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Direct Search Optimization in Mathematical Modeling and a Watershed Model Application

JOHN C. MONRO

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TN 44 HYDRO 1 Infrared Radiation from Air to Underlying Surface. Vance A. Myers, May 1966. (PB-170 664)

ESSA Technical Memoranda

- WBTM HYDRO 2 Annotated Bibliography of ESSA Publications of Hydrometeorological Interest. J. L. H. Paulhus, February 1967. (Superseded by WBTM HYDRO 8)
- WBTM HYDRO 3 The Role of Persistence, Instability, and Moisture in the Intense Rainstorms in Eastern Colorado, June 14-17, 1965. F. K. Schwarz, February 1967. (PB-174 609)
- WBTM HYDRO 4 Elements of River Forecasting. Marshall M. Richards and Joseph A. Strahl, October 1967. (Superseded by WBTM HYDRO 9)
- WBTM HYDRO 5 Meteorological Estimation of Extreme Precipitation for Spillway Design Floods. Vance A. Myers, October 1967. (PB-177 687)
- WBTM HYDRO 6 Annotated Bibliography of ESSA Publications of Hydrometeorological Interest. J. L. H. Paulhus, November 1967. (Superseded by WBTM HYDRO 8)
- WBTM HYDRO 7 Meteorology of Major Storms in Western Colorado and Eastern Utah. Robert L. Weaver, January 1968. (PB-177 491)
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- WBTM HYDRO 9 Elements of River Forecasting (Revised). Marshall M. Richards and Joseph A. Strahl, March 1969. (PB-185 969)
- WBTM HYDRO 10 Flood Warning Benefit Evaluation - Susquehanna River Basin (Urban Residences). Harold J. Day, March 1970. (PB-190 984)
- WBTM HYDRO 11 Joint Probability Method of Tide Frequency Analysis Applied to Atlantic City and Long Beach Island, N.J. Vance A. Myers, April 1970. (PB-192 745)

DIRECT SEARCH OPTIMIZATION IN MATHEMATICAL MODELING
AND A WATERSHED MODEL APPLICATION

John C. Monro
National Weather Service

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.

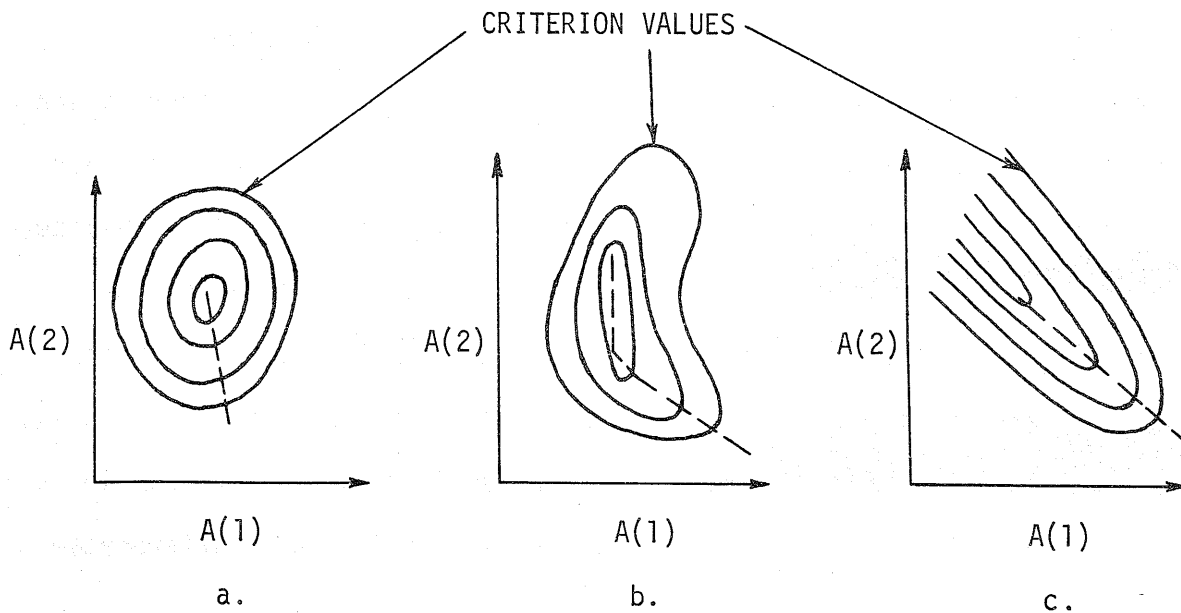


Figure 1.-- Contours of equal criterion value delineating that ridge which leads to the highest peak on a response surface

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 $I = 1, 2, \dots, N$, 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 (δ), 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 δ . 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:

$$\zeta^i(1) = \left[\begin{array}{l} \text{present value of} \\ \text{coefficient 1} \end{array} \right] - \left[\begin{array}{l} \text{previous local excursion} \\ \text{value of coefficient 1} \end{array} \right]$$

where:

