.016	728.041	90.06	61969.3	.0477	.7781
.00	20.02	.012	709.630	94.55	67883.3	.3316	.5330
.00	22.88	.008	634.365	97.11	73314.1	.6664	.3508
.00	25.74	.004	661.107	93.39	73471.0	.9160	.2219
.00	28.60	.000	642.766	95.77	83556.2	1.1396	.1406
.06	14.30	.016	734.233	87.17	59154.2	-.1203	.9332
.06	17.16	.012	724.012	93.17	65731.2	.2039	.6500
.06	20.02	.008	702.340	96.54	71853.9	.5369	.4434
.06	22.88	.004	679.690	93.23	77629.0	.8672	.3000
.06	25.74	.000	662.731	98.75	83351.6	1.1156	.2143
.12	11.44	.016	732.183	82.93	55759.8	-.3505	1.1203
.12	14.30	.012	735.835	91.17	63261.4	.1197	.7367
.12	17.16	.008	719.626	95.70	70113.3	.4912	.5492
.12	20.02	.004	699.421	97.96	76641.0	.8092	.3895
.12	22.88	.000	634.367	98.67	83214.4	1.0902	.2992
.18	11.44	.012	742.663	83.20	60188.5	-.0609	.9502
.18	14.30	.008	735.965	94.48	63027.1	.3750	.6719
.18	17.16	.004	719.809	97.55	75505.9	.7414	.4910
.18	20.02	.000	707.729	98.51	83153.6	1.0025	.3957
.24	8.58	.012	739.654	83.65	56374.3	-.2937	1.1500
.24	11.44	.008	749.647	92.63	65442.4	.2291	.8156
.24	14.30	.004	740.360	96.93	74139.9	.6594	.6072
.24	17.16	.000	732.870	98.22	83252.1	1.0336	.5063
.30	8.58	.008	757.533	89.76	62142.3	.0395	.9875
.30	11.44	.004	760.304	95.98	72464.3	.5534	.7418
.30	14.30	.000	760.072	97.75	83614.7	1.0039	.6375
.36	5.72	.008	753.401	84.99	57779.1	-.2187	1.1992
.36	8.58	.004	777.965	94.51	70284.5	.4283	.3998
.36	11.44	.000	789.267	96.99	84513.1	.9731	.7926
.42	5.72	.004	789.791	92.15	67276.2	.2527	1.0871
.42	8.58	.000	820.796	95.75	86456.1	.9025	.9826
.48	5.72	.000	855.463	93.51	90961.2	.9326	1.2258

CHAPTER IV

CONCLUSIONS AND RECOMMENDATIONS

Certain conclusions arise from the investigation conducted. No one nonlinear programming technique or one problem formulation can be shown to be best for all situations. The intent here has only been to explore several formulations for a specific algorithm, and to investigate the results.

The Type IA formulation lends itself to a firm fixing of a constraint level for any secondary response. The algorithm chosen here does not give the best results when used in conjunction with this explicit manner of considering constraints. Application of nonlinear programming algorithms specifically designed for the constrained problem might prove a fruitful area for further investigation.

Implicit consideration of constraints, as in Type IB, yields better results for optimum operating conditions then does either the Type IA, investigated here, or the original method used, usually Lagrange multipliers. As in the latter case, minor constraint violations occur. From the response surface literature it becomes evident that such violations are of minimal importance. Since the overall results obtained for the implicitly considered constraint problem are better than those of the explicitly considered constraint problem it appears that the former is to be preferred generally. While the investigation conducted here does not consider other types of algorithms it seems that for the algorithm used here, a modified Hooke and Jeeves Pattern Search Technique, if some responses are to be restated and treated as constraints, then implicit treatment of such constraints is to be preferred to explicit treatment.

Of the models investigated, and in the absence of specific requirements on the responses, the weighting function approach provides possibly the best approach to the multiple response problem. The approach is not confined to a fixed level for the secondary response as in the Umland and Smith approach. It also avoids the inherent inaccuracy of graphical analysis, as that of Myers and Carter, while possessing the attributes of simplicity and ease of marginal analysis. The tabular form of the results lends itself to simple evaluation of tradeoff values by the decision-maker for two responses, and to a certain extent, larger numbers of responses. While such analysis can be accomplished with other methods, notably Myers and Carter, that method remains a graphical solution. While relatively accurate data can be extracted from graphs, and the nature of the response surface problem does not demand extreme accuracy, the method of eventually arriving at such simple graphs is quite complex. The weighting function approach reduces the highly subjective area of decision making to a readily available tabular form and the approach is relatively simple for the typical response surface problem found in the literature. Discussion of the extension of the weighting function approach to problems with a larger number of objective functions has been undertaken and the conclusion seems to be that, while the extension is difficult, it is not impossible. The same conclusion cannot be arrived at when previous work in the area is considered. The approach of Myers and Carter is dependent upon the nature of the fitted curves and, as such, application may be impossible for some problems. Their method of holding certain of the Lagrange multipliers fixed while varying others presents the same sort of difficulty as the weighting function with respect to number of iterations. Additionally, there is an intuitive interpretation and appeal for the weighted objective function which might aid the decision-maker.

