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OPTIMIZATION OF A COMPUTER SIMULATION RESPONSE

by

Dennis E. Smith

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Based on results to date, the statistical techniques of Response Surface Methodology (RSM) appear to be well-adapted to use in seeking an optimum simulation response. This report summarizes the optimum-seeking problem, reviews the framework of RSM, and describes an "automated RSM" computer program which has been developed as an alternative to manual applications of these statistical techniques. Program interface and data preparation are discussed. In addition, easily-followed examples are presented to illustrate program output and major aspects of the RSM optimum-seeking process.

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I. BACKGROUND

Because of their complexity, many problems of operations research or management science cannot be examined analytically, but instead must be attacked by means of computer simulation. This paper discusses the task of obtaining an optimum computer simulation solution, and describes a computer program for aiding in this task. This computer program incorporates the statistical techniques of Response Surface Methodology.

Throughout this paper, a computer simulation will be regarded as a "black box" in which the values of input parameters, or factors, are combined in some manner to produce output parameters. The input parameters may be classified into two categories: (1) controllable factors and (2) uncontrollable factors. Controllable factors are those input parameters having values which may be directly controlled by the appropriate decision maker in the real world. Uncontrollable factors, on the other hand, are those input parameters over which the decision maker has no direct control.

For example, in a simulation in which a U. S. Navy task force is protected from an attacking enemy submarine by destroyer escorts, the range at which the submarine can be detected is a function of controllable factors (such as speed, bearing, and maneuverability) describing escort tactics. Factors which pertain to weather conditions and the submarine's tactics are classified as uncontrollable.

The specific topic addressed in this paper is the determination of those values of continuous controllable factors which produce the optimum value of one output parameter of interest. It should be noted that there are two basic assumptions in this problem definition. One is that each of the controllable factors is continuous; the other is that the optimum value of a single output parameter is to be found. In actual practice, the former assumption may be relaxed somewhat in that discrete factors may be considered if they are reasonably approximated as continuous.

In a sense, this type of problem-solving situation is similar to an optimization problem to be solved by analytical techniques (e.g., linear programming). The major difference is that no explicit objective function is stated and, in fact, such a function exists only implicitly in the multitude of computer instructions in the programs comprising the simulation. Thus, the task of finding the best solution cannot rely on those analytical methods which depend on an explicit objective function.

Methods to aid in the quest for an optimum simulation solution may be thought of as comprising two general types: (1) internal methods and (2) external methods. Internal methods are those methods which involve tinkering with the inner workings (the mathematical relationships and computer programming) of the simulation black box. Thus, these methods are incorporated directly into the black box during simulation development.

There are a number of internal methods. For example, analytical techniques of optimization may be programmed for use in selected portions of the models. Thus, within a restricted section of the model, an optimum may be identified, subject to conditional constraints.

Another procedure involves consideration of approximations or expected values instead of dealing directly with underlying probability distributions. This procedure may restructure the model to make it more amenable to classical optimization techniques.

Unlike internal methods, external methods do not affect development of the mathematical model or computer programs which compose the simulation black box, and are, therefore, independent of simulation construction. These methods specify search strategies or decision rules for experimenting with different values of the controllable factors, usually using the output of the black box as feedback. Although a number of search strategies have been suggested, there are four primary techniques which serve as a basis for most other ones. These are: (1) Factorial Design, (2) Random Search, (3) Single-Factor method, and (4) Response Surface Methodology (RSM).

It can readily be seen that, because of their independence of both the mathematical model underlying the simulation and the associated computer programs, external methods have a much wider area of applicability than do internal methods. This is doubly true when one reflects that models and simulations tend to evolve, being revised at a number of stages. In view of this situation, an internal method incorporated into an original model may have to be altered or deleted.

In addition, should someone desire to use an existing simulation in an attempt to determine an optimum solution to some problem, the application of any internal method would require that the computer programs be revised and modified. On the other hand, external methods could be used without any changes to the simulation structure. Furthermore, optimization in the simulation situation usually, at some stage, relies on external methods to provide a search of the relevant parameter space.

There is evidence [6,7] that response surface methodology (RSM) is the external method which offers the greatest payoff under the assumptions (continuous controllable factors, single output to be optimized) that have been made. Thus, this paper concentrates on the use of RSM in computer simulation situations.

II. RESPONSE SURFACE METHODOLOGY

Under the assumptions mentioned previously, when k controllable factors are involved in the simulation, the output parameter or response lies on a surface in (k + 1) - dimensional space if statistical variation is disregarded. This surface is often referred to as the response surface.