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

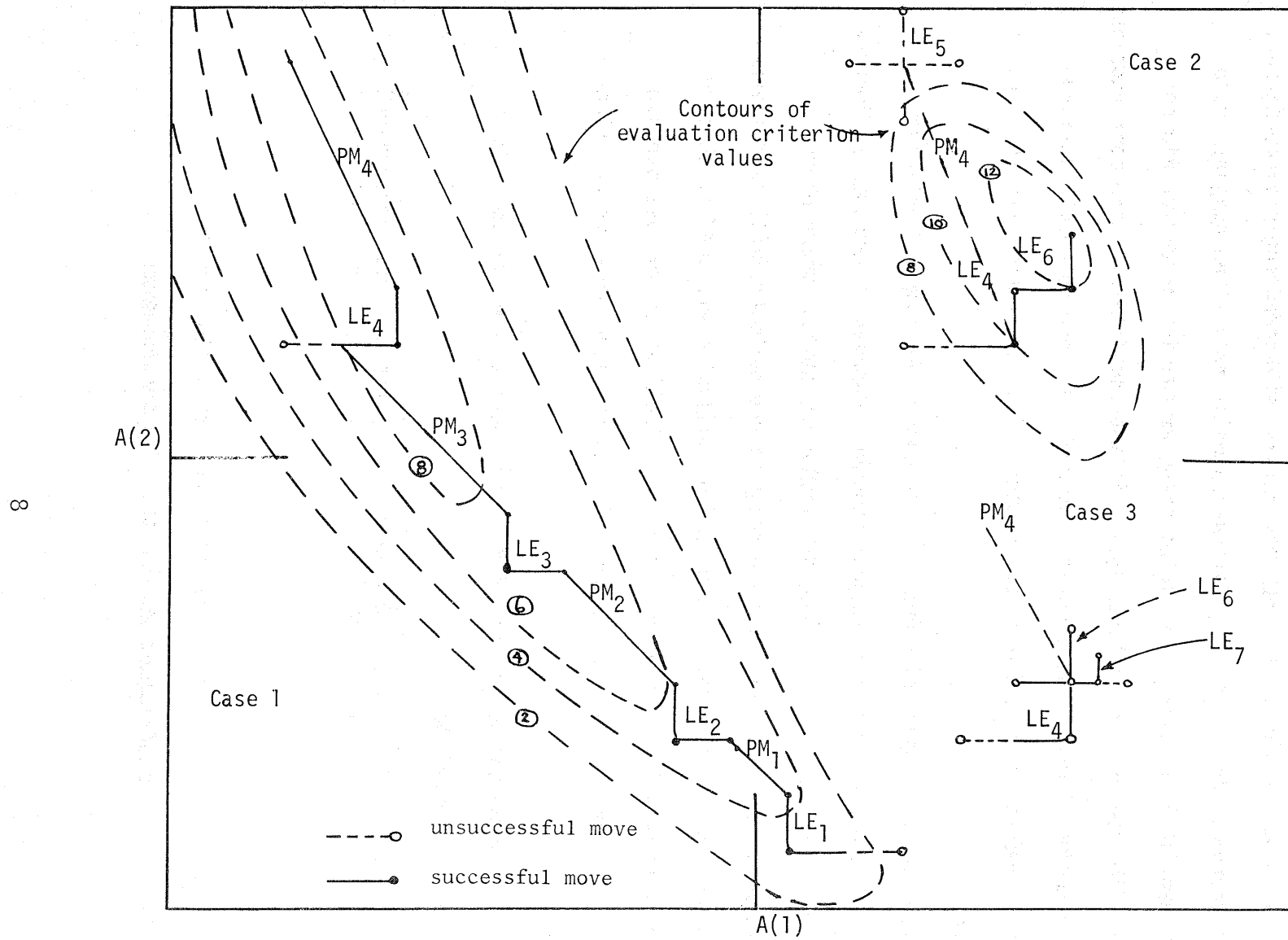


Figure 2.--Pattern Search moves resulting in delineation of ridges on response surfaces.

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, PM₄), 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 specifying 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):

$$\text{Initial: } A^0(1) = B^0(1)$$

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

$$LE._1 : BA^1(1) = A^0(1) - \text{DELTA}(1)$$

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

$$A^1(1) = A^0(1) - 2 * \text{DELTA}(1)$$

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

$$LE._2 : BA^2(1) = A^1(1) - \text{DELTA}(1)$$

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

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

$$A^2(1) = 2 * [A^1(1) - \text{DELTA}(1)] - [A^0(1) - \text{DELTA}(1)]$$

$$A^2(1) = 2 * [A^0(1) - 3 * \text{DELTA}(1)] - [A^0(1) - \text{DELTA}(1)]$$

$$A^2(1) = A^0(1) - 5 * \text{DELTA}(1)$$

or

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

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

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

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

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

$$A^3(1) = 2 * [A^2(1) - \text{DELTA}(1)] - [A^1(1) - \text{DELTA}(1)]$$

since

$$A^2(1) = A^0(1) - 5 * \text{DELTA}(1)$$

$$A^1(1) = A^0(1) - 2 * \text{DELTA}(1)$$

then

$$A^3(1) = A^0(1) - 9 * \text{DELTA}(1)$$

or

$$A^3(1) = A^2(1) - 4 * \text{DELTA}(1)$$

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

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

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

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

$$A^4(1) = 2 * [A^3(1) + \text{DELTA}(1)] - [A^2(1) - \text{DELTA}(1)]$$

since

$$A^3(1) = A^0(1) - 9 * \text{DELTA}(1)$$

$$A^2(1) = A^0(1) - 5 * \text{DELTA}(1)$$

then

$$A^4(1) = A^0(1) - 10 * \text{DELTA}(1)$$

or

$$A^4(1) = A^3(1) - 1 * \text{DELTA}(1)$$

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

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.