Recommendations for continuation of this line of investigation fall into two categories; (1) application of different nonlinear programming algorithms, and (2) development of different problem formulations. With respect to the first, it seems that application of different algorithms could be fruitful from the aspect of determining degrees of efficiency measured against degrees of complexity. Particularly in the area of constrained optimization, algorithms specifically designed to handle the constrained case provide an entirely new approach. It would seem that gradient techniques, Zoutendijk's Methods of Feasible Directions (19), or Fiacco and McCormick's (5) Penalty function approaches, provide possibilities for exploration. However in such application, simplicity and speed, especially in view of the typical response surface problem size, may be sacrificed.

Other problem formulations need also to be investigated. Particularly the interactive techniques and their application to larger scale problems. Geoffrion (7), for instance, deserves consideration. In his approach a preference function receives information from the local functions, as to both function values and operating conditions. Decisions are then made relative to new data based on this information which is then distributed to the local functions and the cycle continues. Parts of this approach have been used here particularly the assignment of the weights involved. Completely interactive techniques have not been investigated and any extension of the methods shown here to large scale problems must include such methods.

APPENDIX A

COMPUTER PROGRAMS - MODIFIED HOOKE-JEEVES PATTERN SEARCH

Weighting Function Model - Umland and Smith Problem

```
      DIMENSION X(2,2),G(13),S(2),D(2,2),XM(2,2000),Y(2)
     X,P(2),X1(2,2),Q(2)
      A=0.0
      B=1.0
      M=0
      KL=1
      READ(5,21)Z,STEP,PR,GR,JTEMP,JT
   26 FORMAT(/,3X,F3.1,5X,F3.1)
      DO 2 J=1,2
      S(J)=STEP
    2 CONTINUE
      READ(5,21)(XM(I,KL),I=1,2)
      DO 114 J=1,2
      READ(5,21)(D(I,J),I=1,2)
   21 FORMAT( )
  114 CONTINUE
  115 JK=10
      KB=KL+1
      DO 34 I=1,2
      XM(I,KB)=XM(I,KL)
   34 CONTINUE
    6 J=1
      CALL ACCEL(A,B,J,JK,G,Z,ZKL,ZTEMP,XM,KB)
  110 DO 81 J=1,2
      DO 111 I=1,2
      X(I,J)=XM(I,KB)+(S(J)*D(I,J))
  111 CONTINUE
   80 CALL EVAL(X,Y,J,A,B,Q,P)
    9 FORMAT(5X,F20.10,5X,I2,)
      IF(JT.GT.J)GO TO 11
      GO TO 50
   11 JT=JT-1
      GO TO 82
   50 IF(Y(J).LE.Z) GO TO 60
      Z=Y(J)
```

```
82 DO 32 I=1,2
   XM(I,KB)=X(I,J)
32 CONTINUE
   GO TO 81
60 IF(JT.LT.J) GO TO 56
   GO TO 57
56 JT=J
   MC=2
   GO TO 55
57 JT=JT+1
   MC=-1
55 DO 31 N=1,2
   X1(N,J)=X(N,J)-(MC*S(J)*D(N,J))
   X(N,J)=X1(N,J)
31 CONTINUE
   GO TO 80
27 FORMAT(/,3(F20.10))
81 CONTINUE
   JT=0
   M=M+1
   IF(KCOUNT.EQ.1)GO TO 150
   IF(Z.LE.ZKL)GO TO 70
   GO TO 68
150 IF(Z.LE.ZKL)GO TO 71
68 KS=KB+1
   DO 37 I=1,2
   XM(I,KS)=(2*XM(I,KB))-XM(I,KL)
   XM(I,KL)=XM(I,KB)
   XM(I,KB)=XM(I,KS)
   ZKL=Z
   KCOUNT=1
37 CONTINUE
   GO TO 6
71 IF(ZTEMP.LE.ZKL)GO TO 72
   ZKL=ZTEMP
   Z=ZTEMP
   GO TO 68
72 DO 38 I=1,2
   XM(I,KB)=XM(I,KL)
   KCOUNT=0
38 CONTINUE
   GO TO 6
70 DO 112 J=1,2
    S(J)=.5*S(J)
112 CONTINUE
   JT=0
   DO 113 J=1,2
   IF(S(J).GT.GR) GO TO 110
113 CONTINUE
```

```
      CALL  EVAL(X,Y,J,A,B,Q,P)
      IF(NB.EQ.1)GO TO 500
      WRITE(6,52)A,B,Q(J),P(J),(XM(I,KB),I=1,2)
      NB=1
      GO TO 501
  500 WRITE(6,53)A,B,Q(J),P(J),(XM(I,KB),I=1,2)
   52 FORMAT(9X,'WEIGHTS',7X,'YP',9X,'YS',13X,'OPTIMAL X',
     X,2(/),8X,F4.2,1X,F4.2,4X,F7.4,4X,F7.4,2X,2(F10.5))
   53 FORMAT(/,8X,F4.2,1X,F4.2,4X,F7.4,4X,F7.4,2X,2(F10.5))
   23 FORMAT(3(F20.6))
   24 FORMAT(2(F20.6),4X,I8,4X,I4)
  501 A=A+.1
      B=B-.1
      IF(A.GE.1.0)GO TO 88
      Z=-100000000
      DO 116 I=1,2
      XM(I,KL)=0.0
  116 CONTINUE
      KCOUNT=0
      DO 117 J=1,2
      S(J)=STEP
  117 CONTINUE
      JT=0
      GO TO 115
   88 END


      SUBROUTINE ACCEL(A,B,J,JK,G,Z,ZKL,ZTEMP,XM,KB)
      DIMENSION XM(2,2000),X(2,2),G(13),XC(2)
      DO 82 I=1,2
      XC(I)=XM(I,KB)
   12 FORMAT(2(F15.7))
      X(I,J)=XC(I)
   82 CONTINUE
      YK=((55.84+(7.31*XC(1))+(26.65*XC(2))-(3.03*(XC(1)
     X**2))-(6.96*(XC(2)**2))+(2.69*XC(1)*XC(2)))*A)
     X+(B*(85.72+(21.85*XC(1))+(8.59*XC(2))-(9.2*(XC(1)
     X**2))-(5.18*(XC(2)**2))-(6.26*XC(1)*XC(2))))
      IF(JK.EQ.10)GO TO 47
      ZTEMP=YK
      GO TO 10
   47 Z=YK
      ZKL=Z
      JK=2
   10 RETURN
      END
```

```
      SUBROUTINE EVAL(X,Y,J,A,B,Q,P)
      DIMENSION X(2,2),Q(2),P(2),Y(2)
      Q(J)=55.84+(7.31*X(1,J))+(26.65*X(2,J))-(3.03*(X(1,J)
     X**2))-(6.96*(X(2,J)**2))+(2.69*X(1,J)*X(2,J))
      P(J)=85.72+(21.85*X(1,J))+(8.59*X(2,J))-(9.2*(X(1,J)
     X**2))-(5.18*(X(2,J)**2))-(6.26*X(1,J)*X(2,J))
      Y(J)=(A*Q(J))+(B*P(J))
      RETURN
      END
```

