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Direct Search Optimization in Mathematical Modeling and a Watershed Model Application

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DIRECT SEARCH OPTIMIZATION IN MATHEMATICAL MODELING AND A WATERSHED MODEL APPLICATION

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ABSTRACT. The purpose of this report is to describe and demonstrate the application of Pattern Search, a direct search optimization technique, to mathematical modeling. Pattern Search is explained in three ways: geometrically, verbally, and mathematically. Examples are given to demonstrate the uses of this technique. Input/output data are provided that may be used to check the accuracy of a duplication of the computer program. (Appendix B). It is shown that Pattern Search is a powerful technique for the objective determination of optimal values for model coefficients. The technique is applied to a Watershed Model.

INTRODUCTION

There has been an increasing need for the objective determination of an optimal set of coefficients for conceptual models. Models may be described by a single equation or by interconnected equations; a watershed model is an example of a multi-equation model. The optimization technique to be described provides objectivity in parameterizing conceptual models.

In the application of an optimization procedure, it is necessary to specify the basis upon which the best set (optimal set) of coefficients is to be judged. This must be an index dependent on the values of the coefficients of the system under study. The index is referred to as the evaluation criterion and is generally minimized or maximized in the optimization procedure. In this study the index consists of only a single criterion of model performance. This does not imply that a combination of criteria is not possible.

Optimization techniques are usually divided into two methods: direct and indirect. Indirect methods involve mathematical manipulation of the objective function. First derivative equations with respect to each of the system coefficients are generated and set to zero. The solutions of these normal equations provide the optimum (optimal values for the coefficients) since the roots of the equations are also the location of the optimum. Because the indirect method determines the optimal coefficient values without examining any non-optimal solutions, indirect methods are very effective when they can be applied.

Direct methods start at an arbitrary point, as defined by the selected initial values for the coefficients, and proceed stepwise, sequentially examining trial values of the coefficients in an attempt to reach the optimum. At each stage of optimization there is successive improvement to the value of the evaluation criterion. The trial points are determined by a simple strategy that is usually based on the past changes to the coefficients.

Direct search techniques are especially useful where an analytic expression for the objective function is too complicated to be manipulated by the indirect method. Some advantages of direct search techniques:

a) they require no knowledge of the form of the system of equations being optimized, (this is especially important in the optimum parameterization of conceptual models, where it may be necessary to evaluate many inter-connected equations to obtain the desired coefficients).

b) they provide for objective parameterization.

c) they are well adapted for solution by digital computer.

A particular direct search technique, Pattern Search, which is a modified version of the original Pattern Search as developed by Hooke and Jeeves (1961) will be described. Pattern Search has an advantage over most other direct search techniques in that its structure is so simple.

PATTERN SEARCH: GEOMETRIC DESCRIPTION

In working with the Pattern Search technique it is helpful to first visualize a geometric picture of the process taking place. The Pattern Search technique attempts to establish a pattern of coefficient adjustments that will rapidly minimize (or maximize) the evaluation criterion.

If we consider a model with N coefficients to be optimized, then we are working with a N+1 dimensional problem (an N+1 hyperspace). The evaluation criterion defines the N+1 th dimension. Since it is impossible to visualize a problem with greater than three spatial dimensions, a three dimensional case is considered. Let coefficients 1 and 2, A(1), A(2), be represented on the x-y plane and the evaluation criterion, Z, in the z direction. It is, however, necessary to remember that we will be dealing with a very simple case. Therefore, we should not be too literal in the following interpretations for higher dimensional problems.

Combinations of A(1) and A(2) values define a criterion value Z. The set of Z values will define the response surface and this response surface may be pictured as a mountain range. The highest peak would be the global optimum value of the evaluation criterion for a maximization search, (the lowest valley point for a minimization search). The corresponding A(1) and A(2) values are the optimal values for coefficients 1 and 2 respectively. There may be several peaks, lower than the highest (separated by valleys), which are local optimums.

The Pattern Search technique attempts to define the pattern of coefficient adjustments that will follow the ridge that leads to the highest peak on the response surface. The response surface (mountains) can be climbed rapidly only if there is a consistent direction of a ridge to the peak. As shown in figure 1, the contour lines of equal criterion value indicate a consistent direction to the optimum for cases a and c, but not for case b.

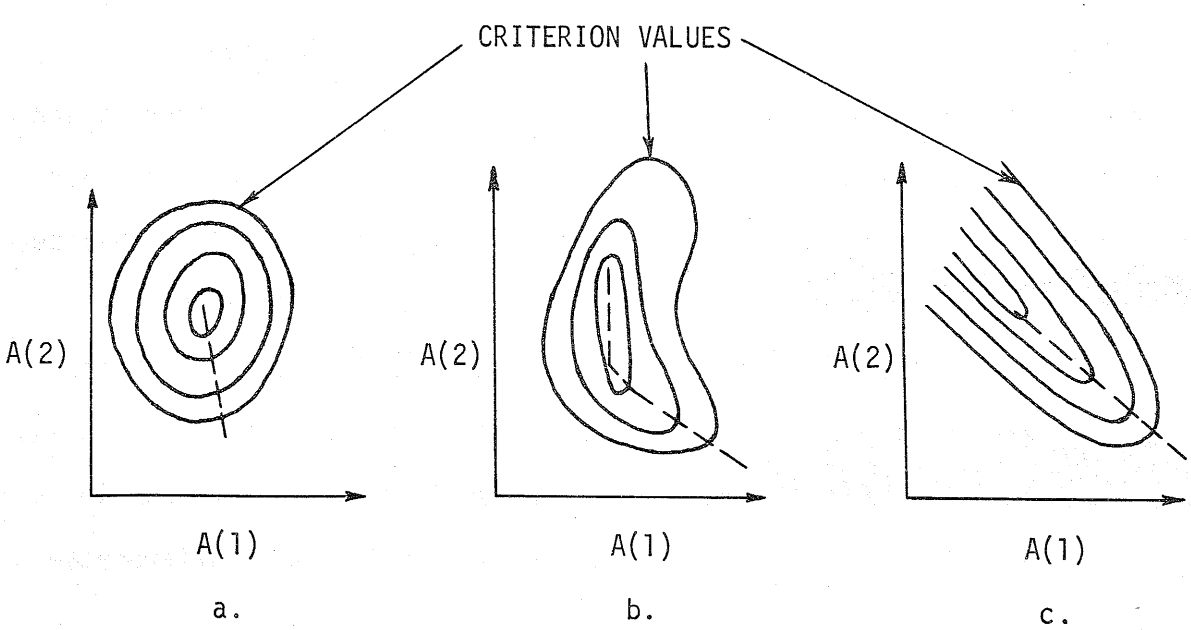

Figure 1.-- Contours of equal criterion value delineating that ridge which leads to the highest peak on a response surface

If there are several peaks, i.e. the response surface is not a unimodal function, then it is possible that the search technique will climb a "local" mountain and not the "global" mountain. The initial values assigned to the coefficients will, in general, determine which mountain is to be climbed.

However, to obtain reasonable certainty of global optimum values for the coefficients, it is necessary to perform a series of optimization studies with different initial values for the coefficients. The best evaluation criterion determines which coefficient combination would be selected.

PATTERN SEARCH: VERBAL DESCRIPTION

The process consists of starting with an initial set of coefficient values, A(I), where I = 1,2,......N, successively adjusting them and testing the results. There are two types of adjustments known as "Local Excursion" (LE) and "Pattern Move" (PM). Pattern move is the most distinguishing feature of this technique, and it is this feature that contrasts the technique with a pure trial-and-error search.

The differences between the two types of adjustments, LE and PM, are as follows. In a local excursion, the coefficient increment (delta), is a fixed quantity, or a percentage of the present coefficient value. An adjustment is made only if it improves the optimizing criterion. In a pattern move, the size of the adjustment applied to each coefficient is determined from the trend of its past local excursions and is, in general much larger than the local excursion delta. The resulting optimizing criterion is not used to accept or reject this move.

The optimizing evaluation criterion is arbitrary and the choice is left to the modeler. The choice may be the sum of the squares of the differences between the model output and the observed values; for example, for a watershed model it might be the sum of the squares of the errors in simulated and observed mean daily discharge values. For curve fitting, it might be the sum of the squares of the errors in observed and predicted data points. It may be the minimum value of the function itself. The criterion might also be absolute differences, logarithmic differences, maximum errors, etc., between observed and predicted system outputs. In general, the "best fit" coefficients will depend on the modeler's choice of what will be the criterion.

Before starting the optimizing process, each coefficient has an initial value and a delta assigned to it. The initial value of these coefficients may be the result of a best fit guess or of a random choice routine. The delta value is arbitrarily selected, but should be small compared to its corresponding coefficient value and the delta may differ for various coefficients.

The system (model) output and the criterion function are calculated with the system coefficients at their initial values. These calculations are performed in the "Main" computer program and examples are given in appendices C, D, and E. The calculated criterion value represents its "base" value.

The first step in optimization is a local excursion. The initial value of the first coefficient A(1) is increased by its delta. The Main Program is re-run with this change coefficient value and the original values for the remaining coefficients. If the evaluation criterion is now better than its base value, the first coefficient is held at its new value and the criterion base value reset to its improved value. If the criterion is not improved, the delta value is subtracted from the initial value and the program re-run. If this improves the criterion, the new value is held. The original value is retained if in both cases the optimizing evaluation criterion did not improve. The second coefficient, A(2), is then subjected to the same process and, for a dimensional problem greater than 3, the process would continue until all coefficients had been so treated. This would complete the local excursion.

An example is given in figure 2. In case 1, A(1) was first given a plus delta and the criterion did not improve. However, there was an improvement with a negative delta. Then A(2), plus its delta, improved the evaluation criterion value, corresponding to the adjusted A(1) coefficient and the original A(2) value. Since we have adjusted all coefficients and there was improvement to the criterion, the local excursion has been completed. This establishes the pattern for the pattern move, which is the next step.

In this move the magnitude of the increment applied to the first coefficient is equal to:

$$\zeta^{i}(1) = \begin{bmatrix}\text{present value of} \\ \text{coefficient 1}\end{bmatrix} - \begin{bmatrix}\text{previous local excursion} \\ \text{value of coefficient 1}\end{bmatrix}$$

where:

$\zeta^{i}(1)$: the pattern increment applied to the first coefficient during the i th pattern move.

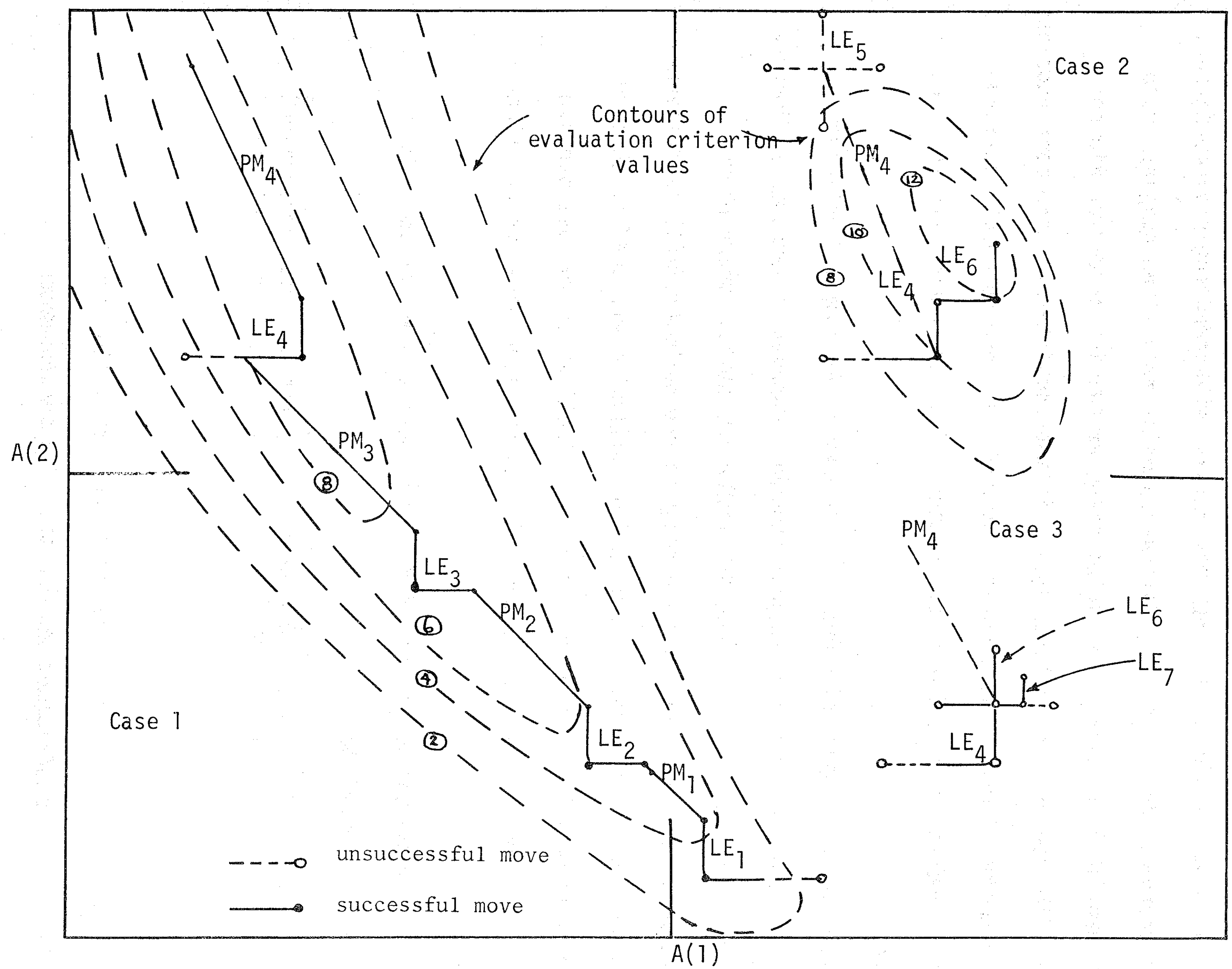

Figure 2.--Pattern Search moves resulting in delineation of ridges on response surfaces.

The pattern move adjustment for a given coefficient for any given pattern move can be calculated by the following equation:

$$\zeta^{i}(I) = N(I) * DELTA(I)$$

$$N(I) = n_1(I) - n_2(I)$$

where:

$n_1(I)$: the number of previous successful (+) local excursions for A(I)

$n_2(I)$: the number of previous successful (-) local excursions for A(I)

Pattern move adjustment values for coefficient A(1), for case 1, may be determined by use of table 1.

Table 1. -- Pattern move adjustment values for coefficient A(1) of case 1, figure 2

Pattern Move (i)	$n_1(1)$	$n_2(1)$	N(1)	$\zeta^{i}(1)$
1	0	1	-1	-1*DELTA(1)
2	0	2	-2	-2*DELTA(1)
3	0	3	-3	-3*DELTA(1)
4	1	3	-2	-2*DELTA(1)

The logic of the pattern move is the increasing size of the pattern move adjustment for each coefficient, as long as the local excursions of that coefficient have shown a persistence of direction. When this persistence ceases to exist, the pattern move adjustment reduces (for coefficient A(1), figure 2, case 1, PM_4), and eventually reverses direction.