The basis of response surface methodology, which is a blending of statistical experimental design and regression analysis, was developed in a paper by Box and Wilson [1]. RSM makes use of the initial assumption that the response surface can, in any local region, be well-approximated by a hyperplane. That is, a good approximation to the response surface in any locality is given by the equation

$$\alpha_o + \sum_{1}^{k} \alpha_i X_i$$

If an experimental region (i.e., a locality) is defined by the boundaries $L_i \leq X_i \leq U_i$, i = 1,...,k, it is often convenient to code the largest value of each factor as + 1 and the smallest value of each factor as - 1. For example, if factor X_j were to be investigated in the interval $20 \leq X_j \leq 60$, the coding would be given by

$$x_j = \frac{X_j - 40}{20}$$

so that $x_j = -1$ is equivalent to $X_j = 20$, and $x_j = +1$ is equivalent to $X_j = 60$. If the factors $X_1,\ldots,X_k$ are transformed into the coded factors $x_1,\ldots,x_k$ in this manner, the equation

$$\alpha_o + \sum_1^k \alpha_i X_i$$

is transformed into the equation

$$\beta_o + \sum_1^k \beta_i x_i \quad .$$

Thus, an estimate $\hat{y}$ of the value of the response y at the coded point $(x_1,\ldots,x_k)$ would be given by

$$\hat{y} = b_o + \sum_1^k b_i x_i \ ,$$

where b_i, obtained from an initial experiment (usually a 2^{k-p} fractional factorial [2,3,5]) by least squares, is an estimate of β_i.

The estimates $(b_1,\ldots,b_k)$ determine the estimated gradient direction known as the path of steepest ascent. This path, which provides the approximate direction of predicted maximum response, is followed until there is no improvement in the observed response, at which time the whole process may be repeated, usually within a smaller experimental region.

When the initial assumption of an approximating hyperplane no longer appears valid, additional experiments may be conducted to estimate the curvature of the response surface. The usual design in this situation is a central composite design [2,3,5], which may be constructed by adding axial points to an existing fractional factorial.

If necessary, ridge analysis [4] may be used to continue optimum-seeking on the approximating curved (i.e., second order) surface. Ridge analysis is the analogue of the steepest ascent procedure used in conjunction with the hyperplane (i.e., first order) approximation.

III. A COMPUTER PROGRAM FOR AUTOMATED RSM

Because of the independence of RSM from the underlying simulation, it is possible to automate its application to a large extent. Such automation eliminates the requirement that a person applying RSM techniques must be relatively knowledgeable about their underlying statistical and mathematical bases.

The following sections of this paper describe an automated RSM computer program[1] which is now available to simulation users. This program, which may be used for constrained or unconstrained optimum-seeking in conjunction with deterministic or Monte Carlo simulations, should prove valuable in obtaining improved simulation solutions, while at the same time reducing analyst effort and shortening overall time to solution. In addition, and somewhat paradoxically, optimum-seeking by means of the RSM program may often result in a smaller investment in total computer time than that required by an analyst's manual search involving the same number of simulation runs. This surprising situation occurs because execution time for the program tends to be less than the corresponding time requirements of repetitive simulation loading and input processing in the manual mode.

The automated RSM program, which can process up to 15 controllable factors subject to a maximum of 25 linear constraints,[2] is coded as a maximizing program. It treats a minimization problem by changing

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[1] Developed under Office of Naval Research Contract No. N00014-74-C-0148.

[2] A larger number of controllable factors and/or constraints may be processed if the dimensions of the appropriate arrays in the program are increased.

the sign of all responses obtained and maximizing the changed responses. That is, the program maximizes the negative of the original responses. (All information printed as output is, however, in terms of the original responses.)

Two versions of the RSM program are available. One, labeled RSMC, is for problems in which there are linear constraints on the input parameters. The other, labeled RSMU, is a shorter version designed for problems involving unconstrained optimum-seeking. Each version of this American National Standard FORTRAN IV program is designed to function as an executive program which may be easily interfaced with an existing FORTRAN simulation.

Program version RSMU, which is composed of a main program and 24 subroutines on 1690 cards (including 454 comment cards), requires 23,280 bytes of core memory on the IBM 370/Model 168 when using the FORTRAN IV (H) compiler. The RSMC version, which consists of a main program and 30 subroutines on 2349 cards (including 604 comment cards), requires 32,148 bytes.

The automated RSM program incorporates the general RSM procedures described in the previous section. In addition to permitting optimum-seeking subject to user-specified constraints on the controllable factors, the program also allows the user to conduct the RSM search in suitably-sized blocks of simulation runs to permit flexible scheduling of computer processing time.

The following sections summarize the automated RSM program. More detailed information about the program is provided in two volumes [8,9] of a report which serves as a user's guide. Both volumes are available from the National Technical Information Service (NTIS). Copies of the program may be obtained from Desmatics, Inc.

A. PROGRAM DESCRIPTION

The automated RSM program comprises a number of subroutines which are required for conducting the optimum-seeking search. This search consists of five phases:

(1) First-order design phase

(2) Steepest-ascent phase

(3) Factor screening phase

(4) Second-order design phase

(5) Ridge analysis phase.

The first-order design phase generates a 2^{k-p} fractional factorial of minimal size to permit a first-order (i.e., hyperplane) approximation to the response surface. Using the results of these runs, this phase calculates the path of steepest ascent. The steepest ascent phase then monitors simulation runs along this path. When runs on the path fail to provide improvement in observed response, control returns to the first-order design phase, which generates a new fractional factorial about the point (i.e., the controllable factor values) which yielded the best observed response.