Explicit Constraint Consideration - Myers and Carter No. 1

```
      DIMENSION X(3,3),S(3),D(3,3),XM(3,2000),Y(3),X1(3,3)
     X,P(3)
      M=0
      KL=1
      READ(5,21)Z,STEP,PR,GR,JTEMP,JT
   26 FORMAT(/,3X,F3.1,5X,F3.1)
      DO 2 J=1,3
      S(J)=STEP
    2 CONTINUE
      READ(5,21)(XM(I,KL),I=1,3)
      DO 114 J=1,3
      READ(5,21)(D(I,J),I=1,3)
   21 FORMAT( )
  114 CONTINUE
  115 JK=10
      KB=KL+1
      DO 34 I=1,3
      XM(I,KB)=XM(I,KL)
      J=1
      X(I,J)=XM(I,KB)
   34 CONTINUE
      J=1
    6 CALL EVAL(X,Z,ZTEMP,ZKL,Y,J,JK,P)
  110 DO 81 J=1,3
      DO 111 I=1,3
      X(I,J)=XM(I,KB)+(S(J)*D(I,J))
  111 CONTINUE
      DO 33 I=1,3
      IF(X(I,J).GT.2.5)X(I,J)=2.5
      IF(X(I,J).LT.-2.5)X(I,J)=-2.5
   33 CONTINUE
   80 CALL EVAL(X,Z,ZTEMP,ZKL,Y,J,JK,P)
      IF(JT.GT.J)GO TO 11
      GO TO 50
   11 JT=JT-1
      GO TO 82
   50 IF(Y(J).LE.Z) GO TO 60
      IF(P(J).GT.0.0) GO TO 60
      Z=Y(J)
   82 DO 32 I=1,3
      XM(I,KB)=X(I,J)
   32 CONTINUE
      GO TO 81
   60 IF(JT.LT.J) GO TO 56
      GO TO 57
```

```
 56 JT=J
    MC=1
    GO TO 55
 57 JT=JT+1
    MC=0
 55 DO 31 N=1,3
    X1(N,J)=XM(N,KB)-(MC*S(J)*D(N,J))
    X(N,J)=X1(N,J)
 31 CONTINUE
    GO TO 80
 27 FORMAT(/,3(F20.10))
 81 CONTINUE
    JT=0
    M=M+1
    IF(KCOUNT.EQ.1)GO TO 150
    IF(Z.LE.ZKL)GO TO 70
    GO TO 68
150 IF(Z.LE.ZKL)GO TO 71
 68 KS=KB+1
    DO 37 I=1,3
    XM(I,KS)=(2*XM(I,KB))-XM(I,KL)
    IF(XM(I,KS).GT.2.5)XM(I,KS)=2.5
    IF(XM(I,KS).LT.-2.5)XM(I,KS)=-2.5
    XM(I,KL)=XM(I,KB)
    XM(I,KB)=XM(I,KS)
    X(I,J)=XM(I,KB)
 37 CONTINUE
    KCOUNT=1
    ZKL=Z
 77 JK=8
    GO TO 6
 71 IF(ZTEMP.LE.ZKL)GO TO 72
    ZKL=ZTEMP
    Z=ZTEMP
    GO TO 68
 72 DO 38 I=1,3
    XM(I,KB)=XM(I,KL)
    X(I,J)=XM(I,KB)
    KCOUNT=0
 38 CONTINUE
    JK=8
    GO TO 6
 70 DO 112 J=1,3
     S(J)=.5*S(J)
112 CONTINUE
```

```
      JT=0
      DO 113 J=1,3
      IF(S(J).GT.GR) GO TO 110
  113 CONTINUE
      CALL EVAL(X,Z,ZTEMP,ZKL,Y,J,JK,P)
      PD=P(J)+65.
      WRITE(6,53)Y(J),PD
   53 FORMAT(2X,'YP=',F10.4,5X,'YS=',F10.4)
      WRITE(6,54)(XM(I,KB),I=1,3)
   54 FORMAT(3X,'OPTIMAL X=',3(F12.5))
   23 FORMAT(3(F20.6))
      WRITE(6,24)Z,Y(J),M
   24 FORMAT(2(F20.6),4X,I8,4X,I4)
      END

      SUBROUTINE EVAL(X,Z,ZTEMP,ZKL,Y,J,JK,P)
      DIMENSION X(3,3),P(3),Y(3)
      Y(J)=65.39+(9.24*X(1,J))+(6.36*X(2,J))+(5.22*X(3,J))-
     X(7.23*(X(1,J)**2))-(7.76*(X(2,J)**2))-(13.11*(X(3,J)
     X**2))-(13.68*X(1,J)*X(2,J))-(18.92*X(1,J)*X(3,J))
     X-(14.68*X(2,J)*X(3,J))
      P(J)=-8.58+(4.65*X(1,J))+(8.39*X(2,J))+(2.56*X(3,J))+
     X(5.25*(X(1,J)**2))+(5.62*(X(2,J)**2))+(4.22*(X(3,J)
     X**2))+(8.74*X(1,J)*X(2,J))+(2.32*X(1,J)*X(3,J))+(3.78
     X*X(2,J)*X(3,J))
      IF(JK.EQ.10)GO TO 47
      IF(JK.EQ.9)GO TO 10
      IF(P(J).GT.0.0)GO TO 11
      ZTEMP=Y(J)
   12 JK=9
      GO TO 10
   47 Z=Y(J)
      ZKL=Z
      JK=9
      GO TO 10
   11 ZTEMP=-100000
      GO TO 12
   23 FORMAT(5X,2(F20.10))
   10 RETURN
      END
```