The process, local excursions alternating with pattern moves, continues until there is deterioration of results. Three distinct situations are possible, with corresponding corrective measures, and they are as follows:

(a) the evaluation criterion value is poorer after, than before a pattern move and cannot be corrected by the subsequent local excursion. The indication is that the pattern move adjustments have become too large, (figure 2, case 2, PM_4). The large pattern moves precludes the fine adjustments that must be made to individual coefficients to provide the needed interrelationship among them. Since the old pattern cannot be continued, it is abandoned and we back track one cycle, adopting the values of the coefficients resulting from the last local excursion. The pattern move increments must then be reset to their original small values.

(b) the pattern move improves results, but the following local excursion does not. A resolution maneuver is in order. In a resolution maneuver the local excursion deltas are halved, which enables a more refined excursion to be made.

(c) a pattern has been abandoned (destroyed) and the following local excursion does not improve results. A resolution maneuver is made and the deltas are halved, (figure 2, case 3, LE_4).

When the deltas have been halved a preselected number of times the solution is considered complete. The length of computer time for the procedure may be controlled by specifiying the maximum number of local excursions that may be used.

PATTERN SEARCH: MATHEMATICAL DESCRIPTION

The following mathematical description refers to the cases presented in figure 2. Only mathematics for coefficient A(1) will be presented. Define:

$A^i(1)$: the value of coefficient 1 after the i th pattern move.

$BA^i(1)$: the value of coefficient 1 after the i th local excursion.

$B^i(1)$: the value of coefficient 1 after the i th local excursion

$LE._i$: the i th local excursion

$PM._i$: the i th pattern move

Case 1 (typical mathematics):

Initial: $A^0(1) = B^0(1)$

$BA^0(1) = A^0(1)$

$LE._1$: $BA^1(1) = A^0(1) - DELTA(1)$

$PM._1$: $A^1(1) = 2 * BA^1(1) - B^0(1)$

$A^1(1) = A^0(1) - 2 * DELTA(1)$

$B^1(1) = BA^1(1)$

$LE._2$: $BA^2(1) = A^1(1) - DELTA(1)$

$PM._2$: $A^2(1) = 2 * BA^2(1) - B^1(1)$

$A^2(1) = 2 * BA^2(1) - BA^1(1)$

$A^2(1) = 2 * \left[A^1(1) - DELTA(1)\right] - \left[A^0(1) - DELTA(1)\right]$

$A^2(1) = 2 * \left[A^0(1) - 3 * DELTA(1)\right] - \left[A^0(1) - DELTA(1)\right]$

$A^2(1) = A^0(1) - 5 * DELTA(1)$

or

$A^2(1) = A^1(1) - 3\ DELTA(1)$

$B^2(1) = BA^2(1)$

$LE._3$: $BA^3(1) = A^2(1) - DELTA(1)$

$PM._3$: $A^3(1) = 2 * BA^3(1) - B^2(1)$

$A^3(1) = 2 * BA^3(1) - BA^2(1)$

$A^3(1) = 2 * \left[A^2(1) - DELTA(1)\right] - \left[A^1(1) - DELTA(1)\right]$

since

$A^2(1) = A^0(1) - 5 * DELTA(1)$

$A^1(1) = A^0(1) - 2 * DELTA(1)$

then

$A^3(1) = A^0(1) - 9 * DELTA (1)$

or

$A^3(1) = A^2(1) - 4 * DELTA(1)$

$B^3(1) = BA^3(1)$

$LE._4$: $BA^4(1) = A^3(1) + DELTA(1)$

$PM._4$: $A^4(1) = 2 * BA^4(1) - B^3(1)$

$A^4(1) = 2 * BA^4(1) - BA^3(1)$

$A^4(1) = 2 * \left[A^3(1) + DELTA(1)\right] - \left[A^2(1) - DELTA(1)\right]$

since

$A^3(1) = A^0(1) - 9 * DELTA(1)$

$A^2(1) = A^0(1) - 5 * DELTA(1)$

then

$A^4(1) = A^0(1) - 10 * DELTA(1)$

or

$A^4(1) = A^3(1) - 1 * DELTA(1)$

$B^4(1) = BA^4(1)$

Case 2 (destroying a pattern):

LE.$_5$: $BA^5(1) = A^4(1)$

and

the value of the objective function was better prior to PM_4.

PM.$_5$: destroy pattern

$BA^5(1) = BA^4(1)$

$BA^5(1) = A^3(1) + DELTA(1)$

$B^5(1) = BA^5(1)$

Case 3 (halve delta-resolution):

LE_5 : $BA^5(1) = A^4(1)$

and

the value of the objective function was better prior to PM.$_4$.

PM.$_5$: destroy pattern

$BA^5(1) = BA^4(1)$

$BA^5(1) = A^3(1) + DELTA(1)$

$B^5(1) = BA^5(1)$

LE.$_6$: $BA^6(1) = BA^5(1)$

$BA^6(1) = A^3(1) + DELTA(1)$

[since there is no improvement to the objective function halve DELTA(1)]

LE.$_7$: $BA^6(1) = A^3(1) + DELTA(1)/2$

CONCLUDING REMARKS

Pattern Search is a powerful technique for objectively determining optimal values for model coefficients. However, we must realize some potential problems that might arise when using this direct search optimization technique.

Although the optimization time increases only with the first power of the number of coefficients being optimized, a large dimensional problem may take an excessive amount of computer time. When there is a large amount of interaction between system coefficients, as in most watershed models, optimization may proceed slowly because it is occasionally difficult to establish large pattern moves.

To be reasonably certain that global optimum values for the coefficients have been attained, we may need to perform a series of optimization studies with different initial values for the coefficients.

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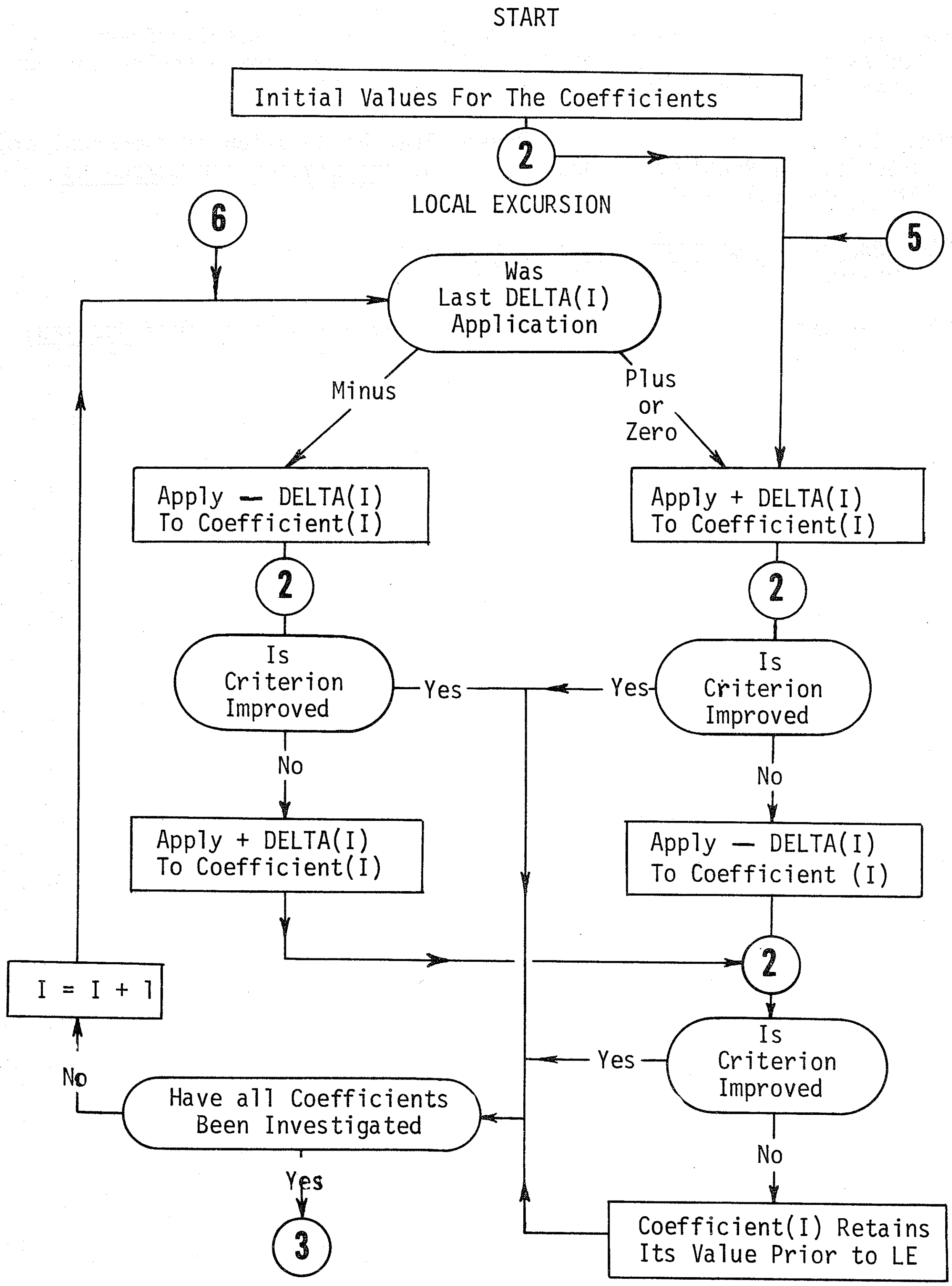
APPENDIX A

FLOW CHART



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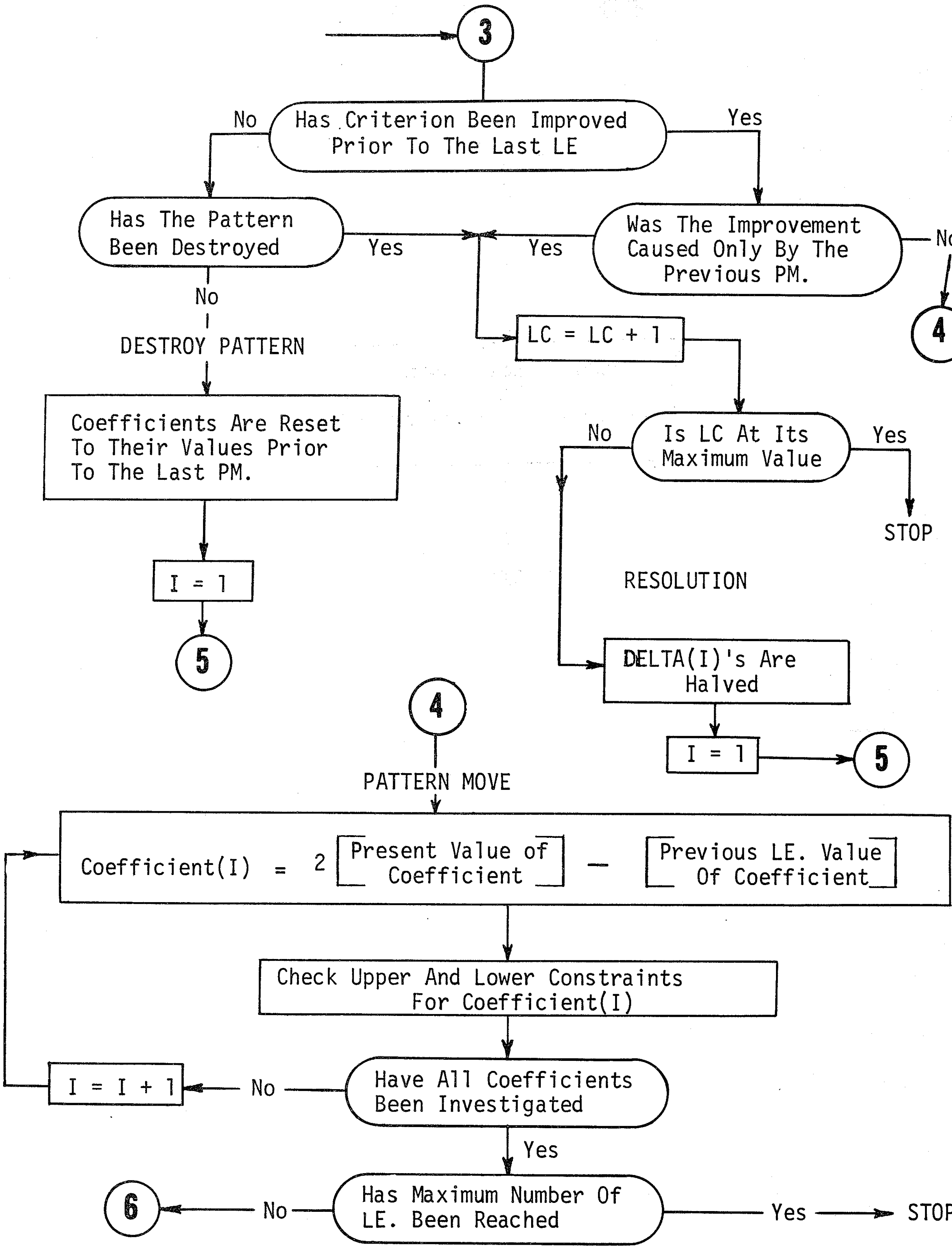

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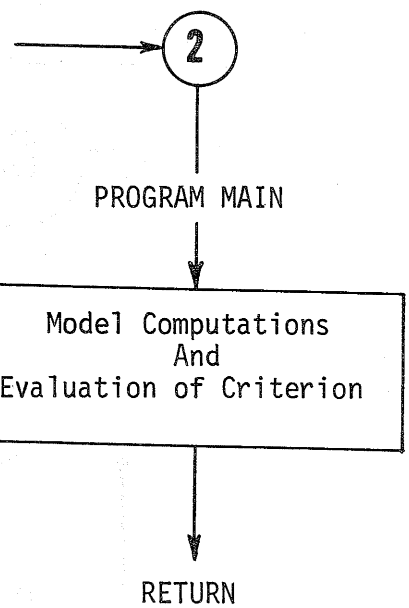