When the fractional factorials are found not to provide a reasonable path of steepest ascent because of an unsuitable approximation to the response surface, the second-order design phase is entered. This module augments the existing fractional factorial with additional simulation runs in order to form a central composite design which permits estimation of quadratic effects (i.e., curvature of the response surface). Using the observed responses obtained from the simulation runs in this design, the ridge analysis phase guides the search for an improved solution by means of ridge analysis.

The factor screening phase permits efficiency in the expenditure of simulation runs in later stages of the search for an improved solution. This is accomplished by eliminating from consideration those controllable factors which were observed in the first-order design phase to have little or no effect on the observed response. Because the fractional factorial provides an estimate of the effect that each factor has on the observed response, the relative importance of each factor is judged by comparing its estimated effect with its estimated standard error, which is also obtained from the fractional factorial. If the estimated effect is larger than its estimated standard error, the factor is retained in the search. Otherwise, the factor is set equal to the value corresponding to the simulation run which has produced the best observed response, and is not varied in succeeding stages of the search.

A constraint option is available for specifying linear constraints on the controllable factors. Should constraints be specified, the program conducts its search subject to them. When a constraint is encountered within a fractional factorial or a central composite design, the complete design is shifted away from the violated constraint. When a constraint is encountered while runs are being made on a search path, the search direction is revised so that it lies in the restrictive hyperplane defined by the constraint.

Although the complete RSM search may be conducted within a single run of the automated program, use of the restart option permits the user to have the search made in blocks of runs. This option provides flexibility in scheduling computer time and protects the processing investment in the event of errors in the data input. After the last simulation run in a block, a file of pertinent data is created. Using this restart data file as input to the RSM program, the user may resume optimum-seeking by continuing the processing of simulation runs. The overall RSM search may be restarted any number of times at any phase.

B. PROGRAM INTERFACE AND DATA INPUT

The automated RSM program begins its optimum-seeking with k controllable factors $X_1,\ldots,X_k$ under investigation and a maximum of n points in the k-dimensional space to be run in the simulation with m iterations at each point. In other words, each of the n points in the k-dimensional factor space determines the values of the controllable factors for which a simulation run consisting of m iterations is to be made. In a deterministic simulation where no random variation exists in responses observed at the same point, only one iteration ($m = 1$) would be used. For a Monte Carlo simulation, however, random variation does exist in responses observed at the same point. To contend with this random variation, several iterations ($m > 1$) may be used to obtain an average observed response at each of the n points.

To apply the automated RSM program, the user must input values of k, m, and n, an initial point for the search, and a step size Δ_i for each factor X_i, $i = 1,\ldots,k$. In addition, the program must be interfaced with the simulation to which it is to be applied. This, however, is a relatively straightforward task, which requires that the response and all controllable factors occur in COMMON statements within the simulation. This may require defining new COMMON statements, if necessary.

A short interface routine must also be prepared. Upon entry to the simulation, this routine should define the values of the factors to be used in the simulation run. Upon exit from the simulation, the routine should define the value of the observed response to be used in the RSM program.

Input to RSMU, the program version for unconstrained optimum-seeking, consists of:

(1) A master parameter card which supplies information about the search to be conducted and the options desired

(2) A set of design specification cards, which contain information from which the initial fractional factorial design is constructed.

RSMC, the version for constrained optimum-seeking, requires an additional set of constraint-specification cards. On a run where restart input is used (for either RSMU or RSMC), only a new master parameter card is required in addition to the existing restart data file.

C. PROGRAM OUTPUT

For each simulation run that is made, the RSM program provides output which includes the observed responses for each of the m iterations comprising a simulation run, the average observed response for that run, the values of the controllable factors corresponding to that run, and an indication when the response is the "best" (maximum on the k-dimensional surface) that has been observed. In addition, RSMC (the version for constrained optimum-seeking) prints the constraints inputted by the user and provides information pertinent to constraint processing. The final output at the conclusion of the search consists of the best observed response and the corresponding factor values.

Instead of a detailed description of the RSM program output, this section presents two simple examples of RSM application to illustrate the type of printed output provided by RSMU and RSMC. It should be noted that in the examples, explicit mathematical function were used as the "simulations" for which an optimum solution was to be found. The use of known functions, rather than simulations involving unknown response surfaces, provides normative information which may prove valuable to the potential user in examining the automated RSM program output.

1. Example No. 1

The first example uses the response surface

$$y = 10\ (-2X_4^2 + X_5^2 - 4X_4X_5 + 96X_4 + 48X_5 - 960)$$

as a deterministic "simulation". Input data to the RSMU program version defined an unconstrained maximum-seeking problem involving five controllable factors.

The starting point for the search was given as

$$(X_1, X_2, X_3, X_4, X_5) = (10.0, 10.0, 0.0, 0.0, 0.0)$$

with corresponding step sizes

$$(\Delta_1, \Delta_2, \Delta_3, \Delta_4, \Delta_5) = (1.0, 1.0, 2.0, 2.0, 2.0).$$

An upper limit of 30 simulation runs of one iteration each was specified, with all 30 runs to be made in one pass of the RSMU program. It should be noted that the response surface, which is determined by X_4 and X_5 only, is a saddle surface centered at the point $X_4 = 16.0$, $X_5 = 8.0$.