Implicit Constraint Consideration - Myers and Carter NO. 2

```
      DIMENSION X(2,2),P(2),S(2),D(2,2),XM(2,2000),Y(2)
     X,Q(2),XI(2,2)
      M=0
      KL=1
      READ(5,21)Z,STEP,PR,GR,JTEMP,JT,BASE
   26 FORMAT(/,3X,F3.1,5X,F3.1)
      DO 2 J=1,2
      S(J)=STEP
    2 CONTINUE
      READ(5,21)(XM(I,KL),I=1,2)
      DO 114 J=1,2
      READ(5,21)(D(I,J),I=1,2)
   21 FORMAT( )
  114 CONTINUE
  115 JK=10
      KB=KL+1
      DO 34 I=1,2
      XM(I,KB)=XM(I,KL)
      J=1
      X(I,J)=XM(I,KB)
   34 CONTINUE
      J=1
    6 CALL EVAL(X,Z,ZTEMP,ZKL,Y,J,JK,P,Q)
  110 DO 81 J=1,2
      DO 111 I=1,2
      X(I,J)=XM(I,KB)+(S(J)*D(I,J))
  111 CONTINUE
   80 CALL EVAL(X,Z,ZTEMP,ZKL,Y,J,JK,P,Q)
    9 FORMAT(5X,F20.10,5X,I2,)
      IF(JT.GT.J)GO TO 11
      GO TO 50
   11 JT=JT-1
      GO TO 82
   50 IF(Y(J).LE.Z) GO TO 60
      Z=Y(J)
   82 DO 32 I=1,2
      XM(I,KB)=X(I,J)
   32 CONTINUE
      GO TO 81
   60 IF(JT.LT.J) GO TO 56
```

```
      GO TO 57
   56 JT=J
      MC=2
      GO TO 55
   57 JT=JT+1
      MC=-1
   55 DO 31 N=1,2
      X1(N,J)=X(N,J)-(MC*S(J)*D(N,J))
      X(N,J)=X1(N,J)
   31 CONTINUE
      GO TO 80
   27 FORMAT(/,3(F20.10))
   81 CONTINUE
      JT=0
      M=M+1
      IF(KCOUNT.EQ.1)GO TO 150
      IF(Z.LE.ZKL)GO TO 70
      GO TO 68
  150 IF(Z.LE.ZKL)GO TO 71
   68 KS=KB+1
      DO 37 I=1,2
      XM(I,KS)=(2*XM(I,KB))-XM(I,KL)
      XM(I,KL)=XM(I,KB)
      XM(I,KB)=XM(I,KS)
      ZKL=Z
      KCOUNT=1
   37 CONTINUE
      JK =8
      GO TO 6
   71 IF(ZTEMP.LE.ZKL)GO TO 72
      ZKL=ZTEMP
      Z=ZTEMP
      GO TO 68
   72 DO 38 I=1,2
      XM(I,KB)=XM(I,KL)
      X(I,J)=XM(I,KB)
      KCOUNT=0
   38 CONTINUE
      JK=8
      GO TO 6
   70 DO 112 J=1,2
       S(J)=.5*S(J)
  112 CONTINUE
      JT=0
      DO 113 J=1,2
```

```
      IF(S(J).GT.GR) GO TO 110
  113 CONTINUE
      CALL EVAL(X,Z,ZTEMP,ZKL,Y,J,JK,P,Q)
      PD=BASE+P(J)
      WRITE(6,53)Q(J),PD
   53 FORMAT(2X,'YP=',F10.4,5X,'YS=',F10.4)
      WRITE(6,54)(XM(I,KB),I=1,2)
   54 FORMAT(3X,'OPTIMAL X=',3(F12.5))
   23 FORMAT(3(F20.6))
      WRITE(6,59)Z,M
   59 FORMAT(5X,'YTOT=',F10.5,10X,I10)
   24 FORMAT(2(F20.6),4X,I8,4X,I4)
      END

      SUBROUTINE EVAL(X,Z,ZTEMP,ZKL,Y,J,JK,P,Q)
      DIMENSION X(2,2),Q(2),T(2),R(2),P(2),Y(2)
      Q(J)=53.69+(7.26*X(1,J))-(10.33*X(2,J))+(7.22*(X
     X(1,J)**2))+(6.43*(X(2,J)**2))+(11.36*X(1,J)*X(2,J))
      P(J)=-1.83-(1.01*X(1,J))-(8.61*X(2,J))+(1.4*(X
     X(1,J)**2))-(8.76*(X(2,J)**2))-(7.2*X(1,J)*X(2,J))
      R(J)=-4.0+P(J)
      T(J)=-1+(X(1,J)**2)+(X(2,J)**2)
      IF(P(J).LT.0.0)GO TO 71
      VAL1=0
   81 IF(R(J).GT.0.0)GO TO 72
      VAL2=0
   82 IF(T(J).GT.0.0)GO TO 73
      VAL3=0
   83 VAL=VAL1+VAL2+VAL3
      GO TO 21
   71 VAL1=P(J)**2
      ZTEMP=-100000000
      GO TO 81
   72 VAL2=R(J)**2
      ZTEMP=-100000000
      GO TO 82
   73 VAL3=T(J)**2
      ZTEMP=-10000000
      GO TO 83
   21 Y(J)=Q(J)-(1000*VAL)
      IF(JK.EQ.10)GO TO 47
      IF(JK.EQ.9)GO TO 10
      ZTEMP=Y(J)
   12 JK=9
      GO TO 10
   47 Z=Y(J)
      ZKL=Z
      JK=9
   10 RETURN
      END
```