APPENDIX B

PROGRAM LISTING

```
      SUBROUTINE OPT
C     ******************************************************************
C     ******************************************************************
C     PATTERN  SEARCH  WITH  MODIFICATIONS
C     ******************************************************************
C     DEFINITION  OF  PROGRAM  VARIABLES
C
C     NUMA= NUMBER OF A(I) COEFFICIENTS TO BE OPTIMIZED
C
C     A(I)= VALUE OF COFFICIENT I AFTER LAST PATTERN MOVE
C
C     B(I)= VALUE OF COEFFICIENT I AFTER PREVIOUS LOCAL EXCURSION
C
C     BA(I)= VALUE OF COEFFICIENT I AFTER PRESENT LOCAL EXCURSION
C
C     NPER= IF = 1 DDELTA(I) MUST BE IN PERCENT/100
C           IF = 0 DDELTA(I) MUST BE AN ABSOLUTE VALUE
C
C     DDELTA(I)= WHEN NPER=1  DELTA(I)=ABS(DDELTA(I)*A(I))
C                WHEN NPER=0  DELTA(I)=DDELTA(I)
C
C     DELTA(I)= INCREMENT ADDED OR SUBTRACTED TO A(I) DURING A LOCAL EXCURSION
C
C     CHECKL(I)= LOWER CONSTRAINT ON A(I)
C
C     CHECKH(I)= UPPER CONSTRAINT ON A(I)
C
C     OPTIM= VALUE OF THE OPTIMIZATION CRITERION
C
C     NN= NUMBER OF TIMES MAIN PROGRAM HAS CALLED OPT
C
C     NSIGN(I)=  NSIGN(I)=0  THEN + DELTA(I) APPLIED FIRST
C                NSIGN(I)=1  - DELTA(I) APPLIED FIRST
C
C     MAXN= MAXIMUM NUMBER OF TIMES MAIN PROGRAM MAY CALL OPT BEFORE
C                 OPTIMIZATION IS ABORTED
C
C     KC= MAXIMUM NUMBER OF TIMES DELTA(I) MAY BE HALVED BEFORE
C        OPTIMIZATION IS TERMINATED (MAXN OVER-RIDES KC)
C     ******************************************************************
C     ******************************************************************
C     THIS PROGRAM IN ITS PRESENT FORM IS FOR MINIMIZATION
C             TO CONVERT TO A MAXIMIZATION FORMAT
C       REPLACE                                WITH
C     IF(YS.GT.YY) GO TO 1008               IF(YS.LT.YY) GO TO 1008
C   8 IF(YX.GT.YS) GO TO 11               8 IF(YX.LT.YS) GO TO 11
C     IF(YS.GT.YY) GO TO 1007               IF(YS.LT.YY) GO TO 1007
C  16 IF(YX.GT.YS) GO TO 19              16 IF(YX.LT.YS) GO TO 19
C     ******************************************************************
C     ******************************************************************
      COMMON A(18),DDELTA(18),CHECKL(18),CHECKH(18)
      COMMON OPTIM,NUMA,NSTART,NPER,KC,MAXN
      DIMENSION DELTA(18),BA(18),B(18),NSIGN(18),LES(18)
      DIMENSION ICLOSEL(18),ICLOSEH(18)
```

```
      IF (NSTART.GT.0) GO TO 2
C     ******************************************************************
C     INITIALIZATION  ROUTINE
C     ******************************************************************
      DO 1 I=1,NUMA
      LES(I)=0
      BA(I)=A(I)
      B(I)=A(I)
      ICLOSEL(I)=0
      ICLOSEH(I)=0
      IF (NPER.GT.0) GO TO 100
      DELTA(I)=DDELTA(I)
      GO TO 101
  100 DELTA(I)=ABS(DDELTA(I)*A(I))
  101 CC=A(I)-1.01*DELTA(I)
      IF(CC.LE.CHECKL(I)) GO TO 3000
      CC=A(I)+1.01*DELTA(I)
      IF(CC.GE.CHECKH(I)) GO TO 3000
    1 CONTINUE
      PRINT 1000
 1000 FORMAT(1H1)
      LC=0
      IT=1
      IZY=0
      NN=0
      NCOUN=1
      ICOUN=0
      IFIRS=0
      LDELT=0
      NSTART=1
      NSAVE=0
      PRINT 3,(I,I=1,NUMA)
      PRINT 221
  221 FORMAT(21X*INITIAL VALUES OF THE COEFFICIENTS*)
C     ******************************************************************
    2 YS=OPTIM
      NN=NN+1
      IF(NN.GT.MAXN) GO TO 7000
      IF(IFIRS.EQ.1) GO TO 4
      YX=OPTIM
      YY=YX
      IFIRS=1
    4 PRINT 5,NCOUN,NN,YS,(A(I),I=1,NUMA)
    5 FORMAT(I6,I5,E10.3,18F6.3)
    3 FORMAT(* TRIAL  RUN CRITERION*18(3H A(,I2,1H)))
   44 IF(LES(IT).EQ.1) GO TO 14
      IF(IZY.GT.0) GO TO 8
      IF(YS.GT.YY) GO TO 1008
      NSAVE=1
      YX=YS
      YY=YS
 1008 PRINT 3,(I,I=1,NUMA)
    6 IZY=IZY+1
      IT=IZY
```

```
      IF(LES(IZY).EQ.1) GO TO 107
  108 LL=0
C     ******************************************************************
C     ******************************************************************
C     LOCAL  EXCURSION  ROUTINE
C     ******************************************************************
C     LOCAL  EXCURSION  WITH  +  DELTA(I)  FIRST
C     ******************************************************************
      A(IZY)=A(IZY)+DELTA(IZY)
      NSIGN(IZY)=0
      IF(ICLOSEH(IZY).EQ.0) GO TO 7
      LL=LL+1
      GO TO 88
    7 LL=LL+1
      GO TO 6000
    8 IF(YX.GT.YS) GO TO 11
   88 GO TO (9,10,12),LL
    9 A(IZY)=A(IZY)-2.0*DELTA(IZY)
      NSIGN(IZY)=1
      IF(ICLOSEL(IZY).EQ.1) GO TO 10
      GO TO 7
   10 A(IZY)=A(IZY)+DELTA(IZY)
      NSIGN(IZY)=0
      GO TO 12
   11 YX=YS
   12 IF(IZY.LT.NUMA) GO TO 6
      IT=1
      IZY=0
      IF(YY.EQ.YX) GO TO 25
      YY=YX
      GO TO 210
C     ******************************************************************
C     LOCAL  EXCURSION  WITH  -  DELTA(I)  FIRST
C     ******************************************************************
   14 IF(IZY.GT.0) GO TO 16
      IF(YS.GT.YY) GO TO 1007
      NSAVE=1
      YX=YS
      YY=YS
 1007 PRINT 3,(I,I=1,NUMA)
  106 IZY=IZY+1
      IT=IZY
      IF(LES(IZY).EQ.0) GO TO 108
  107 LL=0
      A(IZY)=A(IZY)-DELTA(IZY)
      NSIGN(IZY)=1
      IF(ICLOSEL(IZY).EQ.0) GO TO 15
      LL=LL+1
      GO TO 166
   15 LL=LL+1
      GO TO 6000
   16 IF(YX.GT.YS) GO TO 19
  166 GO TO(17,18,20),LL
   17 A(IZY)=A(IZY)+2.0*DELTA(IZY)
```

```
      NSIGN(IZY)=0
      IF(ICLOSEH(IZY).EQ.1) GO TO 18
      GO TO 15
   18 A(IZY)=A(IZY)-DELTA(IZY)
      NSIGN(IZY)=1
      GO TO 20
   19 YX=YS
   20 IF(IZY.LT.NUMA) GO TO 106
      IT=1
      IZY=0
      IF(YY.EQ.YX) GO TO 25
      YY=YX
C     ******************************************************************
  210 IF(NPER.EQ.0) GO TO 22
      DO 21 I=1,NUMA
      DELTA(I)=ABS(DDELTA(I)*A(I))
   21 CONTINUE
   22 LC=0
      NSAVE=0
      PRINT 5,NCOUN,NN,YY,(A(I),I=1,NUMA)
      PRINT 220
  220 FORMAT(21X*PATTERN  MOVE*)
      NCOUN=NCOUN+1
C     ******************************************************************
C     PATTERN  MOVE  ROUTINE
C     ******************************************************************
      DO 24 I=1,NUMA
      LES(I)=NSIGN(I)
      BA(I)=A(I)
      A(I)=2.0*A(I)-B(I)
C     ******************************************************************
C     CHECK  UPPER  AND  LOWER  CONSTRAINTS
C     ******************************************************************
      CC=A(I)-1.01*DELTA(I)
      CD=A(I)+1.01*DELTA(I)
      IF(CC.GT.CHECKL(I)) GO TO 103
      ICLOSEL(I)=1
      A(I)=BA(I)
      GO TO 104
  103 ICLOSEL(I)=0
  104 IF(CD.LT.CHECKH(I)) GO TO 105
      ICLOSEH(I)=1
      A(I)=BA(I)
      GO TO 23
  105 ICLOSEH(I)=0
   23 B(I)=BA(I)
   24 CONTINUE
      GO TO 6000
C     ******************************************************************
   25 LC=LC+1
C     ******************************************************************
C     DESTROY  PRESENT  PATTERN
C     ******************************************************************
      IF(LC-1)7000,26,28
```

```
   26 IF(NSAVE.EQ.1) GO TO 260
      DO 27 I=1,NUMA
      A(I)=BA(I)
   27 CONTINUE
      ICOUN=ICOUN+1
      GO TO 30
   28 IF(LDELT.GE.KC) GO TO 7000
C     ****************************************************************
C     HALVE  DELTA(I)  (RESOLUTION)
C     ****************************************************************
  260 NSAVE=0
      DO 29 I=1,NUMA
      DDELTA(I)=DDELTA(I)*0.5
      DELTA(I)=DELTA(I)*0.5
   29 CONTINUE
      LDELT=LDELT+1
   30 PRINT 31,ICOUN,LDELT
   31 FORMAT(20X,*PATTERN=*I4*   RESOLUTION=*I5)
      PRINT 5,NCOUN,NN,YY,(A(I),I=1,NUMA)
      GO TO 44
 6000 RETURN
 3000 PRINT 5000,I
 5000 FORMAT(1X*THE INITIAL VALUE FOR A(*I2*)IS TOO CLOSE TO ITS CONSTRA
     1INT CHECK ALL INITIAL VALUES, MAKE APPROPRIATE CORRECTIONS AND RE-
     2START*)
      PRINT 3,(I,I=1,NUMA)
      PRINT 5,NCOUN,NN,YS,(A(I),I=1,NUMA)
 7000 STOP
      END
```

APPENDIX C

MINIMIZATION OF A FUNCTION

Introduction

Direct optimization techniques can, in many cases, find the minimum of a function that, by other means, would be mathematically intractable. This will be demonstrated by a simple example. Since this example can be solved by the indirect method, it will merely be a demonstration of the technique. The example also provides input/output data that may be used to check the accuracy of a duplication of the computer program SUBROUTINE OPT.

The modified pattern search method was applied to the test function devised by Rosenbrock(1):

$$Y = 100 \left[A(2) - A(1)^2\right]^2 + \left[1 - A(1)^2\right]$$

Figure 3 shows the response surface. The response surface is analogous to a shallow-curved valley. The minimum is at A(1)=A(2)=1. The minimum may be found by the classical (indirect) method:

$$\frac{\partial y}{\partial A(1)} = 200 \left[A(2) - A^2(1)\right] \left[-2A(1)\right] -2 \left[1-A(1)\right] = 0$$

$$-200\ A(2)A(1) + 200\ A^3(1) + A(1) -1 = 0$$

$$\frac{\partial y}{\partial A(2)} = 200 \left[A(2) - A^2(1)\right] = 0$$

$$A(2) = A^2(1)$$

---

(1)Rosenbrock, H.H., "An Automatic Method for Finding the Greatest or Least Value of a Function," Computer Journal, Vol. 3, No. 3, October, 1960, 175-184.

therefore

$$-200\ A^3(1) + 200\ A^3(1) + A(1) - 1 = 0$$

$$A(1) = 1$$

then

$$A(2) = 1^2 = 1$$

It should be of interest to investigate the efficiency of optimization with pattern search on such a complicated response surface. The initial value for A(1) is -1.20 and for A(2), 1.00. Figure 4 shows the values of A(1) and A(2) after each pattern move.

Initially, the optimization procedure developed a pattern in a direction that could not lead to the optimimum as shown in Figure 4. The pattern then reduces in size and reverses direction. We observe the continued growth of the pattern moves from A(1) = -1, A(2) = 1, to the neighborhood of the origin. At this point the pattern is destroyed, and the technique then follows the response surface valley to the vicinity of the optimum. The computer output details the entire process. Optimization was arbitrarily aborted when the number of runs equaled 250.

Although the indirect method, for this case, is much more efficient than pattern search, pattern search is obviously superior to pure "trial and error." In an operational sense, the direct search technique would normally only be used when the indirect method cannot be applied.

Program Listing

```
      PROGRAM MAIN(INPUT,OUTPUT)
      COMMON A(18),DDELTA(18),CHECKL(18),CHECKH(18)
      COMMON OPTIM,NUMA,NSTART,NPER,KC,MAXN
      READ 1,NUMA,NPER,KC,MAXN
      READ 2,(A(I),I=1,NUMA)
      READ 2,(DDELTA(I),I=1,NUMA)
      READ 2,(CHECKL(I),I=1,NUMA)
      READ 2,(CHECKH(I),I=1,NUMA)
      NSTART=0
8000  Y=100.0*(A(2)-A(1)**2)**2+(1.0-A(1))**2
      OPTIM=Y
      CALL OPT
      GO TO 8000
    1 FORMAT(3I2,I5)
    2 FORMAT(10F6.4)
      END
```