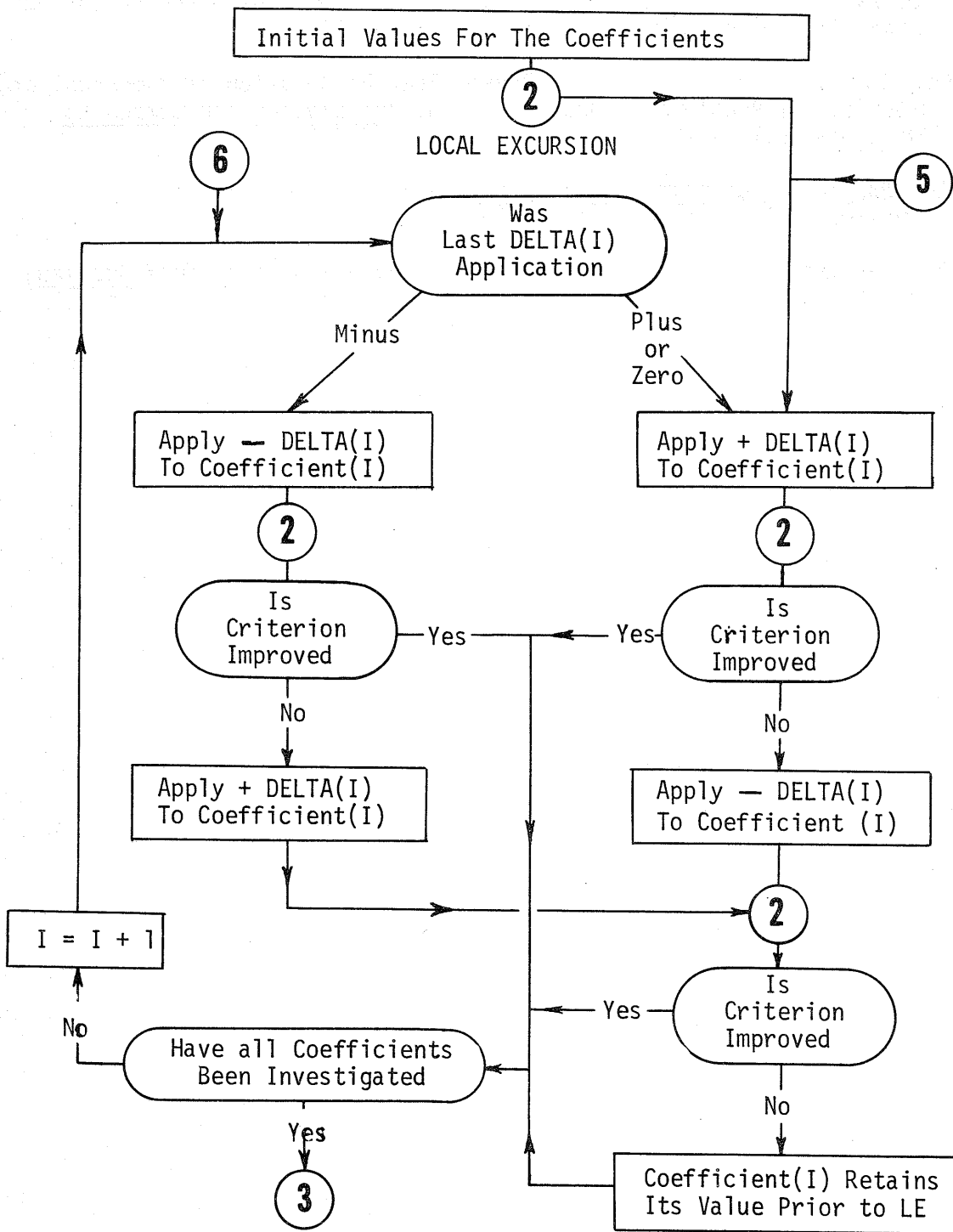
To be reasonably certain that global optimum values for the coefficients have been attained, we may need to perform a series of optimization studies with different initial values for the coefficients.