APPENDIX B

TABLES OF RESULTS

Table 9. Explicit Constraint Consideration for Umland-Smith Problem

Step	Start Pt.	y_P	y_S	x_1	x_2	iter.
$y_S \geq 90.0\%$						
0.1	0.0,1.0	88.6441	90.0001	1.03359	1.50000	26
	0.5,0.5	88.4564	90.0007	1.20527	1.40000	27
0.01	1.22,0.35	88.6568	90.0002	1.05162	1.49100	45
	0.5,0.5	87.8472	90.0004	1.32656	1.31000	31
	1.8,-0.023	86.3742	90.0010	1.47894	1.17300	29
	0.4,1.3	88.4842	90.0011	1.19628	1.40600	34
	0.3,0.6	88.6079	90.0004	1.14297	1.44000	30
	1.01,-0.35	88.6621	90.0011	1.07266	1.48000	44
0.001	0.5,0.5	87.6731	90.0009	1.35032	1.29040	50
$Y_S \geq 92.5\%$						
0.5	1.0,0.0	83.6472	92.5005	1.44019	1.00000	30
0.1	1.0,0.0	81.9840	92.5004	1.53242	0.90000	27
	0.7,0.7	86.0908	92.5006	1.20332	1.20000	21
	0.7,0.6	85.0380	92.5008	1.33301	1.10000	22
0.01	1.0,0.0	81.1059	92.5013	1.57225	0.82231	27
	0.5,0.5	85.8748	92.5006	1.23722	1.17600	34
	0.6,1.1	86.5219	92.5005	0.90491	1.34700	24
	1.4,0.344	86.5857	92.5008	1.07603	1.28000	85
	0.7,0.7	85.9219	92.5005	1.23034	1.18100	28
	0.7,0.6	85.4274	92.5013	1.29322	1.13300	33
$y_S \geq 95.0\%$						
0.5	1.0,0.5	82.9725	95.0000	1.13367	1.00000	30
	1.2,0.2	82.3168	95.0004	1.21196	0.94609	37
0.1	1.2,0.2	82.9600	95.0008	1.12969	1.00000	24
	1.0,0.5	79.9925	95.0010	1.37969	0.80000	21
0.01	1.2,0.2	82.7399	95.0002	1.16234	0.98000	39
	1.0,1.0	83.3139	95.0001	1.05359	1.04000	19
	0.5,0.8	83.4485	95.0001	0.94438	1.08000	30
	1.0,0.5	80.5246	95.0012	1.34953	0.83000	30
	1.22,0.351	82.2655	95.0002	1.21736	0.94225	57
0.001	1.2,0.2	81.4626	95.0000	1.28700	0.88700	76