Input Data Listing

I	A(I)	DDELTA(I)	CHECKL(I)	CHECKH(I)
1	-1.20	0.01	-9.00	10.00
2	1.00	0.01	-9.00	10.00

NUMA = 2

NPER = 0

KC = 10

MAXN = 250

Computer Output

```
TRIAL  RUN CRITERION A( 1) A( 2) A(
                  INITIAL VALUES OF THE COEFFICIENTS
   1     1  .242E+02-1.200 1.000
TRIAL  RUN CRITERION A( 1) A( 2) A(
   1     2  .221E+02-1.190 1.000
   1     3  .213E+02-1.190 1.010
   1     3  .213E+02-1.190 1.010
                  PATTERN  MOVE
   2     4  .186E+02-1.180 1.020
TRIAL  RUN CRITERION A( 1) A( 2) A(
   2     5  .169E+02-1.170 1.020
   2     6  .162E+02-1.170 1.030
   2     6  .162E+02-1.170 1.030
                  PATTERN  MOVE
   3     7  .120E+02-1.150 1.050
TRIAL  RUN CRITERION A( 1) A( 2) A(
   3     8  .108E+02-1.140 1.050
   3     9  .103E+02-1.140 1.060
   3     9  .103E+02-1.140 1.060
                  PATTERN  MOVE
   4    10  .647E+01-1.110 1.090
TRIAL  RUN CRITERION A( 1) A( 2) A(
   4    11  .585E+01-1.100 1.090
   4    12  .562E+01-1.100 1.100
   4    12  .562E+01-1.100 1.100
                  PATTERN  MOVE
   5    13  .427E+01-1.060 1.140
TRIAL  RUN CRITERION A( 1) A( 2) A(
   5    14  .434E+01-1.050 1.140
   5    15  .429E+01-1.070 1.140
   5    16  .431E+01-1.060 1.150
   5    17  .425E+01-1.060 1.130
   5    17  .425E+01-1.060 1.130
                  PATTERN  MOVE
   6    18  .551E+01-1.020 1.160
TRIAL  RUN CRITERION A( 1) A( 2) A(
   6    19  .600E+01-1.010 1.160
   6    20  .510E+01-1.030 1.160
   6    21  .528E+01-1.020 1.150
   6    22  .576E+01-1.020 1.170
                PATTERN=    1    RESOLUTION=     0
   6    22  .425E+01-1.060 1.130
TRIAL  RUN CRITERION A( 1) A( 2) A(
   6    23  .428E+01-1.050 1.130
   6    24  .431E+01-1.070 1.130
   6    25  .424E+01-1.060 1.120
   6    25  .424E+01-1.060 1.120
                  PATTERN  MOVE
   7    26  .426E+01-1.060 1.110
TRIAL  RUN CRITERION A( 1) A( 2) A(
   7    27  .421E+01-1.050 1.110
   7    28  .420E+01-1.050 1.100
   7    28  .420E+01-1.050 1.100
                  PATTERN  MOVE
   8    29  .416E+01-1.040 1.080
TRIAL  RUN CRITERION A( 1) A( 2) A(
   8    30  .416E+01-1.030 1.080
   8    31  .413E+01-1.030 1.070
   8    31  .413E+01-1.030 1.070
                  PATTERN  MOVE
   9    32  .408E+01-1.010 1.040

TRIAL  RUN CRITERION A( 1) A( 2) A(
   9    33  .416E+01-1.000 1.040
   9    34  .408E+01-1.020 1.040
   9    35  .405E+01-1.010 1.030
   9    35  .405E+01-1.010 1.030
                  PATTERN  MOVE
  10    36  .397E+01 -.990  .990
TRIAL  RUN CRITERION A( 1) A( 2) A(
  10    37  .401E+01 -.980  .990
  10    38  .401E+01-1.000  .990
  10    39  .396E+01 -.990  .980
  10    39  .396E+01 -.990  .980
                  PATTERN  MOVE
  11    40  .389E+01 -.970  .930
TRIAL  RUN CRITERION A( 1) A( 2) A(
  11    41  .385E+01 -.960  .930
  11    42  .384E+01 -.960  .920
  11    42  .384E+01 -.960  .920
                  PATTERN  MOVE
  12    43  .373E+01 -.930  .860
TRIAL  RUN CRITERION A( 1) A( 2) A(
  12    44  .370E+01 -.920  .860
  12    45  .369E+01 -.920  .850
  12    45  .369E+01 -.920  .850
                  PATTERN  MOVE
  13    46  .354E+01 -.880  .780
TRIAL  RUN CRITERION A( 1) A( 2) A(
  13    47  .355E+01 -.870  .780
  13    48  .359E+01 -.890  .780
  13    49  .354E+01 -.880  .770
  13    49  .354E+01 -.880  .770
                  PATTERN  MOVE
  14    50  .341E+01 -.840  .690
TRIAL  RUN CRITERION A( 1) A( 2) A(
  14    51  .335E+01 -.830  .690
  14    52  .336E+01 -.830  .680
  14    53  .336E+01 -.830  .700
  14    53  .335E+01 -.830  .690
                  PATTERN  MOVE
  15    54  .317E+01 -.780  .610
TRIAL  RUN CRITERION A( 1) A( 2) A(
  15    55  .316E+01 -.770  .610
  15    56  .314E+01 -.770  .600
  15    56  .314E+01 -.770  .600
                  PATTERN  MOVE
  16    57  .293E+01 -.710  .510
TRIAL  RUN CRITERION A( 1) A( 2) A(
  16    58  .293E+01 -.700  .510
  16    59  .297E+01 -.720  .510
  16    60  .293E+01 -.710  .500
  16    60  .293E+01 -.710  .500
                  PATTERN  MOVE
  17    61  .277E+01 -.650  .400
TRIAL  RUN CRITERION A( 1) A( 2) A(
  17    62  .270E+01 -.640  .400
  17    63  .273E+01 -.640  .390
  17    64  .269E+01 -.640  .410
  17    64  .269E+01 -.640  .410
                  PATTERN  MOVE
  18    65  .247E+01 -.570  .320
TRIAL  RUN CRITERION A( 1) A( 2) A(
  18    66  .244E+01 -.560  .320
  18    67  .246E+01 -.560  .330
  18    68  .243E+01 -.560  .310
  18    68  .243E+01 -.560  .310
                  PATTERN  MOVE
```

```
   19    69   .223E+01 -.480   .210
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   19    70   .217E+01 -.470   .210
   19    71   .220E+01 -.470   .200
   19    72   .216E+01 -.470   .220
   19    72   .216E+01 -.470   .220
                        PATTERN   MOVE
   20    73   .193E+01 -.380   .130
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   20    74   .188E+01 -.370   .130
   20    75   .188E+01 -.370   .140
   20    75   .188E+01 -.370   .140
                        PATTERN   MOVE
   21    76   .163E+01 -.270   .060
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   21    77   .159E+01 -.260   .060
   21    78   .159E+01 -.260   .070
   21    78   .159E+01 -.260   .070
                        PATTERN   MOVE
   22    79   .137E+01 -.150  -.000
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   22    80   .134E+01 -.140  -.000
   22    81   .131E+01 -.140   .010
   22    81   .131E+01 -.140   .010
                        PATTERN   MOVE
   23    82   .129E+01 -.020  -.050
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   23    83   .127E+01 -.010  -.050
   23    84   .118E+01 -.010  -.040
   23    84   .118E+01 -.010  -.040
                        PATTERN   MOVE
   24    85   .186E+01  .120  -.090
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   24    86   .190E+01  .130  -.090
   24    87   .183E+01  .110  -.090
   24    88   .167E+01  .120  -.080
   24    89   .208E+01  .120  -.100
                      PATTERN=    2    RESOLUTION=      0
   24    89   .118E+01 -.010  -.040
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   24    90   .116E+01  .000  -.040
   24    91   .109E+01  .000  -.030
   24    91   .109E+01  .000  -.030
                        PATTERN   MOVE
   25    92   .102E+01  .010  -.020
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   25    93   .100E+01  .020  -.020
   25    94   .971E+00  .020  -.010
   25    94   .971E+00  .020  -.010
                        PATTERN   MOVE
   26    95   .929E+00  .040   .010
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   26    96   .908E+00  .050   .010
   26    97   .933E+00  .050   .020
   26    98   .903E+00  .050  -.000
   26    98   .903E+00  .050  -.000
                        PATTERN   MOVE
   27    99   .848E+00  .080   .010
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   27   100   .828E+00  .090   .010
   27   101   .835E+00  .090  -.000
   27   102   .842E+00  .090   .020
   27   102   .828E+00  .090   .010
                        PATTERN   MOVE
   28   103   .758E+00  .130   .020
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
```

```
   28   104   .740E+00   .140   .020
   28   105   .749E+00   .140   .010
   28   106   .750E+00   .140   .030
   28   106   .740E+00   .140   .020
                        PATTERN   MOVE
   29   107   .660E+00   .190   .030
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   29   108   .650E+00   .200   .030
   29   109   .680E+00   .200   .020
   29   110   .640E+00   .200   .040
   29   110   .640E+00   .200   .040
                        PATTERN   MOVE
   30   111   .553E+00   .260   .060
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   30   112   .550E+00   .270   .060
   30   113   .534E+00   .270   .070
   30   113   .534E+00   .270   .070
                        PATTERN   MOVE
   31   114   .460E+00   .340   .100
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   31   115   .473E+00   .350   .100
   31   116   .457E+00   .330   .100
   31   117   .449E+00   .330   .110
   31   117   .449E+00   .330   .110
                        PATTERN   MOVE
   32   118   .373E+00   .390   .150
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   32   119   .388E+00   .380   .150
   32   120   .370E+00   .400   .150
   32   121   .360E+00   .400   .160
   32   121   .360E+00   .400   .160
                        PATTERN   MOVE
   33   122   .293E+00   .470   .210
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   33   123   .312E+00   .480   .210
   33   124   .292E+00   .460   .210
   33   125   .299E+00   .460   .220
   33   126   .305E+00   .460   .200
   33   126   .292E+00   .460   .210
                        PATTERN   MOVE
   34   127   .241E+00   .520   .260
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   34   128   .240E+00   .510   .260
   34   129   .250E+00   .510   .270
   34   130   .250E+00   .510   .250
   34   130   .240E+00   .510   .260
                        PATTERN   MOVE
   35   131   .195E+00   .560   .310
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   35   132   .208E+00   .550   .310
   35   133   .207E+00   .570   .310
   35   134   .198E+00   .560   .320
   35   135   .212E+00   .560   .300
                      PATTERN=    2    RESOLUTION=
   35   135   .195E+00   .560   .310
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   35   136   .198E+00   .555   .310
   35   137   .198E+00   .565   .310
   35   138   .194E+00   .560   .315
   35   138   .194E+00   .560   .315
                        PATTERN   MOVE
   36   139   .153E+00   .610   .370
TRIAL   RUN CRITERION A( 1)  A( 2)  A(
   36   140   .158E+00   .605   .370
   36   141   .155E+00   .615   .370
   36   142   .153E+00   .610   .375
```

Computer Output--Continued

```
   36  143  .157E+00  .610  .365
                    PATTERN=   2   RESOLUTION=    2
   36  143  .153E+00  .610  .370
TRIAL  RUN CRITERION A( 1) A( 2) A(
   36  144  .154E+00  .608  .370
   36  145  .153E+00  .613  .370
   36  146  .152E+00  .610  .372
   36  146  .152E+00  .610  .372
                     PATTERN  MOVE
   37  147  .119E+00  .660  .430
TRIAL  RUN CRITERION A( 1) A( 2) A(
   37  148  .118E+00  .658  .430
   37  149  .117E+00  .658  .432
   37  149  .117E+00  .658  .432
                     PATTERN  MOVE
   38  150  .891E-01  .705  .492
TRIAL  RUN CRITERION A( 1) A( 2) A(
   38  151  .886E-01  .703  .492
   38  152  .887E-01  .703  .495
   38  153  .897E-01  .703  .490
   38  153  .886E-01  .703  .492
                     PATTERN  MOVE
   39  154  .677E-01  .748  .552
TRIAL  RUN CRITERION A( 1) A( 2) A(
   39  155  .657E-01  .745  .552
   39  156  .650E-01  .745  .555
   39  156  .650E-01  .745  .555
                     PATTERN  MOVE
   40  157  .459E-01  .788  .617
TRIAL  RUN CRITERION A( 1) A( 2) A(
   40  158  .464E-01  .785  .617
   40  159  .485E-01  .790  .617
   40  160  .452E-01  .788  .620
   40  160  .452E-01  .788  .620
                     PATTERN  MOVE
   41  161  .304E-01  .830  .685
TRIAL  RUN CRITERION A( 1) A( 2) A(
   41  162  .298E-01  .828  .685
   41  163  .305E-01  .828  .687
   41  164  .303E-01  .828  .682
   41  164  .298E-01  .828  .685
                     PATTERN  MOVE
   42  165  .182E-01  .868  .750
TRIAL  RUN CRITERION A( 1) A( 2) A(
   42  166  .185E-01  .865  .750
   42  167  .217E-01  .870  .750
   42  168  .176E-01  .868  .752
   42  168  .176E-01  .868  .752
                     PATTERN  MOVE
   43  169  .982E-02  .908  .820
TRIAL  RUN CRITERION A( 1) A( 2) A(
   43  170  .912E-02  .905  .820
   43  171  .102E-01  .905  .822
   43  172  .926E-02  .905  .817
   43  172  .912E-02  .905  .820
                     PATTERN  MOVE
   44  173  .337E-02  .943  .887
TRIAL  RUN CRITERION A( 1) A( 2) A(
   44  174  .512E-02  .940  .887
   44  175  .608E-02  .945  .887
   44  176  .359E-02  .943  .890
   44  177  .440E-02  .943  .885
                    PATTERN=   2   RESOLUTION=    3
   44  177  .337E-02  .943  .887
TRIAL  RUN CRITERION A( 1) A( 2) A(
   44  178  .369E-02  .941  .887
```

```
   44  179  .417E-02  .944  .887
   44  180  .333E-02  .943  .889
   44  180  .333E-02  .943  .889
                     PATTERN  MOVE
   45  181  .124E-02  .980  .957
TRIAL  RUN CRITERION A( 1) A( 2) A(
   45  182  .472E-03  .979  .957
   45  183  .515E-03  .979  .959
   45  184  .741E-03  .979  .956
   45  184  .472E-03  .979  .957
                     PATTERN  MOVE
   46  185  .181E-02 1.015 1.026
TRIAL  RUN CRITERION A( 1) A( 2) A(
   46  186  .396E-03 1.014 1.026
   46  187  .193E-03 1.014 1.027
   46  187  .193E-03 1.014 1.027
                     PATTERN  MOVE
   47  188  .294E-02 1.049 1.097
TRIAL  RUN CRITERION A( 1) A( 2) A(
   47  189  .226E-02 1.048 1.097
   47  190  .500E-02 1.050 1.097
   47  191  .250E-02 1.049 1.099
   47  192  .369E-02 1.049 1.096
                    PATTERN=   3   RESOLUTION=    3
   47  192  .193E-03 1.014 1.027
TRIAL  RUN CRITERION A( 1) A( 2) A(
   47  193  .706E-03 1.013 1.027
   47  194  .968E-03 1.015 1.027
   47  195  .302E-03 1.014 1.029
   47  196  .396E-03 1.014 1.026
                    PATTERN=   3   RESOLUTION=    4
   47  196  .193E-03 1.014 1.027
TRIAL  RUN CRITERION A( 1) A( 2) A(
   47  197  .288E-03 1.013 1.027
   47  198  .419E-03 1.014 1.027
   47  199  .208E-03 1.014 1.028
   47  200  .255E-03 1.014 1.027
                    PATTERN=   3   RESOLUTION=    5
   47  200  .193E-03 1.014 1.027
TRIAL  RUN CRITERION A( 1) A( 2) A(
   47  201  .200E-03 1.013 1.027
   47  202  .265E-03 1.014 1.027
   47  203  .191E-03 1.014 1.028
   47  203  .191E-03 1.014 1.028
                     PATTERN  MOVE
   48  204  .208E-03 1.014 1.028
TRIAL  RUN CRITERION A( 1) A( 2) A(
   48  205  .295E-03 1.013 1.028
   48  206  .202E-03 1.014 1.028
   48  207  .245E-03 1.014 1.028
   48  208  .191E-03 1.014 1.028
                    PATTERN=   4   RESOLUTION=    5
   48  208  .191E-03 1.014 1.028
TRIAL  RUN CRITERION A( 1) A( 2) A(
   48  209  .238E-03 1.013 1.028
   48  210  .224E-03 1.014 1.028
   48  211  .208E-03 1.014 1.028
   48  212  .193E-03 1.014 1.027
                    PATTERN=   4   RESOLUTION=    6
   48  212  .191E-03 1.014 1.028
TRIAL  RUN CRITERION A( 1) A( 2) A(
   48  213  .204E-03 1.014 1.028
   48  214  .197E-03 1.014 1.028
   48  215  .197E-03 1.014 1.028
   48  216  .189E-03 1.014 1.028
   48  216  .189E-03 1.014 1.028
```

```
                    PATTERN  MOVE
   49   217   .193E-03 1.014 1.027
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   49   218   .186E-03 1.014 1.027
   49   219   .185E-03 1.014 1.027
   49   219   .185E-03 1.014 1.027
                    PATTERN  MOVE
   50   220   .181E-03 1.013 1.027
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   50   221   .185E-03 1.013 1.027
   50   222   .196E-03 1.014 1.027
   50   223   .184E-03 1.013 1.027
   50   224   .182E-03 1.013 1.027
                 PATTERN=   4    RESOLUTION=     7
   50   224   .181E-03 1.013 1.027
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   50   225   .180E-03 1.013 1.027
   50   226   .179E-03 1.013 1.027
   50   226   .179E-03 1.013 1.027
                    PATTERN  MOVE
   51   227   .174E-03 1.013 1.027
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   51   228   .179E-03 1.013 1.027
   51   229   .174E-03 1.013 1.027
   51   230   .173E-03 1.013 1.026
   51   230   .173E-03 1.013 1.026
                    PATTERN  MOVE
   52   231   .167E-03 1.013 1.026
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   52   232   .169E-03 1.013 1.026
   52   233   .169E-03 1.013 1.026
   52   234   .166E-03 1.013 1.026
   52   234   .166E-03 1.013 1.026
                    PATTERN  MOVE
   53   235   .161E-03 1.013 1.025
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   53   236   .159E-03 1.013 1.025
   53   237   .158E-03 1.013 1.025
   53   237   .158E-03 1.013 1.025
                    PATTERN  MOVE
   54   238   .150E-03 1.012 1.025
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   54   239   .151E-03 1.012 1.025
   54   240   .155E-03 1.012 1.025
   54   241   .151E-03 1.012 1.025
   54   242   .151E-03 1.012 1.025
                 PATTERN=   4    RESOLUTION=     8
   54   242   .150E-03 1.012 1.025
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   54   243   .150E-03 1.012 1.025
   54   244   .150E-03 1.012 1.025
   54   244   .150E-03 1.012 1.025
                    PATTERN  MOVE
   55   245   .142E-03 1.012 1.024
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   55   246   .143E-03 1.012 1.024
   55   247   .142E-03 1.012 1.024
   55   248   .141E-03 1.012 1.024
   55   248   .141E-03 1.012 1.024
                    PATTERN  MOVE
   56   249   .133E-03 1.012 1.023
TRIAL   RUN  CRITERION A( 1) A( 2) A(
   56   250   .134E-03 1.011 1.023
```