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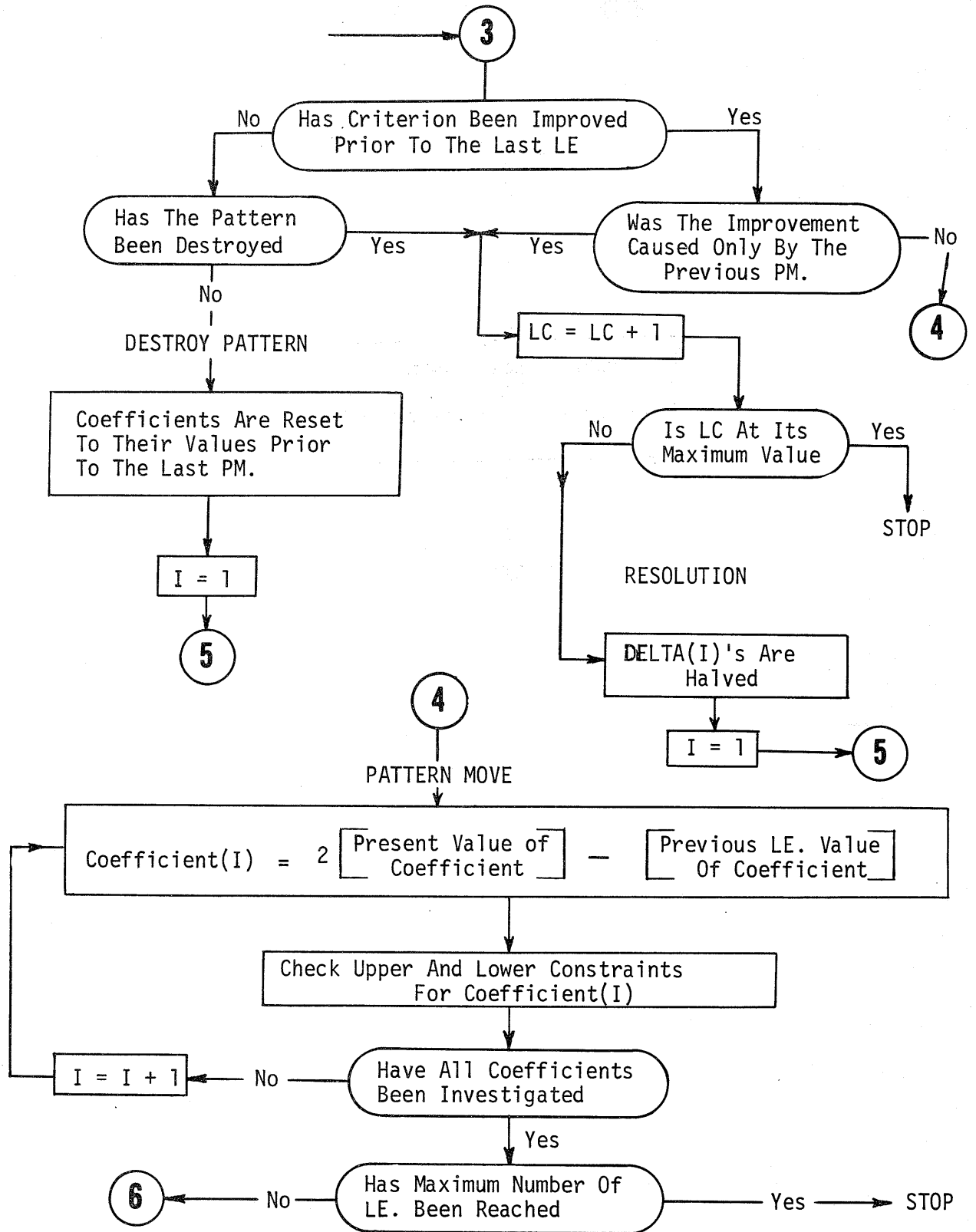
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APPENDIX A
FLOW CHART

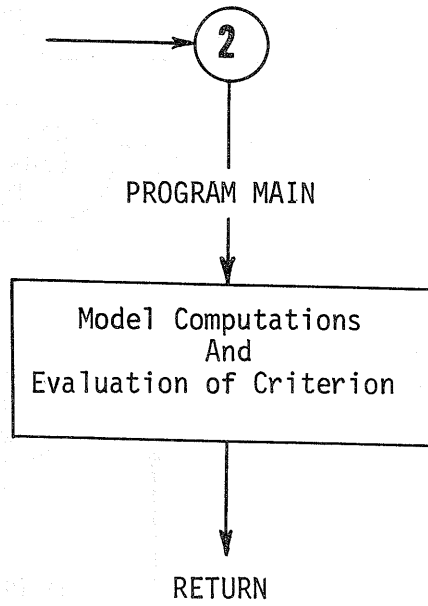
START



FLOW CHART--Continued



FLOW CHART--Continued



APPENDIX B

PROGRAM LISTING

```

SUBROUTINE OPT
*****
*****
PATTERN SEARCH WITH MODIFICATIONS
*****
DEFINITION OF PROGRAM VARIABLES

NUMA= NUMBER OF A(I) COEFFICIENTS TO BE OPTIMIZED

A(I)= VALUE OF COEFFICIENT I AFTER LAST PATTERN MOVE

B(I)= VALUE OF COEFFICIENT I AFTER PREVIOUS LOCAL EXCURSION

BA(I)= VALUE OF COEFFICIENT I AFTER PRESENT LOCAL EXCURSION

NPER= IF = 1 DDELTA(I) MUST BE IN PERCENT/100
      IF = 0 DDELTA(I) MUST BE AN ABSOLUTE VALUE

DDELTA(I)= WHEN NPER=1 DELTA(I)=ABS(DDELTA(I))*A(I)
           WHEN NPER=0 DELTA(I)=DDELTA(I)

DELTA(I)= INCREMENT ADDED OR SUBTRACTED TO A(I) DURING A LOCAL EXCURSION

CHECKL(I)= LOWER CONSTRAINT ON A(I)

CHECKH(I)= UPPER CONSTRAINT ON A(I)

OPTIM= VALUE OF THE OPTIMIZATION CRITERION

NN= NUMBER OF TIMES MAIN PROGRAM HAS CALLED OPT

NSIGN(I)= NSIGN(I)=0 THEN + DELTA(I) APPLIED FIRST
          NSIGN(I)=1 - DELTA(I) APPLIED FIRST

MAXN= MAXIMUM NUMBER OF TIMES MAIN PROGRAM MAY CALL OPT BEFORE
      OPTIMIZATION IS ABORTED

KC= MAXIMUM NUMBER OF TIMES DELTA(I) MAY BE HALVED BEFORE
    OPTIMIZATION IS TERMINATED (MAXN OVER-RIDES KC)
*****
*****
THIS PROGRAM IN ITS PRESENT FORM IS FOR MINIMIZATION
    TO CONVERT TO A MAXIMIZATION FORMAT
    REPLACE                               WITH
    IF(YS.GT.YY) GO TO 1008                IF(YS.LT.YY) GO TO 1008
8  IF(YX.GT.YS) GO TO 11                   8  IF(YX.LT.YS) GO TO 11
    IF(YS.GT.YY) GO TO 1007                IF(YS.LT.YY) GO TO 1007
16 IF(YX.GT.YS) GO TO 19                   16 IF(YX.LT.YS) GO TO 19
*****
*****
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)