Table 10. Implicit Constraint Consideration for Umland-Smith Problem

Step	Start Pt.	y_P	y_S	x_1	x_2	iter.
$y_S \geq 90.0\%$						
0.5	7.0,3.0	88.6442	89.9994	1.03369	1.50000	35
	0.5,0.5	88.6443	89.9994	1.03369	1.50000	22
	-3.0,0.7	88.5513	89.9999	1.17163	1.42217	322
	0.0,0.0	88.6489	89.9997	1.10962	1.45972	559
0.1	0.5,0.5	88.5180	89.9997	1.18480	1.41367	97
	7.0,3.0	88.6623	89.9997	1.08223	1.47497	98
	0.0,0.0	87.7602	89.9998	1.33887	1.30000	29
	-3.0,0.7	87.7602	89.9998	1.33887	1.30000	36
$y_S \geq 92.5\%$						
0.5	0.5,0.5	86.6441	92.4998	1.00562	1.31055	72
	7.0,3.0	86.6441	92.4998	1.00562	1.31055	86
	-3.0,0.7	86.6375	92.4998	1.02649	1.30127	87
	0.0,0.0	86.6441	92.4998	1.00562	1.31055	75
0.1	0.5,0.5	86.5428	92.4998	1.09142	1.26879	193
	7.0,3.0	86.6357	92.4999	1.02930	1.29997	95
	-3.0,0.7	86.6426	92.4990	0.99375	1.31563	69
	0.0,0.0	86.6359	92.4996	1.02930	1.30000	31
$y_S \geq 95.00\%$						
0.5	7.0,3.0	83.4562	94.9992	0.96643	1.07373	719
	0.0,0.0	83.4562	94.9992	0.96643	1.07373	713
	-3.0,0.7	83.4543	94.9993	0.97473	1.07109	72
	0.5,0.5	83.4562	94.9992	0.96643	1.07373	705
0.1	0.0,0.0	82.9606	94.9998	1.12988	1.00000	25
	7.0,3.0	82.9724	94.9999	1.12793	1.00114	100
	0.5,0.5	82.9606	94.9998	1.12988	1.00000	22
	-3.0,0.7	82.9606	94.9998	1.12988	1.00000	33

Table 11. Explicit Constraint Consideration for Myers-Carter Problem No. 1

Step	Start Pt.	y_P	y_S	x_1	x_2	x_3	iter.
0.5	-1.,-1.,0.	72.9136	65.0000	1.5000	-.4922	-.6018	32
0.1	0.,0.,0.	73.7860	65.0000	1.8631	-.9078	-.6072	86
0.01	0.0,0.,0.	72.9132	64.9999	1.5000	-.4925	-.6064	145
	0.,0.,1.0	73.0345	64.9998	1.5390	-.5352	-.6118	133
	0.,0.,-1.0	73.1507	65.0000	1.57812	-.57813	-.6139	46
	0.,-1.0,1.0	72.9136	65.0000	1.5000	-.4922	-.6118	29
	2.0,-2.0,1.0	72.8256	64.9998	1.5000	-1.8125	-.5635	17
	2.0,-2.0,-1.0	73.7412	64.9999	2.2578	-1.4375	-.6115	28
	0.,-1.0,-1.0	73.1507	65.0000	1.5781	-.5781	-.6139	46
	0.,-2.0,1.0	72.9136	65.0000	1.5000	-.4922	-.6018	23
	1.0,0.,0.	73.1507	65.0000	1.5781	-.5781	-.6139	45
	1.0,-1.0,0.	72.9136	65.0000	1.5000	-.4922	-.6018	28
	1.0,-1.0,1.0	72.9136	65.0000	1.5000	-.4922	-.6018	29
	1.0,-1.0,-1.0	72.9136	65.0000	1.5000	-.4922	-.6018	28
	-1.0,0.,0.	73.9145	64.9997	2.1250	-1.250	-.6222	42
	-1.0,0.,1.0	73.0345	64.9998	1.5391	-.5352	-.6118	32
	1.0,-2.0,0.	72.9136	65.0000	1.5000	-.4922	-.6018	28
	-1.0,0.,-1.0	72.9136	64.9998	1.5391	-.5352	-.6118	32
	-1.0,1.0,0.	73.1507	65.0000	1.5782	-.5781	-.6139	48
	-1.0,1.0,-1.0	72.8256	64.9998	2.5000	-1.8125	-.5635	23
	-1.0,-1.0,1.0	72.9136	65.0000	1.5000	-.49219	-.6018	32
	-1.0,-1.0,0.	72.8356	64.9998	2.5000	-1.8125	-.56348	23