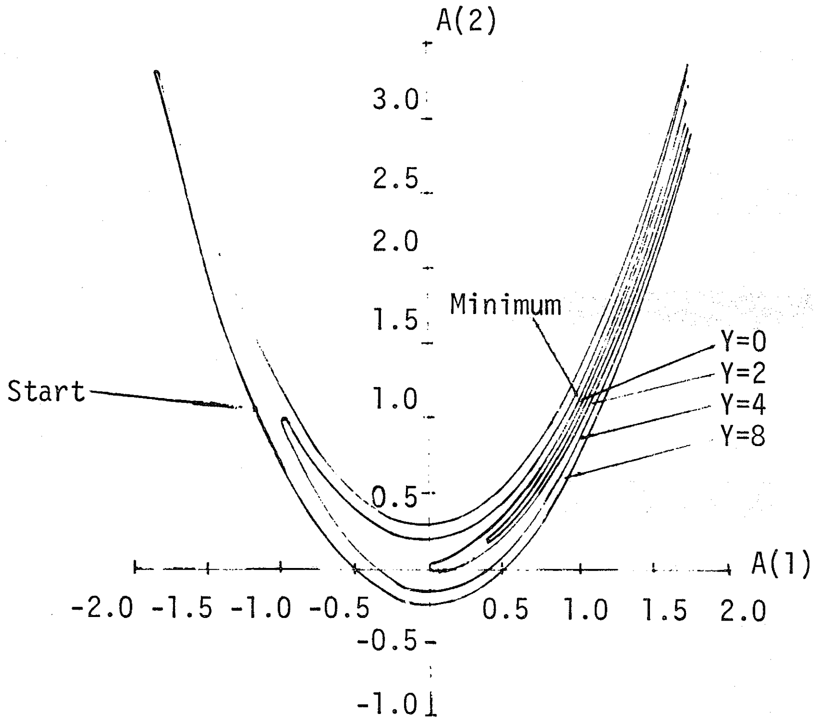


Figure 3.--Response surface resulting from application of the Pattern Search method to the test function of Rosenbrock (1960).

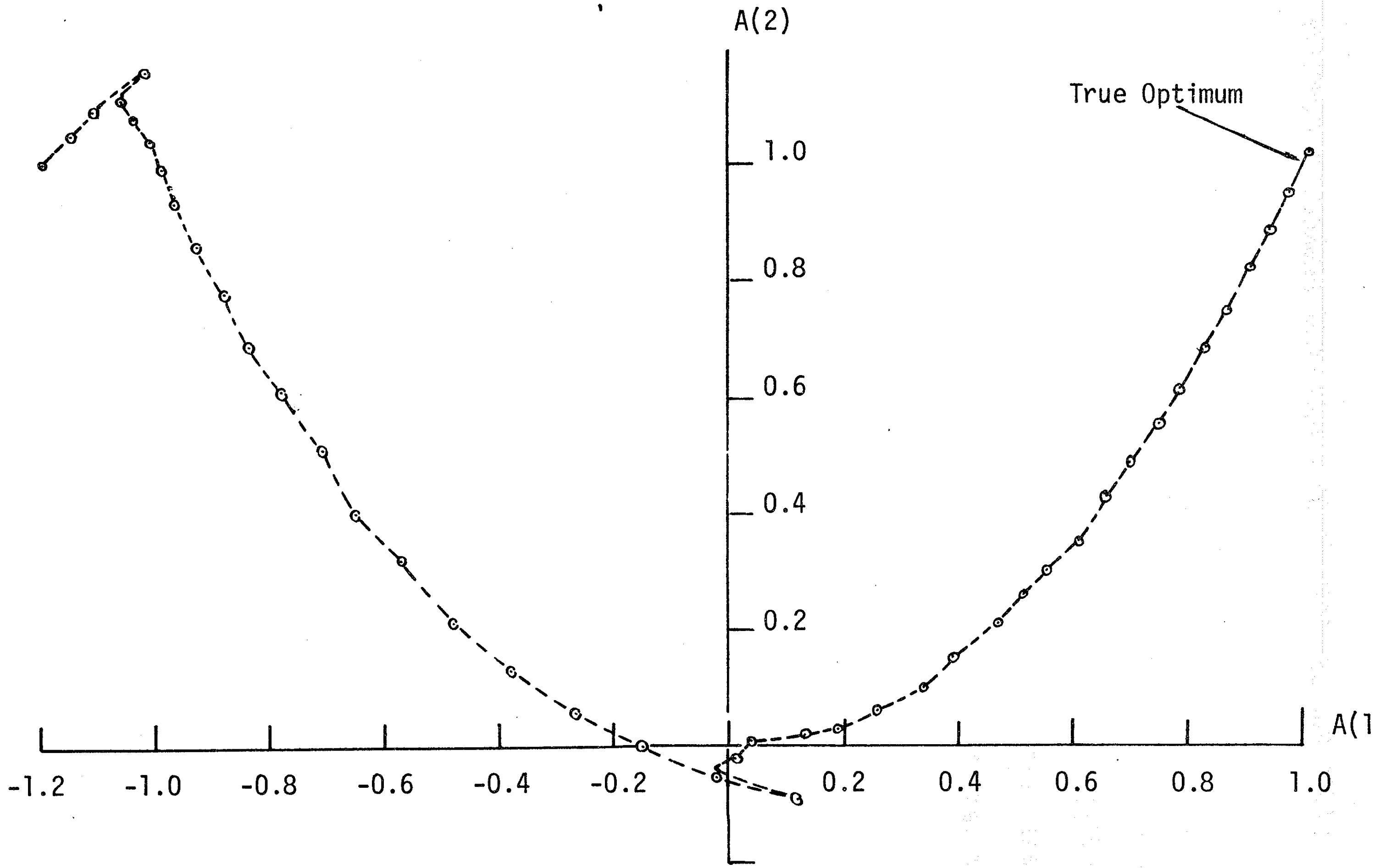


Figure 4.--Successive values of A(1) and A(2) after each Pattern Search move, for the test function of Rosenbrock (1960).

APPENDIX D

LEAST-SQUARES FITTING OF A NONLINEAR REGRESSION FUNCTION

Introduction

Statistical models play important roles in the fields of hydrology and meteorology. This appendix will not treat the mathematics involved, but will describe least-squares curve fitting which is often an important technique in regression and correlation studies.

As an example of a least-squares curve fitting, consider the following functional form that has been used in certain meteorological studies.

$$y_i = A*e^{-B*X_i^C}*COS(D*X_i)$$

where

y_i : smoothed spatial correlation function between the 200 mb. Caribbean zonal wind and the distance between observation stations during the summer months

X_i : distance, in kilometers, between observation stations.

A,B,C,D : parameters of the function.

N : number of data points.

The evaluation criterion will be the sum of the squares of the difference between observed (Y_i) and predicted (y_i) values of the dependent variable; $\sum_i^N (Y_i-y_i)^2$.

The corresponding quantities in the "Main Program" are:

A(1) = A

A(2) = B

A(3) = C

A(4) = D

Y_i = Y(1)

X_i = X(1)

The least-squares analysis, by pattern search, produced what appears to be a good fit, Figure 5. Although it appears that we could have done better, the goodness of fit is limited to the adequacy of the specified equational form. The computer output listing details the entire optimization. Least-squares, by the indirect approach of generating the normal equations, would prove to be mathematically intractable and thus, in this case, pattern search proved to be a useful approach. Optimization was aborted when the number of runs reached 300. At this point, the evaluation criterion was improving only slightly.

We checked to see if a simpler equation could fit the data as well or better than the transcendental function studied. By the indirect method, we fit the following 3rd degree polynomial and it produced slightly better results:

$$\sum (Y_i - y_i)^2 = 7.15 * 10^{-2}$$

$$Y_i = 1.0 + 1.177X_i + 0.297X_i^2 + 0.024X_i^3$$

Program Listing

```
      PROGRAM MAIN(INPUT,OUTPUT)
      COMMON A(18),DDELTA(18),CHECKL(18),CHECKH(18)
      COMMON OPTIM,NUMA,NSTART,NPER,KC,MAXN
      DIMENSION Y(50),X(50)
      READ 1,NUMA,NPER,KC,MAXN
      READ 2,(A(I),I=1,NUMA)
      READ 2,(DDELTA(I),I=1,NUMA)
      READ 2,(CHECKL(I),I=1,NUMA)
      READ 2,(CHECKH(I),I=1,NUMA)
      READ 3,M
      READ 4,(Y(I),X(I),I=1,M)
      NSTART=0
 8000 SUM=0.0
      DO 5 I=1,M
      F=(A(1)*EXP(-A(2)*X(I)**A(3)))*COS(A(4)*X(I))
      SDIF=(F-Y(I))**2
      SUM=SUM+SDIF
    5 CONTINUE
      OPTIM=SUM
      CALL OPT
      GO TO 8000
    1 FORMAT(3I2,I5)
    2 FORMAT(10F6.4)
    3 FORMAT(I3)
    4 FORMAT(2F10.5)
      END
```

Input Data Listing

I	A(I)	DDELTA(I)	CHECKL(I)	CHECKH(I)
1	1.0195	0.01	0.98	1.04
2	1.6391	0.01	-1.00	5.00
3	2.4531	0.01	-1.00	5.00
4	2.4063	0.01	-1.00	5.00

NUMA = 4
NPER = 0
KC = 10
MAXN = 300

I	Y(I)	X(I)	I	Y(I)	X(I)
1	0.760	0.250	10	-0.021	1.150
2	0.581	0.350	11	-0.052	1.250
3	0.434	0.450	12	0.105	1.350
4	0.451	0.550	13	-0.040	1.450
5	0.507	0.650	14	0.021	1.550
6	0.273	0.750	15	-0.023	1.650
7	0.308	0.850	16	-0.020	1.750
8	0.131	0.950	17	0.008	1.850
9	0.125	1.050	18	-0.022	1.950