An examination of the RSMU output shows that an initial fractional factorial involving the five factors was used to determine the steepest ascent path. Simulation runs corresponding to points on this path were made until there was no improvement in the observed response. When this lack of improvement occurred, the factors were examined to determine whether any might be of minor importance and thus be eliminated from further consideration. Based on this examination, factors X_1, X_2, and X_3 were inactivated before a new fractional factorial was constructed. Information from this design revealed that the assumption of a first order (hyperplane) approximation was not reasonable.

Because of this, a second order surface was fit, with the search continuing by means of ridge analysis. Thus, by entering the second order phase, the RSMU program avoided having the search end erroneously in the vicinity of the saddle point, despite the fact that the initial steepest ascent path directed the search to that region.

The following pages exhibit the output produced by RSMU for this problem.

```
RSMU---AUTOMATED RESPONSE SURFACE METHODOLOGY FOR UNCONSTRAINED OPTIMUM-SEEKING
    5 FACTORS
    1 ITERATIONS PER SIMULATION RUN
   30 MAXIMUM NUMBER OF SIMULATION RUNS ALLOCATED
   30 SIMULATION RUNS TO BE USED ON THIS PASS

MAXIMUM RESPONSE DESIRED

   I   STARTING VALUE OF X(I)   VALUE OF DELTA CORRESPONDING TO X(I)
   1        0.100000E 02                   0.100000E 01
   2        0.100000E 02                   0.100000E 01
   3        0.000000E 00                   0.200000E 01
   4        0.000000E 00                   0.200000E 01
   5        0.000000E 00                   0.200000E 01

***********************************************************************************************

RUN     1

OBSERVED RESPONSES ON THE    1  ITERATIONS
                           -0.960000E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.960000E 04      THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                =====================================
                                                                =====================================

VALUES OF X(1),....,X(K) ARE
              0.100000E 02      0.100000E 02      0.000000E 00      0.000000E 00      0.000000E 00

***********************************************************************************************

***********************************************************************************************

RUN     2

OBSERVED RESPONSES ON THE    1  ITERATIONS
                           -0.692000E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.692000E 04      THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                =====================================
                                                                =====================================

VALUES OF X(1),....,X(K) ARE
              0.900000E 01      0.900000E 01     -0.200000E 01      0.200000E 01      0.200000E 01

***********************************************************************************************

***********************************************************************************************

RUN     3

OBSERVED RESPONSES ON THE    1  ITERATIONS
                           -0.126800E 05

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.126800E 05

VALUES OF X(1),....,X(K) ARE
              0.110000E 02      0.900000E 01     -0.200000E 01     -0.200000E 01     -0.200000E 01

***********************************************************************************************
```

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********************************************************************************************************************
RUN     4

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.104400E 05

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.104400E 05

VALUES OF X(1),...,X(K) ARE
                 0.900000E 01        0.110000E 02        -0.200000E 01        -0.200000E 01        0.200000E 01
********************************************************************************************************************

********************************************************************************************************************
RUN     5

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.852000E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.852000E 04

VALUES OF X(1),...,X(K) ARE
                 0.110000E 02        0.110000E 02        -0.200000E 01        0.200000E 01        -0.200000E 01
********************************************************************************************************************

********************************************************************************************************************
RUN     6

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.852000E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.852000E 04

VALUES OF X(1),...,X(K) ARE
                 0.900000E 01        0.900000E 01        0.200000E 01        0.200000E 01        -0.200000E 01
********************************************************************************************************************

********************************************************************************************************************
RUN     7

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.104400E 05

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.104400E 05

VALUES OF X(1),...,X(K) ARE
                 0.110000E 02        0.900000E 01        0.200000E 01        -0.200000E 01        0.200000E 01
********************************************************************************************************************

********************************************************************************************************************
RUN     8
```

```
OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.126800E 05

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.126800E 05

VALUES OF X(1),...,X(K) ARE
                 0.900000E 01        0.110000E 02        0.200000E 01        -0.200000E 01        -0.200000E 01

****************************************************************************************************************

****************************************************************************************************************

RUN      9

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.692000E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.692000E 04

VALUES OF X(1),...,X(K) ARE
                 0.110000E 02        0.110000E 02        0.200000E 01        0.200000E 01        0.200000E 01

****************************************************************************************************************

FRACTIONAL FACTORIAL COMPLETED

DETERMINISTIC SIMULATION ASSUMED

ESTIMATED STANDARD ERROR OF AVERAGE OBSERVED RESPONSE=        0.000000E 00

ACTIVE FACTORS ARE
                      1  2  3  4  5

STEEPEST PATH-----B(0), B(I)S CORRESPONDING TO (CODED) ACTIVE FACTORS IN ORDER LISTED ABOVE

                -0.963555E 04

                 0.000000E 00        0.000000E 00        0.000000E 00        0.192000E 04        0.960000E 03

PREDICTED RANGE RATIO=   0.138946E 02    LACK OF FIT RATIO=   0.999999E 06

EXPLORE PATH

****************************************************************************************************************

RUN     10

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.481981E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.481981E 04       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 ====================================
                                                                 ====================================