Table 12. Implicit Constraint Consideration for Myers-Carter Problem No. 1

Step	Start Pt.	y_P	y_S	x_1	x_2	x_3	iter.
	Penalty = 1000						
0.5	0.,0.,0.	72.8273	65.0001	2.5000	-1.8123	-.5630	25
	-98.,73.,-56.	71.5735	64.9991	1.1392	-.1230	-.5529	36
0.3	0.,0.,0.	73.8772	65.0007	2.0997	-1.2000	-.5405	183
0.1	0.,0.,0.	73.1419	64.9999	1.5752	-.5750	-.6150	47
	Penalty = 100						
0.5	0.,0.,0.	73.3482	65.0034	2.4058	-1.6460	-.5438	1288
	-98.,73.,-56.	71.7244	65.0011	1.1759	-.1603	-.5595	60
0.1	1.0,0.0,0.	72.6647	64.9989	1.4250	-.4125	-.5904	49
	0.,0.,0.5	73.7860	65.0000	1.86309	-.90781	-.60723	86
	0.,0.,0.	73.9442	65.0022	2.0697	-1.1703	-.6014	116
	2.0,-2.0,0.	73.7918	65.0032	2.2469	-1.4113	-.5748	46
	1.0,-1.0,1.0	73.9437	65.0025	2.07774	-1.1807	-.6000	89
	24.0,-5.34,0.	72.9422	65.0039	2.4928	-1.7838	-.5227	105
	-2.1,.554,1.2	73.9439	65.0020	2.07601	-1.17842	-.6002	133
0.01	0.,0.,0.	73.9437	65.0022	2.0553	-1.1519	-.6056	158

Table 13. Weighting Function Results - Myers and Carter No. 2
Increment = 0.1 Initial Stepsize = 0.1

WEIGHTS		YP	YS	OPTIMAL X	
.0	1.0	67.1895	87.7117	.82676	-.56250
.1	.9	67.1895	87.7117	.82676	-.56250
.2	.8	67.2200	87.5977	.73906	-.67363
.3	.7	67.2200	87.5977	.73906	-.67363
.4	.6	67.2200	87.5977	.73906	-.67363
.5	.5	67.2200	87.5977	.73906	-.67363
.6	.4	67.2200	87.5977	.73906	-.67363
.7	.3	67.2200	87.5977	.73906	-.67363
.8	.2	67.2589	87.4961	.71406	-.70000
.9	.1	67.2589	87.4961	.71406	-.70000
1.0	.0	67.2589	87.4961	.71406	-.70000

Table 14. Weighting Function Results - Myers and Carter No. 2
Increment = 0.1 Initial Stepsize = 0.5

WEIGHTS		YP	YS	OPTIMAL X	
.0	1.0	67.1786	87.7247	.79688	-.60413
.1	.9	67.1984	87.6571	.75781	-.65247
.2	.8	67.1984	87.6571	.75781	-.65247
.3	.7	67.1984	87.6571	.75781	-.65247
.4	.6	67.1984	87.6571	.75781	-.65247
.5	.5	67.1984	87.6571	.75781	-.65247
.6	.4	67.1984	87.6571	.75781	-.65247
.7	.3	67.3792	87.2158	.66138	-.75000
.8	.2	70.4500	82.0200	.00000	-1.00000
.9	.1	70.4500	82.0200	.00000	-1.00000
1.0	.0	70.4500	82.0200	.00000	-1.00000

Table 15. Weighting Function Results - Myers and Carter No. 2
Increment = 0.01 Initial Stepsize = 0.1

WEIGHTS		YP	YS	OPTIMAL X	
.70	.30	67.2200	87.5977	.73906	-.67363
.71	.29	67.2200	87.5977	.73906	-.67363
.72	.28	67.2200	87.5977	.73906	-.67363
.73	.27	67.2200	87.5977	.73906	-.67363
.74	.26	67.2200	87.5977	.73906	-.67363
.75	.25	67.2200	87.5977	.73906	-.67363
.76	.24	67.2200	87.5977	.73906	-.67363
.77	.23	67.2589	87.4961	.71406	-.70000
.78	.22	67.2589	87.4961	.71406	-.70000
.79	.21	67.2589	87.4961	.71406	-.70000
.80	.20	67.2589	87.4961	.71406	-.70000

Table 16. Weighting Function Results - Myers and Carter No. 2
Increment = 0.01 Initial Stepsize = 0.5

WEIGHTS		YP	YS	OPTIMAL X	
.70	.30	67.3792	87.2158	.66138	-.75000
.71	.29	67.3792	87.2158	.66138	-.75000
.72	.28	67.3792	87.2158	.66138	-.75000
.73	.27	67.3792	87.2158	.66138	-.75000
.74	.26	67.3792	87.2158	.66138	-.75000
.75	.25	67.3792	87.2158	.66138	-.75000
.76	.24	70.4500	82.0200	.00000	-1.00000
.77	.23	70.4500	82.0200	.00000	-1.00000
.78	.22	70.4500	82.0200	.00000	-1.00000
.79	.21	70.4500	82.0200	.00000	-1.00000
.80	.20	70.4500	82.0200	.00000	-1.00000