Computer Output

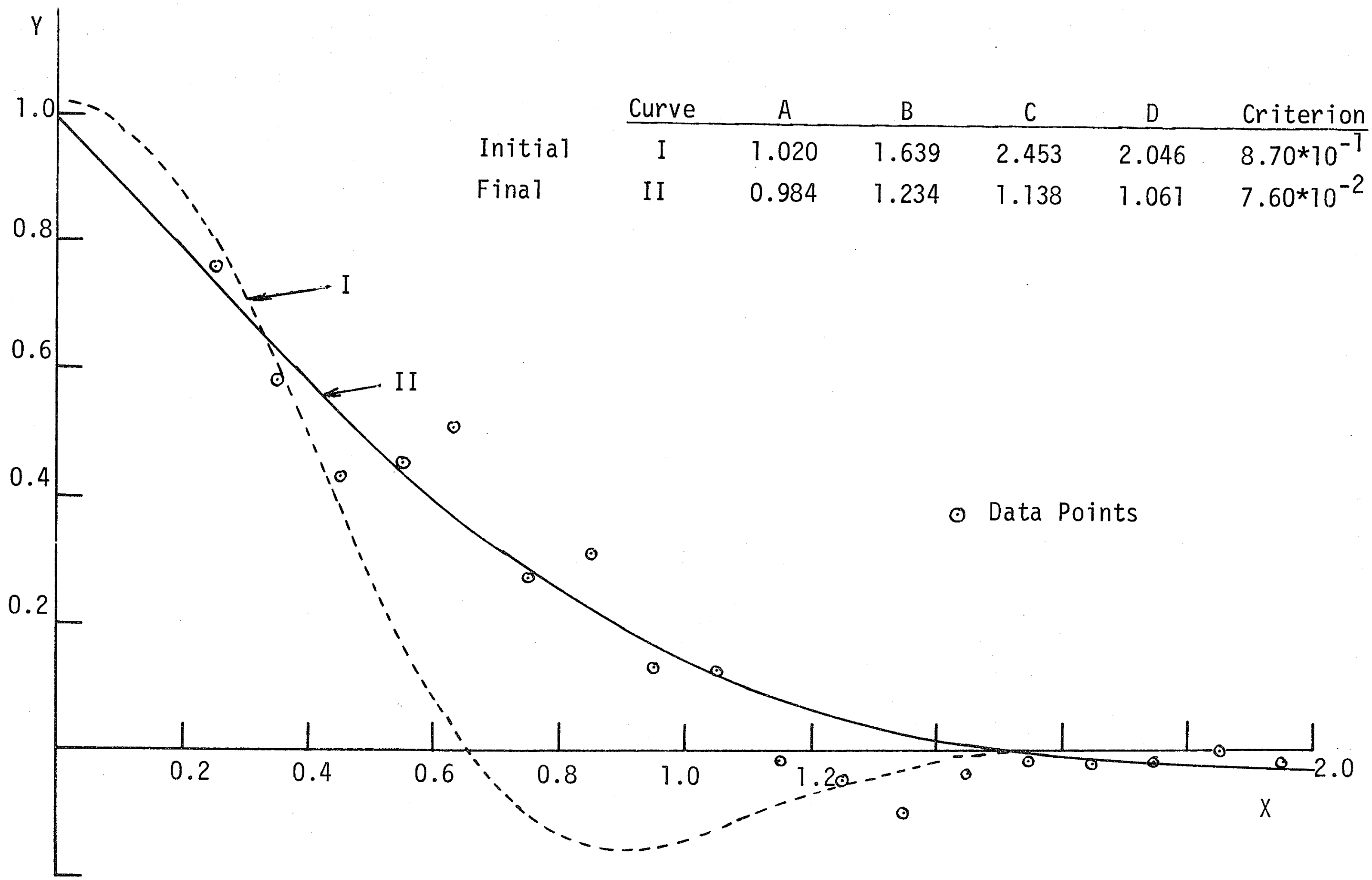
```
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
                 INITIAL VALUES OF THE COEFFICIENTS
    1     1   .870E+00 1.020 1.639 2.453 2.406
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    1     2   .873E+00 1.029 1.639 2.453 2.406
    1     3   .866E+00 1.009 1.639 2.453 2.406
    1     4   .864E+00 1.009 1.649 2.453 2.406
    1     5   .864E+00 1.009 1.649 2.463 2.406
    1     6   .863E+00 1.009 1.649 2.443 2.406
    1     7   .876E+00 1.009 1.649 2.443 2.416
    1     8   .851E+00 1.009 1.649 2.443 2.396
    1     8   .851E+00 1.009 1.649 2.443 2.396
                 PATTERN  MOVE
    2     9   .834E+00  .999 1.659 2.433 2.386
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    2    10   .831E+00  .989 1.659 2.433 2.386
    2    11   .828E+00  .989 1.669 2.433 2.386
    2    12   .828E+00  .989 1.669 2.423 2.386
    2    13   .828E+00  .989 1.669 2.443 2.386
    2    14   .817E+00  .989 1.669 2.443 2.376
    2    14   .817E+00  .989 1.669 2.443 2.376
                 PATTERN  MOVE
    3    15   .789E+00  .989 1.689 2.443 2.356
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    3    16   .791E+00  .999 1.689 2.443 2.356
    3    17   .786E+00  .989 1.699 2.443 2.356
    3    18   .786E+00  .989 1.699 2.453 2.356
    3    19   .775E+00  .989 1.699 2.453 2.346
    3    19   .775E+00  .989 1.699 2.453 2.346
                 PATTERN  MOVE
    4    20   .735E+00  .989 1.729 2.463 2.316
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    4    21   .737E+00  .999 1.729 2.463 2.316
    4    22   .733E+00  .989 1.739 2.463 2.316
    4    23   .733E+00  .989 1.739 2.473 2.316
    4    24   .723E+00  .989 1.739 2.473 2.306
    4    24   .723E+00  .989 1.739 2.473 2.306
                 PATTERN  MOVE
    5    25   .674E+00  .989 1.779 2.493 2.266
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    5    26   .676E+00  .999 1.779 2.493 2.266
    5    27   .673E+00  .989 1.789 2.493 2.266
    5    28   .672E+00  .989 1.789 2.503 2.266
    5    29   .662E+00  .989 1.789 2.503 2.256
    5    29   .662E+00  .989 1.789 2.503 2.256
                 PATTERN  MOVE
    6    30   .608E+00  .989 1.839 2.533 2.206
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    6    31   .609E+00  .999 1.839 2.533 2.206
    6    32   .607E+00  .989 1.849 2.533 2.206
    6    33   .606E+00  .989 1.849 2.543 2.206
    6    34   .597E+00  .989 1.849 2.543 2.196
    6    34   .597E+00  .989 1.849 2.543 2.196
                 PATTERN  MOVE
    7    35   .540E+00  .989 1.909 2.583 2.136
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    7    36   .541E+00  .999 1.909 2.583 2.136
    7    37   .539E+00  .989 1.919 2.583 2.136
    7    38   .539E+00  .989 1.919 2.593 2.136
    7    39   .531E+00  .989 1.919 2.593 2.126
    7    39   .531E+00  .989 1.919 2.593 2.126
                 PATTERN  MOVE
    8    40   .473E+00  .989 1.989 2.643 2.056
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    8    41   .474E+00  .999 1.989 2.643 2.056
    8    42   .473E+00  .989 1.999 2.643 2.056
    8    43   .473E+00  .989 1.999 2.653 2.056
    8    44   .466E+00  .989 1.999 2.653 2.046
    8    44   .466E+00  .989 1.999 2.653 2.046
                 PATTERN  MOVE
    9    45   .411E+00  .989 2.079 2.713 1.966
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
    9    46   .413E+00  .999 2.079 2.713 1.966
    9    47   .411E+00  .989 2.089 2.713 1.966
    9    48   .411E+00  .989 2.089 2.723 1.966
    9    49   .405E+00  .989 2.089 2.723 1.956
    9    49   .405E+00  .989 2.089 2.723 1.956
                 PATTERN  MOVE
   10    50   .357E+00  .989 2.179 2.793 1.866
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   10    51   .359E+00  .999 2.179 2.793 1.866
   10    52   .357E+00  .989 2.189 2.793 1.866
   10    53   .357E+00  .989 2.169 2.793 1.866
   10    54   .357E+00  .989 2.169 2.803 1.866
   10    55   .352E+00  .989 2.169 2.803 1.856
   10    55   .352E+00  .989 2.169 2.803 1.856
                 PATTERN  MOVE
   11    56   .311E+00  .989 2.249 2.883 1.756
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   11    57   .315E+00  .999 2.249 2.883 1.756
   11    58   .311E+00  .989 2.239 2.883 1.756
   11    59   .311E+00  .989 2.239 2.893 1.756
   11    60   .307E+00  .989 2.239 2.893 1.746
   11    60   .307E+00  .989 2.239 2.893 1.746
                 PATTERN  MOVE
   12    61   .277E+00  .989 2.309 2.983 1.636
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   12    62   .282E+00  .999 2.309 2.983 1.636
   12    63   .277E+00  .989 2.299 2.983 1.636
   12    64   .277E+00  .989 2.299 2.993 1.636
   12    65   .277E+00  .989 2.299 2.973 1.636
   12    66   .274E+00  .989 2.299 2.973 1.626
   12    66   .274E+00  .989 2.299 2.973 1.626
                 PATTERN  MOVE
   13    67   .255E+00  .989 2.359 3.053 1.506
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   13    68   .261E+00  .999 2.359 3.053 1.506
   13    69   .255E+00  .989 2.349 3.053 1.506
   13    70   .255E+00  .989 2.349 3.043 1.506
   13    71   .253E+00  .989 2.349 3.043 1.496
   13    71   .253E+00  .989 2.349 3.043 1.496
                 PATTERN  MOVE
   14    72   .247E+00  .989 2.399 3.113 1.366
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   14    73   .255E+00  .999 2.399 3.113 1.366
   14    74   .247E+00  .989 2.389 3.113 1.366
   14    75   .246E+00  .989 2.389 3.103 1.366
   14    76   .246E+00  .989 2.389 3.103 1.356
   14    76   .246E+00  .989 2.389 3.103 1.356
                 PATTERN  MOVE
   15    77   .252E+00  .989 2.429 3.163 1.216
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   15    78   .262E+00  .999 2.429 3.163 1.216
   15    79   .252E+00  .989 2.419 3.163 1.216
   15    80   .252E+00  .989 2.439 3.163 1.216
   15    81   .251E+00  .989 2.429 3.153 1.216
   15    82   .253E+00  .989 2.429 3.173 1.216
```

```
   15    83  .253E+00   .989 2.429 3.163 1.206
   15    84  .252E+00   .989 2.429 3.163 1.226
                  PATTERN=   1   RESOLUTION=      0
   15    84  .246E+00   .989 2.389 3.103 1.356
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   15    85  .254E+00   .999 2.389 3.103 1.356
   15    86  .246E+00   .989 2.379 3.103 1.356
   15    87  .245E+00   .989 2.379 3.093 1.356
   15    88  .245E+00   .989 2.379 3.093 1.346
   15    88  .245E+00   .989 2.379 3.093 1.346
                  PATTERN  MOVE
   16    89  .244E+00   .989 2.369 3.083 1.336
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   16    90  .252E+00   .999 2.369 3.083 1.336
   16    91  .243E+00   .989 2.359 3.083 1.336
   16    92  .243E+00   .989 2.359 3.083 1.336
   16    93  .243E+00   .989 2.359 3.073 1.326
   16    93  .243E+00   .989 2.359 3.073 1.326
                  PATTERN  MOVE
   17    94  .241E+00   .989 2.339 3.053 1.306
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   17    95  .249E+00   .999 2.339 3.053 1.306
   17    96  .240E+00   .989 2.329 3.053 1.306
   17    97  .240E+00   .989 2.329 3.043 1.306
   17    98  .240E+00   .989 2.329 3.043 1.296
   17    98  .240E+00   .989 2.329 3.043 1.296
                  PATTERN  MOVE
   18    99  .237E+00   .989 2.299 3.013 1.266
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   18   100  .246E+00   .999 2.299 3.013 1.266
   18   101  .237E+00   .989 2.289 3.013 1.266
   18   102  .236E+00   .989 2.289 3.003 1.266
   18   103  .236E+00   .989 2.289 3.003 1.256
   18   104  .236E+00   .989 2.289 3.003 1.276
   18   104  .236E+00   .989 2.289 3.003 1.276
                  PATTERN  MOVE
   19   105  .232E+00   .989 2.249 2.963 1.256
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   19   106  .241E+00   .999 2.249 2.963 1.256
   19   107  .232E+00   .989 2.239 2.963 1.256
   19   108  .232E+00   .989 2.239 2.953 1.256
   19   109  .231E+00   .989 2.239 2.953 1.266
   19   109  .231E+00   .989 2.239 2.953 1.266
                  PATTERN  MOVE
   20   110  .227E+00   .989 2.189 2.903 1.256
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   20   111  .236E+00   .999 2.189 2.903 1.256
   20   112  .227E+00   .989 2.179 2.903 1.256
   20   113  .226E+00   .989 2.179 2.893 1.256
   20   114  .226E+00   .989 2.179 2.893 1.266
   20   114  .226E+00   .989 2.179 2.893 1.266
                  PATTERN  MOVE
   21   115  .220E+00   .989 2.119 2.833 1.266
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   21   116  .229E+00   .999 2.119 2.833 1.266
   21   117  .220E+00   .989 2.109 2.833 1.266
   21   118  .219E+00   .989 2.109 2.823 1.266
   21   119  .219E+00   .989 2.109 2.823 1.276
   21   120  .219E+00   .989 2.109 2.823 1.256
   21   120  .219E+00   .989 2.109 2.823 1.256
                  PATTERN  MOVE
   22   121  .213E+00   .989 2.039 2.753 1.246
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   22   122  .221E+00   .999 2.039 2.753 1.246
   22   123  .213E+00   .989 2.029 2.753 1.246
   22   124  .212E+00   .989 2.029 2.743 1.246
   22   125  .212E+00   .989 2.029 2.743 1.236
   22   126  .212E+00   .989 2.029 2.743 1.256
   22   126  .212E+00   .989 2.029 2.743 1.246
                  PATTERN  MOVE
   23   127  .204E+00   .989 1.949 2.663 1.236
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   23   128  .212E+00   .999 1.949 2.663 1.236
   23   129  .204E+00   .989 1.939 2.663 1.236
   23   130  .203E+00   .989 1.939 2.653 1.236
   23   131  .203E+00   .989 1.939 2.653 1.226
   23   132  .203E+00   .989 1.939 2.653 1.246
   23   132  .203E+00   .989 1.939 2.653 1.236
                  PATTERN  MOVE
   24   133  .194E+00   .989 1.849 2.563 1.226
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   24   134  .203E+00   .999 1.849 2.563 1.226
   24   135  .194E+00   .989 1.839 2.563 1.226
   24   136  .194E+00   .989 1.859 2.563 1.226
   24   137  .193E+00   .989 1.859 2.553 1.226
   24   138  .193E+00   .989 1.859 2.553 1.216
   24   139  .193E+00   .989 1.859 2.553 1.236
   24   139  .193E+00   .989 1.859 2.553 1.226
                  PATTERN  MOVE
   25   140  .184E+00   .989 1.779 2.453 1.216
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   25   141  .192E+00   .999 1.779 2.453 1.216
   25   142  .184E+00   .989 1.789 2.453 1.216
   25   143  .183E+00   .989 1.789 2.443 1.216
   25   144  .183E+00   .989 1.789 2.443 1.206
   25   145  .183E+00   .989 1.789 2.443 1.226
   25   145  .183E+00   .989 1.789 2.443 1.216
                  PATTERN  MOVE
   26   146  .172E+00   .989 1.719 2.333 1.206
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   26   147  .179E+00   .999 1.719 2.333 1.206
   26   148  .172E+00   .989 1.729 2.333 1.206
   26   149  .171E+00   .989 1.729 2.323 1.206
   26   150  .171E+00   .989 1.729 2.323 1.196
   26   150  .171E+00   .989 1.729 2.323 1.196
                  PATTERN  MOVE
   27   151  .158E+00   .989 1.669 2.203 1.176
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   27   152  .165E+00   .999 1.669 2.203 1.176
   27   153  .158E+00   .989 1.679 2.203 1.176
   27   154  .157E+00   .989 1.679 2.193 1.176
   27   155  .157E+00   .989 1.679 2.193 1.166
   27   155  .157E+00   .989 1.679 2.193 1.166
                  PATTERN  MOVE
   28   156  .143E+00   .989 1.629 2.063 1.136
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   28   157  .149E+00   .999 1.629 2.063 1.136
   28   158  .143E+00   .989 1.639 2.063 1.136
   28   159  .142E+00   .989 1.639 2.053 1.136
   28   160  .142E+00   .989 1.639 2.053 1.126
   28   160  .142E+00   .989 1.639 2.053 1.126
                  PATTERN  MOVE
   29   161  .127E+00   .989 1.599 1.913 1.086
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   29   162  .132E+00   .999 1.599 1.913 1.086
   29   163  .127E+00   .989 1.609 1.913 1.086
   29   164  .126E+00   .989 1.609 1.903 1.086
   29   165  .126E+00   .989 1.609 1.903 1.076
   29   165  .126E+00   .989 1.609 1.903 1.076
                  PATTERN  MOVE
   30   166  .110E+00   .989 1.579 1.753 1.026
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
```

```
   30  167  .115E+00   .999 1.579 1.753 1.026
   30  168  .110E+00   .989 1.589 1.753 1.026
   30  169  .109E+00   .989 1.589 1.743 1.026
   30  170  .109E+00   .989 1.589 1.743 1.016
   30  171  .109E+00   .989 1.589 1.743 1.036
   30  171  .109E+00   .989 1.589 1.743 1.026
                    PATTERN  MOVE
   31  172  .947E-01   .989 1.569 1.583  .976
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   31  173  .975E-01   .999 1.569 1.583  .976
   31  174  .946E-01   .989 1.579 1.583  .976
   31  175  .938E-01   .989 1.579 1.573  .976
   31  176  .938E-01   .989 1.579 1.573  .966
   31  176  .938E-01   .989 1.579 1.573  .966
                    PATTERN  MOVE
   32  177  .843E-01   .989 1.569 1.403  .906
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   32  178  .855E-01   .999 1.569 1.403  .906
   32  179  .844E-01   .989 1.579 1.403  .906
   32  180  .843E-01   .989 1.559 1.403  .906
   32  181  .839E-01   .989 1.559 1.393  .906
   32  182  .840E-01   .989 1.559 1.393  .896
   32  183  .839E-01   .989 1.559 1.393  .916
   32  183  .839E-01   .989 1.559 1.393  .916
                    PATTERN  MOVE
   33  184  .844E-01   .989 1.539 1.213  .866
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   33  185  .838E-01   .999 1.539 1.213  .866
   33  186  .835E-01   .999 1.529 1.213  .866
   33  187  .838E-01   .999 1.529 1.203  .866
   33  188  .833E-01   .999 1.529 1.223  .866
   33  189  .831E-01   .999 1.529 1.223  .876
   33  189  .831E-01   .999 1.529 1.223  .876
                    PATTERN  MOVE
   34  190  .922E-01 1.009 1.499 1.053  .836
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   34  191  .909E-01 1.019 1.499 1.053  .836
   34  192  .939E-01   .999 1.499 1.053  .836
   34  193  .918E-01 1.009 1.489 1.053  .836
   34  194  .927E-01 1.009 1.509 1.053  .836
   34  195  .913E-01 1.009 1.499 1.063  .836
   34  196  .933E-01 1.009 1.499 1.043  .836
   34  197  .918E-01 1.009 1.499 1.053  .846
   34  198  .927E-01 1.009 1.499 1.053  .826
                  PATTERN=   2    RESOLUTION=      0
   34  198  .831E-01   .999 1.529 1.223  .876
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   34  199  .829E-01 1.009 1.529 1.223  .876
   34  200  .828E-01 1.009 1.519 1.223  .876
   34  201  .828E-01 1.009 1.519 1.233  .876
   34  202  .825E-01 1.009 1.519 1.233  .886
   34  202  .825E-01 1.009 1.519 1.233  .886
                    PATTERN  MOVE
   35  203  .828E-01 1.019 1.509 1.243  .896
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   35  204  .836E-01 1.029 1.509 1.243  .896
   35  205  .822E-01 1.009 1.509 1.243  .896
   35  206  .822E-01 1.009 1.499 1.243  .896
   35  207  .824E-01 1.009 1.499 1.253  .896
   35  208  .821E-01 1.009 1.499 1.233  .896
   35  209  .818E-01 1.009 1.499 1.233  .906
   35  209  .818E-01 1.009 1.499 1.233  .906
                    PATTERN  MOVE
   36  210  .812E-01 1.009 1.479 1.233  .926
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   36  211  .810E-01   .999 1.479 1.233  .926
```

```
   36  212  .809E-01   .999 1.469 1.233  .926
   36  213  .809E-01   .999 1.469 1.223  .926
   36  214  .809E-01   .999 1.469 1.243  .926
   36  215  .807E-01   .999 1.469 1.233  .936
   36  215  .807E-01   .999 1.469 1.233  .936
                    PATTERN  MOVE
   37  216  .798E-01   .999 1.439 1.233  .966
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   37  217  .801E-01 1.009 1.439 1.233  .966
   37  218  .796E-01   .999 1.429 1.233  .966
   37  219  .795E-01   .999 1.429 1.223  .966
   37  220  .795E-01   .999 1.429 1.223  .976
   37  220  .795E-01   .999 1.429 1.223  .976
                    PATTERN  MOVE
   38  221  .785E-01   .999 1.389 1.213 1.016
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   38  222  .786E-01   .989 1.389 1.213 1.016
   38  223  .787E-01 1.009 1.389 1.213 1.016
   38  224  .783E-01   .999 1.379 1.213 1.016
   38  225  .782E-01   .999 1.379 1.203 1.016
   38  226  .783E-01   .999 1.379 1.203 1.026
   38  227  .782E-01   .999 1.379 1.203 1.006
   38  227  .782E-01   .999 1.379 1.203 1.006
                    PATTERN  MOVE
   39  228  .773E-01   .999 1.329 1.183 1.036
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   39  229  .772E-01   .989 1.329 1.183 1.036
   39  230  .770E-01   .989 1.319 1.183 1.036
   39  231  .770E-01   .989 1.319 1.173 1.036
   39  232  .770E-01   .989 1.319 1.193 1.036
   39  233  .770E-01   .989 1.319 1.183 1.026
   39  234  .771E-01   .989 1.319 1.183 1.046
   39  234  .770E-01   .989 1.319 1.183 1.036
                    PATTERN  MOVE
   40  235  .764E-01   .989 1.259 1.163 1.066
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   40  236  .768E-01   .999 1.259 1.163 1.066
   40  237  .763E-01   .989 1.249 1.163 1.066
   40  238  .763E-01   .989 1.249 1.153 1.066
   40  239  .762E-01   .989 1.249 1.153 1.056
   40  239  .762E-01   .989 1.249 1.153 1.056
                    PATTERN  MOVE
   41  240  .769E-01   .989 1.179 1.123 1.076
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   41  241  .778E-01   .999 1.179 1.123 1.076
   41  242  .772E-01   .989 1.169 1.123 1.076
   41  243  .766E-01   .989 1.189 1.123 1.076
   41  244  .767E-01   .989 1.179 1.113 1.076
   41  245  .770E-01   .989 1.179 1.133 1.076
   41  246  .770E-01   .989 1.179 1.123 1.066
   41  247  .768E-01   .989 1.179 1.123 1.086
                  PATTERN=   3    RESOLUTION=      0
   41  247  .762E-01   .989 1.249 1.153 1.056
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   41  248  .768E-01   .999 1.249 1.153 1.056
   41  249  .763E-01   .989 1.239 1.153 1.056
   41  250  .762E-01   .989 1.259 1.153 1.056
   41  251  .762E-01   .989 1.249 1.143 1.056
   41  252  .763E-01   .989 1.249 1.143 1.046
   41  253  .762E-01   .989 1.249 1.143 1.066
   41  253  .762E-01   .989 1.249 1.143 1.056
                    PATTERN  MOVE
   42  254  .762E-01   .989 1.249 1.133 1.056
TRIAL  RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   42  255  .765E-01   .999 1.249 1.133 1.056
   42  256  .761E-01   .989 1.239 1.133 1.056
```

```
   42   257   .761E-01   .989 1.239 1.123 1.056
   42   258   .762E-01   .989 1.239 1.123 1.046
   42   259   .762E-01   .989 1.239 1.123 1.066
   42   259   .761E-01   .989 1.239 1.123 1.056
                      PATTERN  MOVE
   43   260   .762E-01   .989 1.229 1.103 1.056
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   43   261   .764E-01   .999 1.229 1.103 1.056
   43   262   .762E-01   .989 1.219 1.103 1.056
   43   263   .763E-01   .989 1.239 1.103 1.056
   43   264   .763E-01   .989 1.229 1.093 1.056
   43   265   .762E-01   .989 1.229 1.113 1.056
   43   266   .763E-01   .989 1.229 1.103 1.046
   43   267   .762E-01   .989 1.229 1.103 1.066
                    PATTERN=   4    RESOLUTION=      0
   43   267   .761E-01   .989 1.239 1.123 1.056
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   43   268   .765E-01   .999 1.239 1.123 1.056
   43   269   .762E-01   .989 1.229 1.123 1.056
   43   270   .762E-01   .989 1.249 1.123 1.056
   43   271   .762E-01   .989 1.239 1.113 1.056
   43   272   .761E-01   .989 1.239 1.133 1.056
   43   273   .762E-01   .989 1.239 1.123 1.046
   43   274   .762E-01   .989 1.239 1.123 1.066
                    PATTERN=   4    RESOLUTION=      1
   43   274   .761E-01   .989 1.239 1.123 1.056
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   43   275   .763E-01   .994 1.239 1.123 1.056
   43   276   .761E-01   .989 1.234 1.123 1.056
   43   277   .762E-01   .989 1.244 1.123 1.056
   43   278   .761E-01   .989 1.239 1.118 1.056
   43   279   .761E-01   .989 1.239 1.128 1.056
   43   280   .762E-01   .989 1.239 1.128 1.051
   43   281   .761E-01   .989 1.239 1.128 1.061
   43   281   .761E-01   .989 1.239 1.128 1.061
                      PATTERN  MOVE
   44   282   .762E-01   .989 1.239 1.133 1.066
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   44   283   .761E-01   .984 1.239 1.133 1.066
   44   284   .761E-01   .984 1.234 1.133 1.066
   44   285   .761E-01   .984 1.234 1.138 1.066
   44   286   .761E-01   .984 1.234 1.138 1.071
   44   287   .760E-01   .984 1.234 1.138 1.061
   44   287   .760E-01   .984 1.234 1.138 1.061
                      PATTERN  MOVE
   45   288   .761E-01   .984 1.229 1.148 1.061
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   45   289   .763E-01   .989 1.229 1.148 1.061
   45   290   .761E-01   .984 1.224 1.148 1.061
   45   291   .761E-01   .984 1.234 1.148 1.061
   45   292   .761E-01   .984 1.229 1.153 1.061
   45   293   .760E-01   .984 1.229 1.143 1.061
   45   294   .761E-01   .984 1.229 1.148 1.056
   45   295   .761E-01   .984 1.229 1.148 1.066
                    PATTERN=   5    RESOLUTION=      1
   45   295   .760E-01   .984 1.234 1.138 1.061
TRIAL   RUN CRITERION A( 1) A( 2) A( 3) A( 4) A(
   45   296   .762E-01   .989 1.234 1.138 1.061
   45   297   .760E-01   .984 1.229 1.138 1.061
   45   298   .760E-01   .984 1.229 1.143 1.061
   45   299   .760E-01   .984 1.229 1.133 1.061
   45   300   .760E-01   .984 1.229 1.133 1.056
```