VALUES OF X(1),...,X(K) ARE
                 0.100000E 02        0.100000E 02        0.000000E 00        0.466296E 01        0.233148E 01

****************************************************************************************************************

****************************************************************************************************************
```

```
RUN     11

OBSERVED RESPONSES ON THE    1  ITERATIONS
                             -0.299515E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.299515E 04       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),....,X(K) ARE
                 0.100000E 02        0.100000E 02        0.000000E 00        0.706296E 01        0.353148E 01

************************************************************************************************************************

************************************************************************************************************************

RUN     12

OBSERVED RESPONSES ON THE    1  ITERATIONS
                             -0.160248E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.160248E 04       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),....,X(K) ARE
                 0.100000E 02        0.100000E 02        0.000000E 00        0.946296E 01        0.473148E 01

************************************************************************************************************************

************************************************************************************************************************

RUN     13

OBSERVED RESPONSES ON THE    1  ITERATIONS
                             -0.641819E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.641819E 03       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),....,X(K) ARE
                 0.100000E 02        0.100000E 02        0.000000E 00        0.118630E 02        0.593148E 01

************************************************************************************************************************

************************************************************************************************************************

RUN     14

OBSERVED RESPONSES ON THE    1  ITERATIONS
                             -0.113150E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.113150E 03       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),....,X(K) ARE
                 0.100000E 02        0.100000E 02        0.000000E 00        0.142630E 02        0.713148E 01
```

```
****************************************************************************************************

****************************************************************************************************

RUN     15

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.164811E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.164811E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  =====================================
                                                                  =====================================

VALUES OF X(1),...,X(K) ARE
                 0.100000E 02         0.100000E 02         0.000000E 00         0.166629E 02         0.833148E 01

****************************************************************************************************

****************************************************************************************************

RUN     16

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.351810E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.351810E 03

VALUES OF X(1),...,X(K) ARE
                 0.100000E 02         0.100000E 02         0.000000E 00         0.190629E 02         0.953148E 01

****************************************************************************************************

****************************************************************************************************

RUN     17

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          -0.111914E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.111914E 04

VALUES OF X(1),...,X(K) ARE
                 0.100000E 02         0.100000E 02         0.000000E 00         0.214629E 02         0.107315E 02

****************************************************************************************************

SEEK NEW PATH

NUMBER OF B(I)S WITH MAGNITUDE GREATER THAN 2.*SIGMA OF B(I)     2

K IS NOW EQUAL TO     2

ACTIVE FACTORS ARE
                     4   5

   I    STARTING VALUE OF X(I)    VALUE OF DELTA CORRESPONDING TO X(I)
   4         0.166629E 02                    0.100000E 01
   5         0.833148E 01                    0.200000E 01
```

```
****************************************************************************************************

RUN    18

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          0.307225E 01

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS    0.307225E 01       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  =====================================
                                                                  =====================================

VALUES OF X(1),...,X(K) ARE
                   0.100000E 02        0.100000E 02        0.000000E 00        0.156629E 02        0.633148E 01
****************************************************************************************************

****************************************************************************************************

RUN    19

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          0.835187E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS    0.835187E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  =====================================
                                                                  =====================================

VALUES OF X(1),...,X(K) ARE
                   0.100000E 02        0.100000E 02        0.000000E 00        0.176629E 02        0.633148E 01
****************************************************************************************************

****************************************************************************************************

RUN    20

OBSERVED RESPONSES ON THE    1  ITERATIONS
                          0.835189E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS    0.835189E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  =====================================
                                                                  =====================================

VALUES OF X(1),...,X(K) ARE
                   0.100000E 02        0.100000E 02        0.000000E 00        0.156629E 02        0.103315E 02
****************************************************************************************************

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RUN    21

OBSERVED RESPONSES ON THE    1  ITERATIONS
                         -0.156035E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   -0.156035E 03

VALUES OF X(1),...,X(K) ARE
                   0.100000E 02        0.100000E 02        0.000000E 00        0.176629E 02        0.103315E 02
```

```
*************************************************************************************************************

FRACTIONAL FACTORIAL COMPLETED

DETERMINISTIC SIMULATION ASSUMED

ESTIMATED STANDARD ERROR OF AVERAGE OBSERVED RESPONSE=        0.000000E 00

ACTIVE FACTORS ARE
                    4  5

STEEPEST PATH-----B(0), B(I)S CORRESPONDING TO (CODED) ACTIVE FACTORS IN ORDER LISTED ABOVE

               -0.481165E 00

               -0.397767E 02        -0.397766E 02

PREDICTED RANGE RATIO=   0.988261E 00     LACK OF FIT RATIO=   0.999999E 06

PREDICTED RANGE SMALL AND LACK OF FIT LARGE

THUS, ENTER SECOND ORDER PHASE

*****************************************************

*****************************************************

SECOND ORDER DESIGN REQUIRED

*****************************************************

*****************************************************

THE NUMBER OF FACTORS CONSIDERED IN THIS PHASE IS    2
THESE ARE FACTORS   4  5

RUN AXIAL POINTS OF DESIGN

*************************************************************************************************************

RUN    22

OBSERVED RESPONSES ON THE    1  ITERATIONS
                       -0.228384E 00

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.228384E 00

VALUES OF X(1),....,X(K) ARE
                0.100000E 02        0.100000E 02        0.000000E 00        0.152487E 02        0.833148E 01