Table 17. Explicit Constraint Consideration for Myers and Carter No.2

Step	Start Pt.	y_P	y_S	x_1	x_2
0.1	0.5,-0.5	67.5716	86.8056	0.60000	-.80000
0.01	0.5,-0.5	67.2589	87.4961	0.71406	-.70000
	0.0,-0.2	67.5705	86.8046	0.59984	-.80000
	-0.5,-0.5	71.0997	80.9106(infs)	-.24297	-.97000
	0.2,-0.4	67.5256	86.8983	0.61297	-.79000
	-1.0,0.0	53.6500	84.5800	-1.00000	0.00000
0.001	0.2,-0.4	67.5669	86.8152	0.60133	-.79900

Table 18. Implicit Constraint Consideration for Myers and Carter No.2

Step	Start Pt.	y_P	y_S	x_1	x_2
0.5	0.0,0.0	68.0878	83.9998	0.99792	-.09656
0.1	7.0,-3.0	68.0864	84.0013	0.99786	-.09688
	0.0,0.0	69.1847	83.9997	0.26660	-.96563
	-3.0,-7.0	68.0863	84.0013	0.99785	-.09668
	-5.0,3.0	69.1846	83.9997	0.26660	-.96562
	5.0,5.0	68.0863	84.0013	0.99785	-.09668
	2.0,-0.2	69.1824	83.9999	0.26651	-.96551

BIBLIOGRAPHY

1. Box, G.E.P., "The Exploration and Exploitation of Response Surfaces, Some General Considerations and Examples", Biometrics, Vol. 10, p. 16, 1954.

2. Box, M. J., Davies, D., and Swann, W. H., Non-linear Optimization Techniques, Monograph Series, Imperial Chemical Industries Ltd., 1969.

3. Carrol, Charles W., "The Created Response Surface Technique for Optimizing Nonlinear, Restrained Systems", Operations Research, Vol. 9, p. 169-184, 1961.

4. Dyer, James S., An Empirical Investigation of a Man-machine Interactive Approach to the Solution of the Multiple Criteria Problem, Western Management Science Institute, University of California, Los Angeles, 1972.

5. Fiacco, A. V., and McCormick, G. P., Nonlinear Programming: Sequential Unconstrained Minimization Technique, John Wiley and Sons Inc., N. Y.

6. Geoffrion, A. M., Dyer, J. S., and Feinberg, A., An Interactive Approach for Multi-Criterion Optimization, with an Application to the Operation of an Academic Department, Western Management Science Institute, University of California, Los Angeles, Working Paper No. 176, 1972.

7. Geoffrion, A. M., and Hogan, W. W., "Coordination of Two-Level Organizations with Multiple Objectives", Techniques of Optimization, Academic Press Inc., N. Y., 1972.

8. Heller, Nelson B., and Staats, Glenn E., "Response Surface Optimization When Experimental Factors are Subject to Costs and Constraints", Technometrics, Vol. 15, No 1, 1973.

9. Hoerl, Arthur E., "Optimum Solution of Many Variable Equations", Chemical Engineering Progress, Vol. 55, p. 69, 1959.

10. Hooke, R., and Jeeves, T. A., "Direct Search" Solutions of Numerical and Statistical Problems", J. Assoc. Computer. Mach., Vol. 8, p. 212, 1961.

11. Hunter, J. S., "Determination of Optimum Operating Conditions by Experimental Methods: Part II - 1,2,3, Models and Methods" Ind. Quality Control, Vol. 15, No. 6, p. 16-24, No. 7, p. 7-15, No. 8, p. 6-14, 1958, 1959.

12. Lind, E. E., Goldin, J., and Hickman, J. B., "Fitting Yield and Cost Response Surfaces", Chemical Engineering Progress, Vol. 56, p. 62, 1960.

13. Michaels, S. F., and Pengilly, P. J., "Maximum Yield for Specified Cost", Applied Statistics, Vol. 12, p. 189-193, 1963.

14. Miller, James R., Professional Decision-Making: A Procedure for Evaluating Complex Alternatives, Praeger Publishers, N. Y., 1970.

15. Myers, Raymond H., Response Surface Methodology, Allyn and Bacon, Inc., Boston, 1971.

16. Myers, Raymond and Carter, Walter H. Jr., "Response Surface Techniques for Dual Response Systems", Technometrics, Vol. 15, No. 2, 1973.

17. Schrage, R. W., "Optimizing a Catalytic Cracking Operation by the Method of Steepest Ascent and Linear Programming", Operations Research, Vol. 6, p. 498-515, 1958.

18. Umland, A. W., and Smith, W. N., "The Use of LaGrange Multipliers With Response Surfaces", Technometrics, Vol. 1, p. 289-292, 1959.

19. Zoutendijk, G., Methods of Feasible Directions, Amsterdam, Elsevier, 1960.