	Curve	A	B	C	D	Criterion
Initial	I	1.020	1.639	2.453	2.046	$8.70*10^{-1}$
Final	II	0.984	1.234	1.138	1.061	$7.60*10^{-2}$

Figure 5.--Least-squares curve fitting using the Pattern Search method. Dashed curve: transcendental function using initial values of the coefficients. Solid curve: function using final values resulting from Pattern Search method.

APPENDIX E

OPTIMAL PARAMETERIZATION OF A WATERSHED MODEL

Introduction

The watershed model to be described is a modified version of the Stanford Watershed Model IV[1]. The major elements of the modified model are shown in figures 6 and 7. The detailed operations of the model will not be included. However, selected definitions are included, as needed, to present the coefficients being optimized.

Mean basin six-hour precipitation and daily potential evapotranspiration are the data inputs to the model. Water is stored in three distinct soil zones. The upper zone storage simulates the initial watershed response to rainfall and evapotranspiration takes place at the potential rate. The lower zone is the major storage zone and its level of storage determines infiltration rates and inflow to the groundwater storage. Evapotranspiration opportunity controls evapotranspiration rate from the lower zone storage.

The active groundwater storage supplies the base flow to the stream channel. Water passing from the lower zone must first fill the inactive groundwater zone before any water may enter the active zone.

[1] Crawford, N. H., (with Linsley, R. K.), "Digital Simulation in Hydrology: Stanford Watershed Model IV", Technical Paper Number 39, Civil Engineering Dept., Stanford University, July 1966.

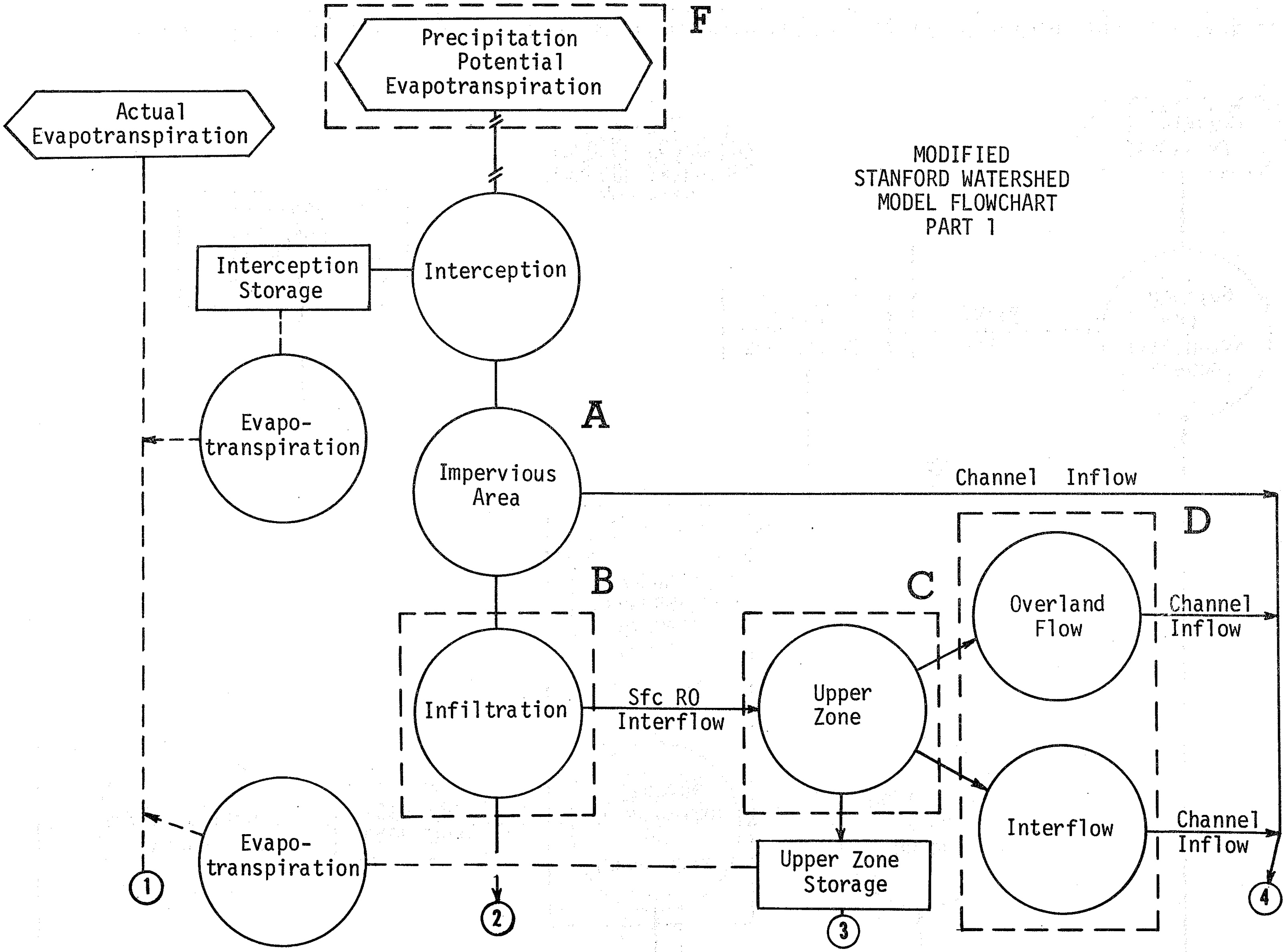


Figure 6.--Flow chart for the Modified Stanford Watershed Model IV (Crawford, 1966). Part 1.