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RUN    23

OBSERVED RESPONSES ON THE    1  ITERATIONS
                       -0.112733E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.112733E 03
```

```
VALUES OF X(1),...,X(K) ARE
                 0.100000E 02        0.100000E 02        0.000000E 00        0.180771E 02        0.833148E 01

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RUN    24

OBSERVED RESPONSES ON THE    1  ITERATIONS
                             0.119771E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.119771E 03       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),...,X(K) ARE
                 0.100000F 02        0.100000E 02        0.000000E 00        0.166629E 02        0.550305E 01

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RUN    25

OBSERVED RESPONSES ON THE    1  ITERATIONS
                             0.726550E 01

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.72655CE 01

VALUES OF X(1),...,X(K) ARE
                 0.100000E 02        0.100000E 02        0.000000E 00        0.166629E 02        0.111599E 02

****************************************************************************************************************

SECOND ORDER DESIGN COMPLETED

ESTIMATED FIRST ORDER, MIXED, SECOND ORDER, AND CONSTANT COEFFICIENTS FOR CODED FACTORS (IN ORDER LISTED ABOVE) ARE

 -0.397765E 02 -0.397767E 02 -0.799999E 02 -0.199997E 02  0.399997E 02 -0.164810E 02

RIDGE TO BE CLIMBED

****************************************************************************************************************

RUN    26

OBSERVED RESPONSES ON THE    1  ITERATIONS
                             0.137926E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.137926E 03       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),...,X(K) ARE
                 0.100000E 02        0.100000E 02        0.000000E 00        0.170671E 02        0.559272E 01

****************************************************************************************************************

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```

```
RUN    27

OBSERVED RESPONSES ON THE    1  ITERATIONS
                           0.307896E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.307896E 03       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),...,X(K) ARE
              0.100000E 02       0.100000E 02       0.000000E 00       0.173916E 02       0.427101E 01

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RUN    28

OBSERVED RESPONSES ON THE    1  ITERATIONS
                           0.534756E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.534756E 03       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),...,X(K) ARE
              0.100000E 02       0.100000E 02       0.000000E 00       0.177086E 02       0.299157E 01

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RUN    29

OBSERVED RESPONSES ON THE    1  ITERATIONS
                           0.798434E 03

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.798434E 03       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),...,X(K) ARE
              0.100000E 02       0.100000E 02       0.000000E 00       0.180020E 02       0.181131E 01

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RUN    30

OBSERVED RESPONSES ON THE    1  ITERATIONS
                           0.110999E 04

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.110999E 04       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),...,X(K) ARE
              0.100000E 02       0.100000E 02       0.000000E 00       0.182922E 02       0.646051E 00
```

```
****************************************************************************************************************************

TERMINATE SEARCH

ALL AVAILABLE RUNS USED

TOTAL OF    30 RUNS, EACH AVERAGING OVER    1  ITERATIONS OF SIMULATION, YIELD
OPTIMUM OBSERVED RESPONSE=     0.110999E 04 FOR    30 TH RUN WITH VALUES OF X(1),...,X(K) EQUAL TO
                  0.100000E 02         0.100000E 02         0.000000E 00         0.182922E 02         0.646051E 00
```

2. Example No. 2

The second example uses the response surface

$$y = 100 - (X_1 - 1)^2 - (X_3 + 2)^2 - (X_4 - 10)^2 + \varepsilon$$

as a "simulation", where ε is a random error term generated from a Normal distribution with mean $\mu = 0$ and standard deviation $\sigma = 2$. This value of the standard deviation is equivalent to 20% of the true response at the starting point for the search.

Input data to the RSMC program version defined a maximum-seeking problem involving four controllable factors, subject to the following six constraints:

$$1.5 - 2X_1 + 3X_3 \geq 0 \text{ (Constraint No. 1)}$$

$$1.5 - X_1 + X_3 \geq 0 \text{ (Constraint No. 2)}$$

$$-7.0 + 5X_1 - X_3 \geq 0 \text{ (Constraint No. 3)}$$

$$7.0 - X_4 \geq 0 \text{ (Constraint No. 4)}$$

$$7.0 - X_3 \geq 0 \text{ (Constraint No. 5)}$$

$$X_4 \geq 0 \text{ (Constraint No. 6)}$$

The starting point for the search was given as

$$(X_1, X_2, X_3, X_4) = (5.0, 5.0, 5.0, 5.0)$$

with corresponding step sizes

$$(\Delta_1, \Delta_2, \Delta_3, \Delta_4) = (0.5, 0.5, 0.5, 0.5).$$

An upper limit of 30 simulation runs of two iterations each was specified, with all 30 runs to be made in one pass of the RSMC program.