```

PROGRAM LISTING--Continued

```

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

```

PROGRAM LISTING--Continued

```

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)

```

PROGRAM LISTING--Continued

```

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

```


PROGRAM LISTING--Continued

```

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(LDELTA.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
LDELTA=LDELTA+1
30 PRINT 31,ICOUN,LDELTA
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
INT 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

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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⁾:

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

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 optimum 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(3)
INITIAL VALUES OF THE COEFFICIENTS				
1	1	.242E+02	-1.200	1.000
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
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
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
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
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
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
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
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
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
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
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
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
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
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
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
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
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
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
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				

Computer Output--Continued

```

                                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

```

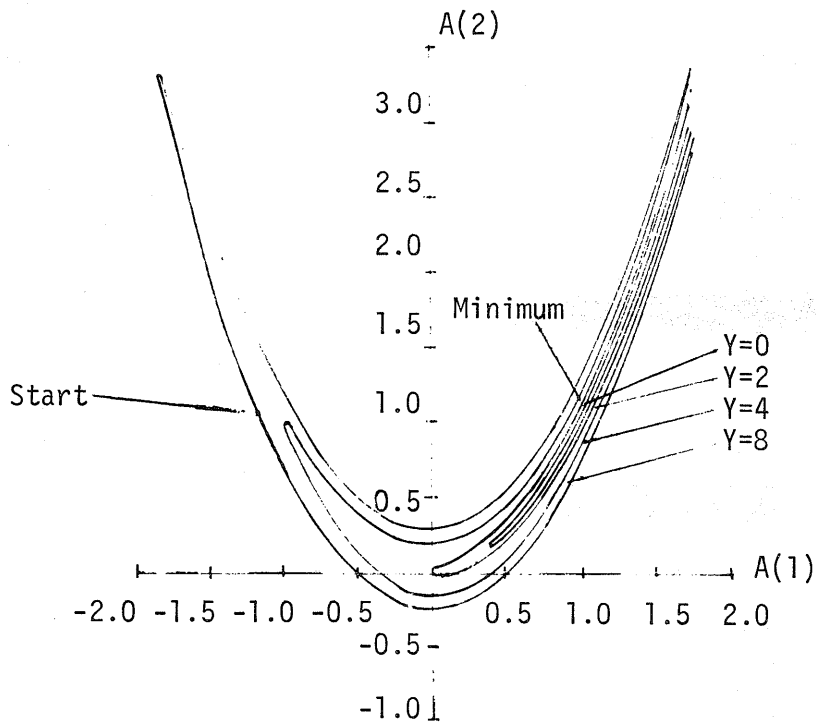


Figure 3.--Response surface resulting from application of the Pattern Search method to the test function of Rosenbrock (1960).

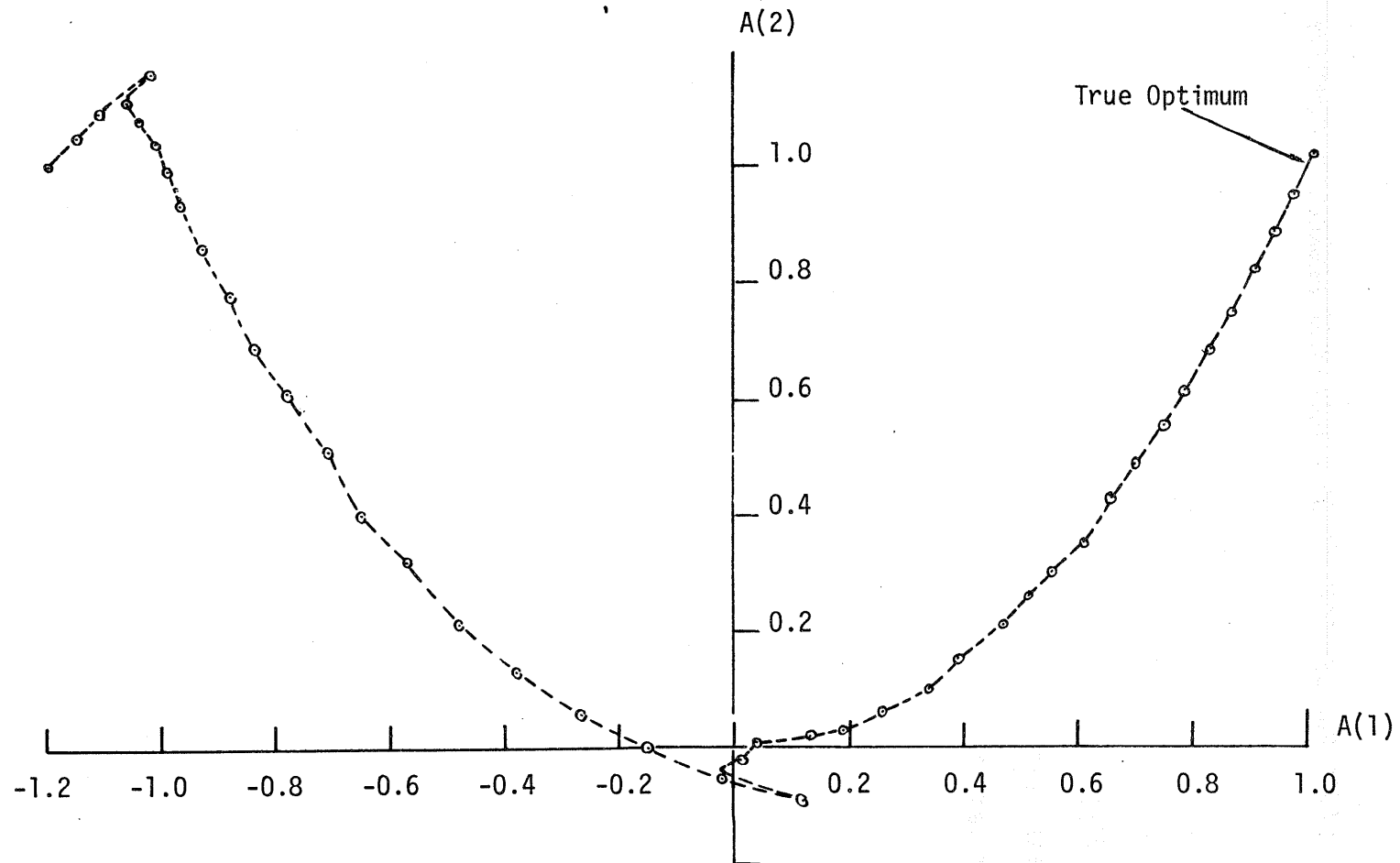


Figure 4.--Successive values of $A(1)$ and $A(2)$ after each Pattern Search move, for the test function of Rosenbrock (1960).

APPENDIX D

LEAST-SQUARES FITTING OF A NONLINEAR REGRESSION FUNCTION

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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; $\sum_{i=1}^N (Y_i - y_i)^2$.

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:

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