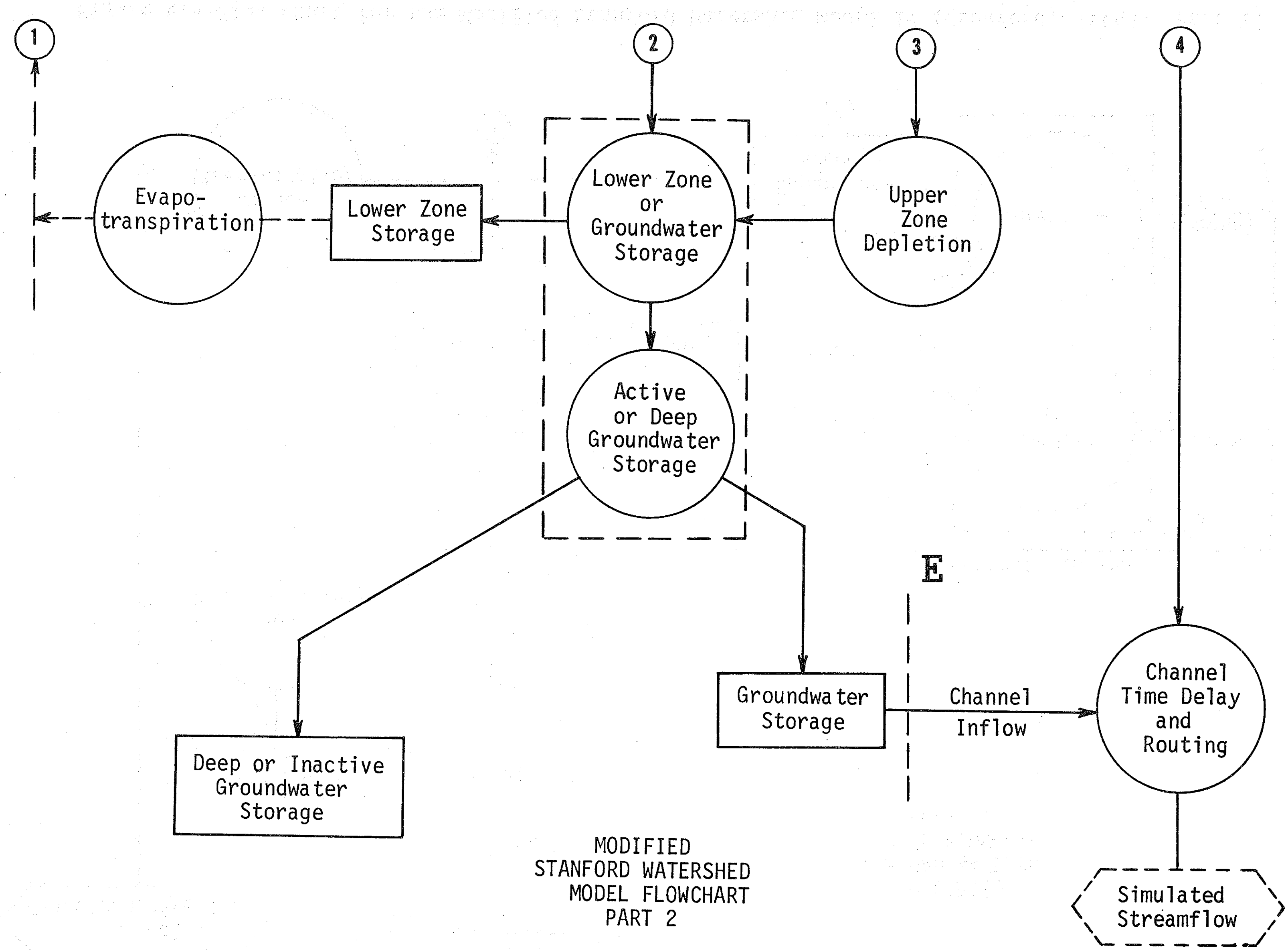


Figure 7.--Flow chart for the Modified Stanford Watershed Model IV (Crawford, 1966). Part 2.

Coefficient Optimization

Seventeen coefficients are subjected to the optimization routine. Six coefficients are used to reduce potential evapotranspiration to "actual" evapotranspiration. There is an upper and lower zone nominal storage value. Two coefficients define the shape of the infiltration curve. There are several routing coefficients. The following definitions give more detail on these coefficients (as a cross-reference the letters in figures 6 and 7 correspond to the model locations used below):

Model Location A

FIA: fraction of the watershed that produces runoff from impervious areas

Model Location B

FLZSN: lower zone nominal storage; an index of the storage limitation for the lower zone

CBI: six hour characteristic rate of infiltration; infiltration rate when the lower zone is at nominal storage

POW: defines the shape of the infiltration curve

Model Location C

UZSN: upper zone nominal storage; an index of the storage limitations for the upper zone

Model Location D

CC: defines the level of interflow relative to overland flow

FKSI: overland flow routing coefficient; percentage of calculated potential overland flow that reaches the channel in six hours

FLIRC: interflow routing coefficient; percentage of calculated interflow that reaches the channel in six hours

Model Location E

FLKK4: complement of the six hour fixed portion of the active groundwater storage recession factor

FKV: defines the magnitude of the variable portion of the active groundwater storage recession factor

FKGS: decay constant for the antecedent accretion to active groundwater storage

Model Location F

E(I): monthly percentage reductions applied to potential evapotranspiration for the months 2, 4, 6, 8, 10, and 12

Evaluation Criterion

The simulation time period is fifty (50) months. This includes four water years for which the evaluation criterion is computed and a two month buffer period prior to the first water year to be simulated. The buffer period allows the model's assumed initial moisture conditions (which are not involved in the optimization) to adjust to "actual" field conditions.

The objective function is the sum of the squared difference between simulated mean daily discharge and observed mean daily discharge. This type of evaluation criterion places more weight on matching peak flows rather than low streamflows. Therefore, the optimal parameterized watershed model will tend to simulate high flows better than the low flows. As mentioned before, the final coefficient values will depend in part on the choice of the type of optimizing criterion and the initial values of the coefficients.

The analysis for the Mad River Basin will be used as an example.

Results

The Mad River above Springfield, Ohio is situated in the west central portion of Ohio. Its basin is 485 square miles in area. This basin is located in a humid climate with an average annual precipitation of 36.9 inches and runoff of 13.2 inches.

The streamflow records are rated as good; however, the mean basin precipitation was computed from 3 recording gages and 4 non-recording gages which are located within or close to the watershed. Daily potential evapotranspiration values were calculated from observations of solar radiation, air temperature, dewpoint and wind at Indianapolis, Indiana.

The results of the optimization are shown in tables 2 and 3, and figure 8.

Table 2.-- The initial coefficient values and the final values obtained by pattern search optimization

Coefficient	Initial Value	Final Value
A(1)=FLZSN	12.000	3.928
A(2)=CBI	2.000	0.516
A(3)=POW	1.500	1.127
A(4)=CC	1.500	0.794
A(5)=UZSN	0.750	0.463
A(6)=FKV	1.250	1.457
A(7)=FIA	0.030	0.050
A(8)=FKGS	0.970	0.876
A(9)=FLIRC	0.100	0.030
A(10)=FKSI	0.750	0.857
A(11)=FLKK4	0.0025	0.0009
A(12)=E(10)	0.600	0.721
A(13)=E(12)	0.350	0.399
A(14)=E(2)	0.300	0.255
A(15)=E(4)	0.750	0.996
A(16)=E(6)	0.950	0.998
A(17)=E(8)	0.700	0.840

Evaluation Criterion

Initial	Final
$69.56*10^7$	$5.469*10^7$

Table 3. -- Statistical summary comparing the simulated and observed streamflow traces

Water Year	Mean Annual Flow (cfs)			Standard Error (cfs)		Correlation Coef.	
	ACT	Init/Final SIM	SIM	Initial	Final	Initial	Final
1956	444	383	399	394	207	.520	.893
1957*	405	507	446	540	168	.566	.967
1958*	674	808	662	615	242	.611	.950
1959*	620	608	633	983	177	.700	.993
1960*	323	396	324	186	129	.449	.783
1961	417	491	396	312	164	.742	.936
1962	405	441	436	400	408	.583	.558

* water years used for coefficient optimization

Summary

The modified Pattern Search optimization routine has been demonstrated to be a good objective watershed parameterization technique. The optimal coefficient values, however, are not to be intrepreted as unique, but rather, as a good set of values among many other possible sets.

Complex models, such as is the watershed model, require modest amounts of computer time. The watershed model takes approximately 1.7 seconds on the CDC 6600 computer to simulate the 50 months of test streamflow record. If one assumes that the average number of runs per optimization study is 500, then the total computation time will be less than fifteen (15) minutes. Thus, under most circumstances, direct search optimization applied to watershed parameterization should not require a prohibitive amount of computer time.

Schematic of the Main and Subroutine Programs

```
      PROGRAM MAIN(INPUT, OUTPUT)
      COMMONA(18),DDELTA(18),CHECKL(18),CHECKH(18)
      COMMON OPTIM,NUMA,NSTART,NPER,KC,MAXN

         (additional MAIN PROGRAM DIMENSION STATEMENTS)

      READ 1,NUMA,NPER,KC,MAXN
      READ 2,(A(I),I=1,NUMA)
      READ 2,(DDELTA(I),I=1,NUMA)
      READ 2,(CHECKL(I),I=1,NUMA)
      READ 2,(CHECKH(I),I=1,NUMA)

         (additional MAIN PROGRAM READ STATEMENTS)

 8000    (start watershed model calculations)

      OPTIM="evaluation criterion"
      CALL OPT
      GO TO 8000
    1 FORMAT(312,15)
    2 FORMAT(10F6.4)

         (additional MAIN PROGRAM FORMAT STATEMENTS)

      END
```

```
      SUBROUTINE OPT
```

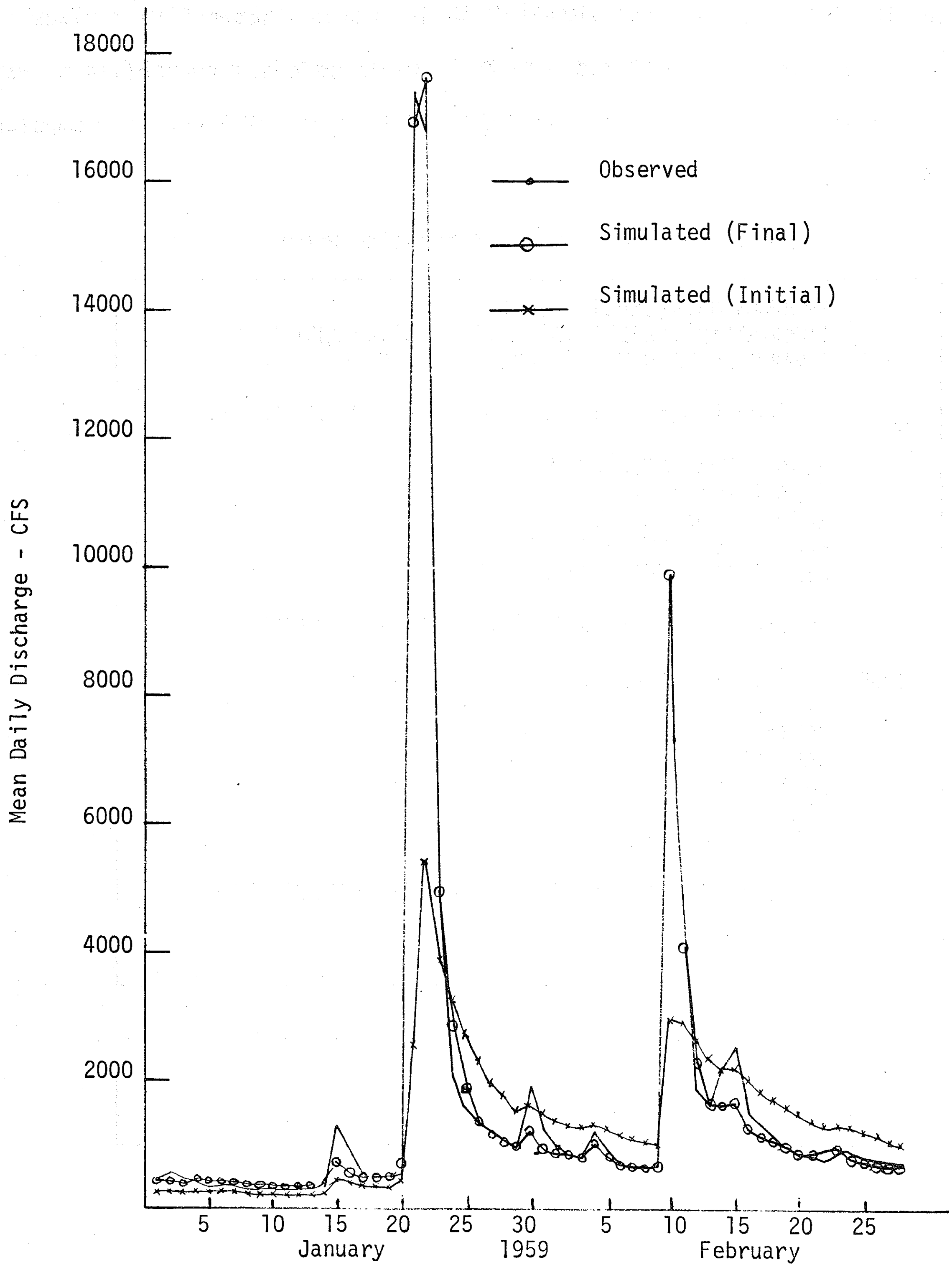


Figure 8.--Selected Portions of the observed streamflow trace for the Mad River Basin, Ohio, the simulated trace using initial coefficient values, and the simulated trace using final values optimized by Pattern Search method.