It can be verified that the true maximum value on the response surface is 84.50 corresponding to the point

$$(1.50,\ X_2,\ 0.50,\ 7.00)$$

where X_2 may assume any value. This point lies at the intersection of the first, third, and fourth constraints listed above.

The RSMC output shows that the steepest ascent path resulting from the initial fractional factorial was followed until constraint No. 4 was encountered. At that time, the revised path direction was determined and then followed until constraints No. 1 and No. 2 were hit. The constrained path direction was again calculated and followed until constraint No. 3 was encountered. Because no further success was predicted in the path direction resulting from consideration of constraint No. 3, the search was terminated. The point identified as optimum by RSMC was

$$(1.51,\ 4.24,\ 0.53,\ 7.00)$$

which corresponded to an observed response of 84.60. Because of the presence of random error, the observed response at this point differs from the true response, which is 84.34.

The following pages exhibit the output produced by RSMC for this problem.

```
RSMC---AUTOMATED RESPONSE SURFACE METHODOLOGY FOR CONSTRAINED OPTIMUM-SEEKING
    4 FACTORS
    2 ITERATIONS PER SIMULATION RUN
   30 MAXIMUM NUMBER OF SIMULATION RUNS ALLOCATED
    6 NUMBER OF CONSTRAINTS
   30 SIMULATION RUNS TO BE USED ON THIS PASS

MAXIMUM RESPONSE DESIRED

    I   STARTING VALUE OF X(I)   VALUE OF DELTA CORRESPONDING TO X(I)
    1        0.500000E 01                       0.500000E 00
    2        0.500000E 01                       0.500000E 00
    3        0.500000E 01                       0.500000E 00
    4        0.500000E 01                       0.500000E 00

CONSTRAINT NO.  1     A( 0)=    0.150000E 01
                      A( 1)=   -0.200000E 01
                      A( 3)=    0.300000E 01

CONSTRAINT NO.  2     A( 0)=    0.150000E 01
                      A( 1)=   -0.100000E 01
                      A( 3)=    0.100000E 01

CONSTRAINT NO.  3     A( 0)=   -0.700000E 01
                      A( 1)=    0.500000E 01
                      A( 3)=   -0.100000E 01

CONSTRAINT NO.  4     A( 0)=    0.700000E 01
                      A( 4)=   -0.100000E 01

CONSTRAINT NO.  5     A( 0)=    0.700000E 01
                      A( 3)=   -0.100000E 01

CONSTRAINT NO.  6     A( 0)=    0.000000E 00
                      A( 4)=    0.100000E 01

ALL POINTS IN THE FRACTIONAL FACTORIAL SATISFY ALL CONSTRAINTS

**************************************************************************************************************

RUN      1

OBSERVED RESPONSES ON THE    2  ITERATIONS
                            0.972513E 01
                            0.950704E 01

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.961608E 01       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 ===================================
                                                                 ===================================

VALUES OF X(1),...,X(K) ARE
                 0.500000E 01        0.500000E 01        0.500000E 01        0.500000E 01

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RUN      2

OBSERVED RESPONSES ON THE    2  ITERATIONS
```

```
                   0.283256E 02
                   0.252176E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.267716E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 =====================================
                                                                 =====================================

VALUES OF X(1),...,X(K) ARE
            0.450000E 01       0.450000E 01       0.450000E 01       0.550000E 01

********************************************************************************************************

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RUN     3

OBSERVED RESPONSES ON THE    2  ITERATIONS
                   0.104118E 02
                   0.875852E 01

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.958515E 01

VALUES OF X(1),...,X(K) ARE
            0.550000E 01       0.450000E 01       0.450000E 01       0.450000E 01

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RUN     4

OBSERVED RESPONSES ON THE    2  ITERATIONS
                   0.125343E 02
                   0.121218E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.123281E 02

VALUES OF X(1),...,X(K) ARE
            0.450000E 01       0.550000E 01       0.450000E 01       0.450000E 01

********************************************************************************************************

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RUN     5

OBSERVED RESPONSES ON THE    2  ITERATIONS
                   0.158140E 02
                   0.147446E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.152793E 02

VALUES OF X(1),...,X(K) ARE
            0.550000E 01       0.550000E 01       0.450000E 01       0.550000E 01

********************************************************************************************************

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RUN     6
```

```
OBSERVED RESPONSES ON THE    2  ITERATIONS
                              0.129421E 02
                              0.105097E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.117259E 02

VALUES OF X(1),....,X(K) ARE
                 0.450000E 01        0.450000E 01        0.550000E 01        0.550000E 01

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RUN     7

OBSERVED RESPONSES ON THE    2  ITERATIONS
                             -0.807004E 01
                             -0.450528E 01

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS  -0.628766E 01

VALUES OF X(1),....,X(K) ARE
                 0.550000E 01        0.450000E 01        0.550000E 01        0.450000E 01

****************************************************************************************************

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RUN     8

OBSERVED RESPONSES ON THE    2  ITERATIONS
                              0.385942E 01
                             -0.276987E 00

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.179121E 01

VALUES OF X(1),....,X(K) ARE
                 0.450000E 01        0.550000E 01        0.550000E 01        0.450000E 01

****************************************************************************************************

****************************************************************************************************

RUN     9

OBSERVED RESPONSES ON THE    2  ITERATIONS
                              0.463258E 01
                              0.491304E 01

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.477281E 01

VALUES OF X(1),....,X(K) ARE
                 0.550000E 01        0.550000E 01        0.550000E 01        0.550000E 01

****************************************************************************************************

FRACTIONAL FACTORIAL COMPLETED

ESTIMATE OF SIGMA OBTAINED FROM ITERATIONS
```

```
ESTIMATED STANDARD ERROR OF AVERAGE OBSERVED RESPONSE=        0.117340E 01

ACTIVE FACTORS ARE
                         1  2  3  4

STEEPEST PATH-----B(0), B(I)S CORRESPONDING TO (CODED) ACTIVE FACTORS IN ORDER LISTED ABOVE

                    0.950916E 01

                   -0.365838E 01       -0.952937E 00       -0.649523E 01        0.514160E 01

PREDICTED RANGE RATIO=   0.923808E 01    LACK OF FIT RATIO=   0.299255E 01

EXPLORE PATH

GOING TOWARD CONSTRAINT NO.    4

**************************************************************************************************************

RUN     10

OBSERVED RESPONSES ON THE    2  ITERATIONS
                                0.448025E 02
                                0.383093E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS    0.415559E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  ===================================
                                                                  ===================================

VALUES OF X(1),...,X(K) ARE
                    0.426073E 01        0.480743E 01        0.368747E 01        0.603899E 01

**************************************************************************************************************

GOING TOWARD CONSTRAINT NO.    4

**************************************************************************************************************

RUN     11

OBSERVED RESPONSES ON THE    2  ITERATIONS
                                0.537808E 02
                                0.568898E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS    0.553353E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  ===================================
                                                                  ===================================

VALUES OF X(1),...,X(K) ARE
                    0.390228E 01        0.471407E 01        0.305107E 01        0.654276E 01

**************************************************************************************************************

GOING TOWARD CONSTRAINT NO.    4

**************************************************************************************************************

RUN     12

OBSERVED RESPONSES ON THE    2  ITERATIONS
```

```
                          0.691874E 02
                          0.647158E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.669516E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  ==================================
                                                                  ==================================

VALUES OF X(1),....,X(K) ARE
                0.357695E 01       0.462932E 01       0.247346E 01       0.700000E 01

************************************************************************************************************

CONSTRAINT  4 HAS BEEN HIT

CONSTRAINTS REQUIRE ALTERED PATH, WHICH IS
               -0.365838E 01      -0.952937E 00      -0.649523E 01       0.000000E 00

GOING TOWARD CONSTRAINT NO.   2

************************************************************************************************************

RUN    13

OBSERVED RESPONSES ON THE    2  ITERATIONS
                          0.756847E 02
                          0.717662E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.737254E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  ==================================
                                                                  ==================================

VALUES OF X(1),....,X(K) ARE
                0.306561E 01       0.449613E 01       0.156561E 01       0.700000E 01

************************************************************************************************************

CONSTRAINT  2 HAS BEEN HIT

CONSTRAINT  1 HAS BEEN HIT

CONSTRAINTS REQUIRE ALTERED PATH, WHICH IS
               -0.585785E 01      -0.952937E 00      -0.390524E 01       0.000000E 00

GOING TOWARD CONSTRAINT NO.   3

************************************************************************************************************

RUN    14

OBSERVED RESPONSES ON THE    2  ITERATIONS
                          0.795124E 02
                          0.804720E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.799922E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                  ==================================
                                                                  ==================================

VALUES OF X(1),....,X(K) ARE
                0.212275E 01       0.434275E 01       0.937038E 00       0.700000E 01
```

```
****************************************************************************************************

GOING TOWARD CONSTRAINT NO.   3

****************************************************************************************************

RUN    15

OBSERVED RESPONSES ON THE    2  ITERATIONS
                          0.829841E 02
                          0.862135E 02

AVERAGE OBSERVED RESPONSE FOR THIS POINT IS   0.845988E 02       THIS IS THE OPTIMUM RESPONSE THUS FAR
                                                                 ===================================
                                                                 ===================================

VALUES OF X(1),....,X(K) ARE
                 0.150505E 01        0.424226E 01        0.525237E 00        0.700000E 01

****************************************************************************************************

CONSTRAINT  3 HAS BEEN HIT

TERMINATE SEARCH

NO FURTHER SUCCESS PREDICTED ON CONSTRAINED PATH


TOTAL OF    15 RUNS, EACH AVERAGING OVER    2  ITERATIONS OF SIMULATION, YIELD
OPTIMUM OBSERVED RESPONSE=     0.845988E 02 FOR    15 TH RUN WITH VALUES OF X(1),....,X(K) EQUAL TO
                 0.150505E 01        0.424226E 01        0.525237E 00        0.700000E 01
```

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