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

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

INITIAL VALUES OF THE COEFFICIENTS							
TRIAL	RUN	CRITERION	A (1)	A (2)	A (3)	A (4)	A (5)
1	1	.870E+00	1.020	1.639	2.453	2.406	
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	
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	
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	
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	
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	
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	
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	
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	
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	
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	
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	
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	
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	
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	
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	

Computer Output--Continued

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				

Computer Output--Continued

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)
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)
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)
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)
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)
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)
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

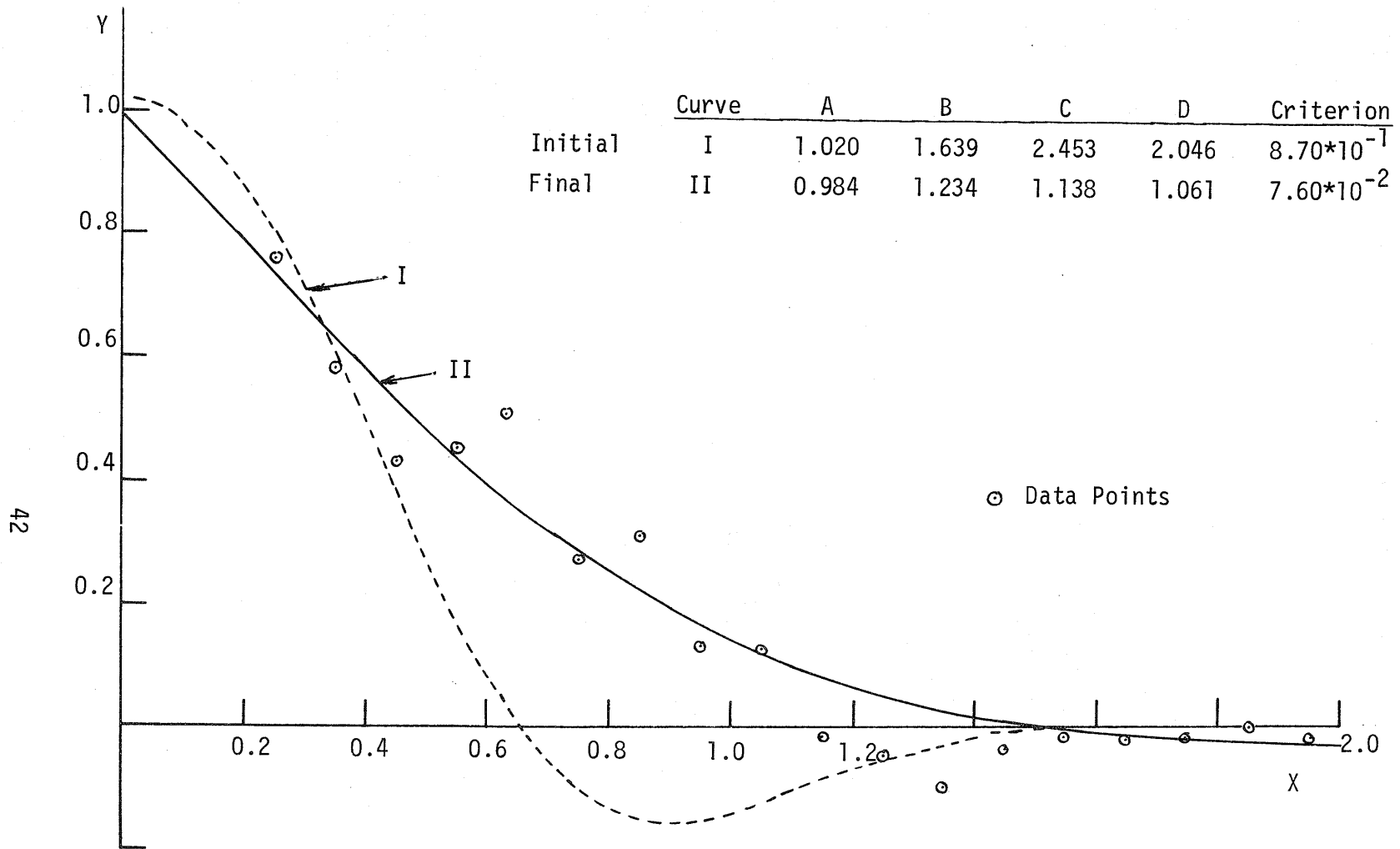


Figure 5.--Least-squares curve fitting using the Pattern Search method. Dashed curve: transcendental function using initial values of the coefficients. Solid curve: function using final values resulting from Pattern Search method.

APPENDIX E

OPTIMAL PARAMETERIZATION OF A WATERSHED MODEL

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Introduction	44
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Schematic of the main and subroutine programs	51

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.

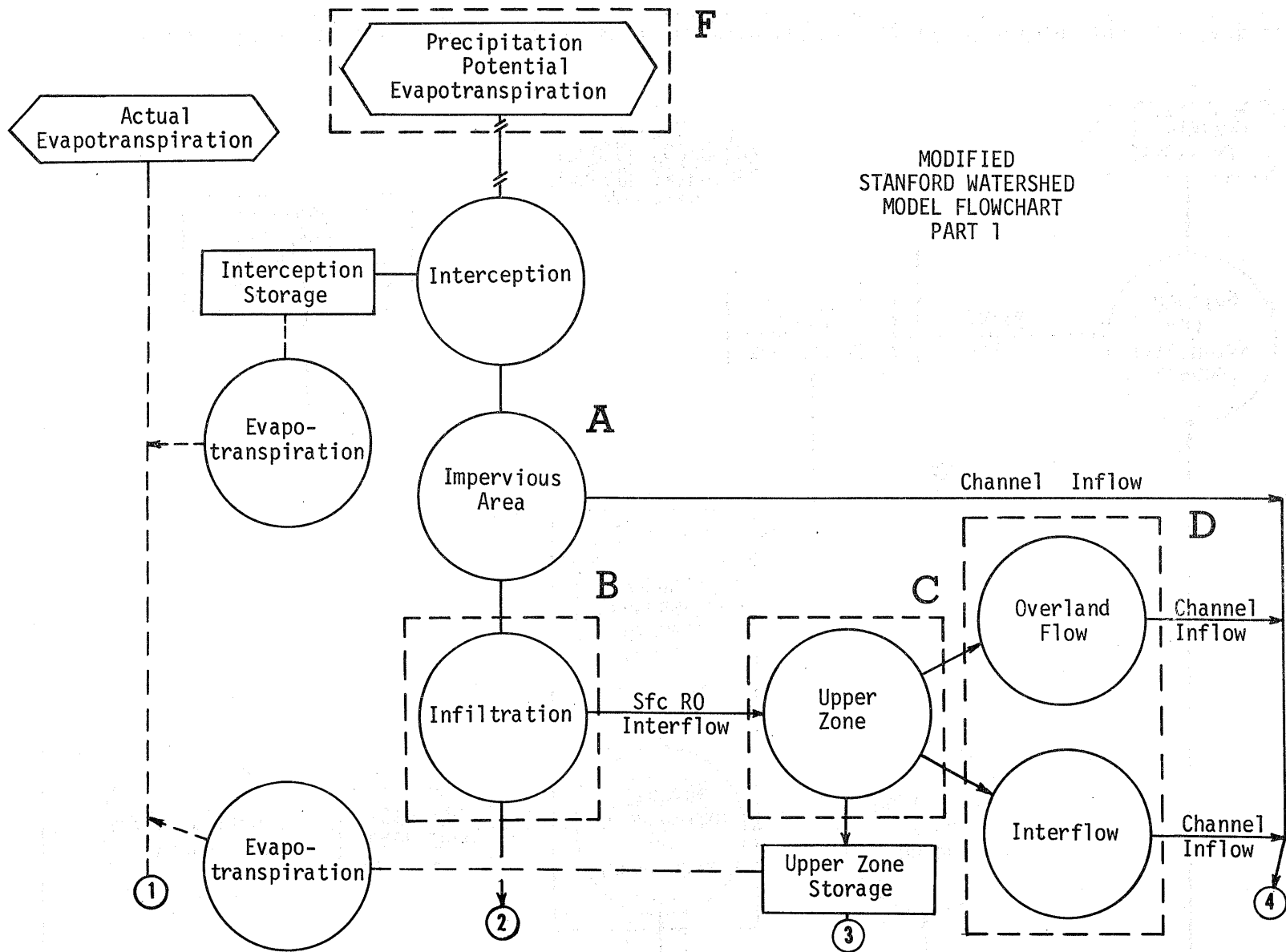
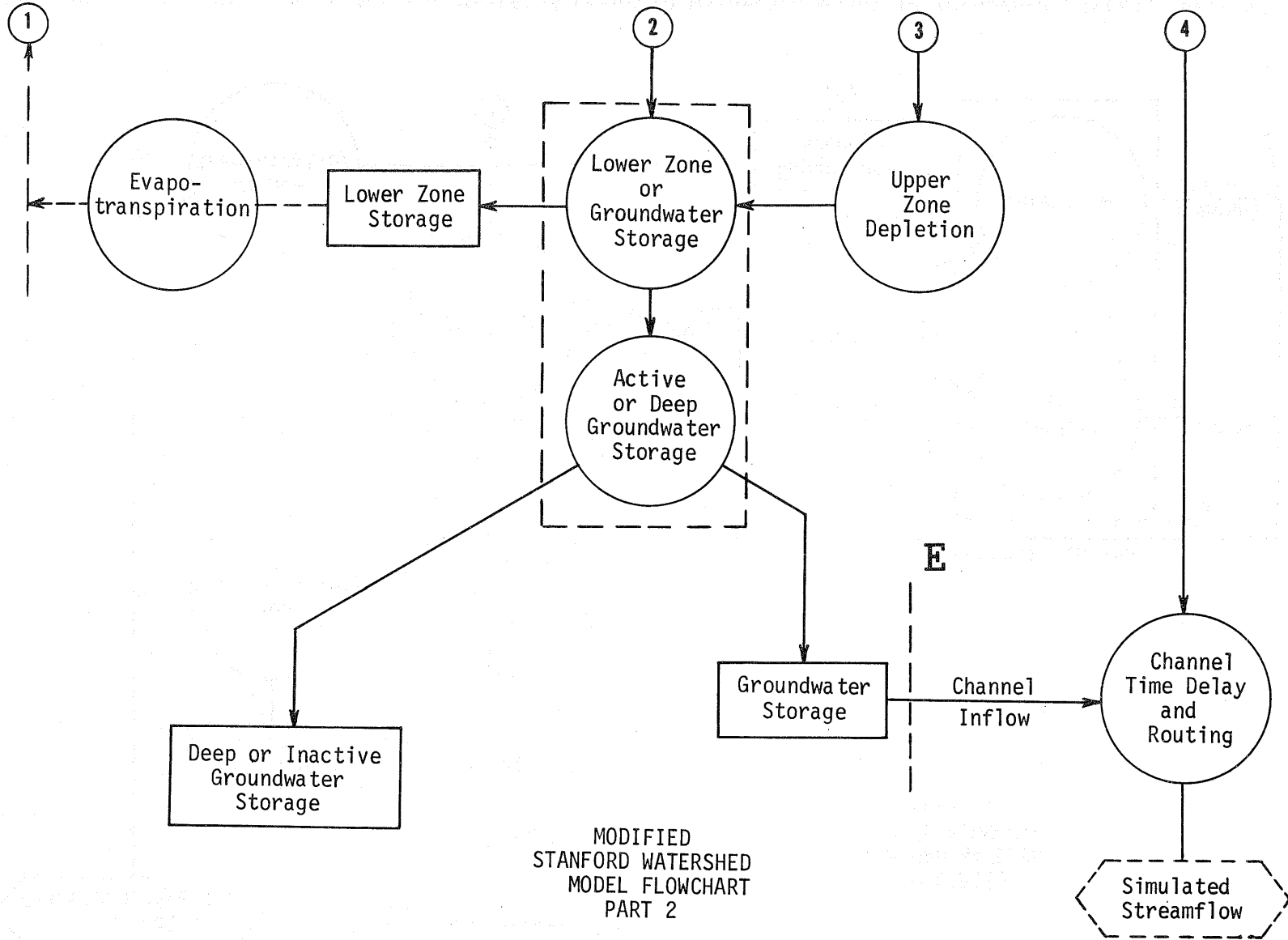


Figure 6.--Flow chart for the Modified Stanford Watershed Model IV (Crawford, 1966). Part 1.



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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

<u>Initial</u>	<u>Final</u>
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		Initial	Final	Initial	Final
		SIM	SIM				
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 interpreted 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(3I2,15)
2  FORMAT(10F6.4)

      (additional MAIN PROGRAM FORMAT STATEMENTS)

END
```

```
SUBROUTINE OPT
```

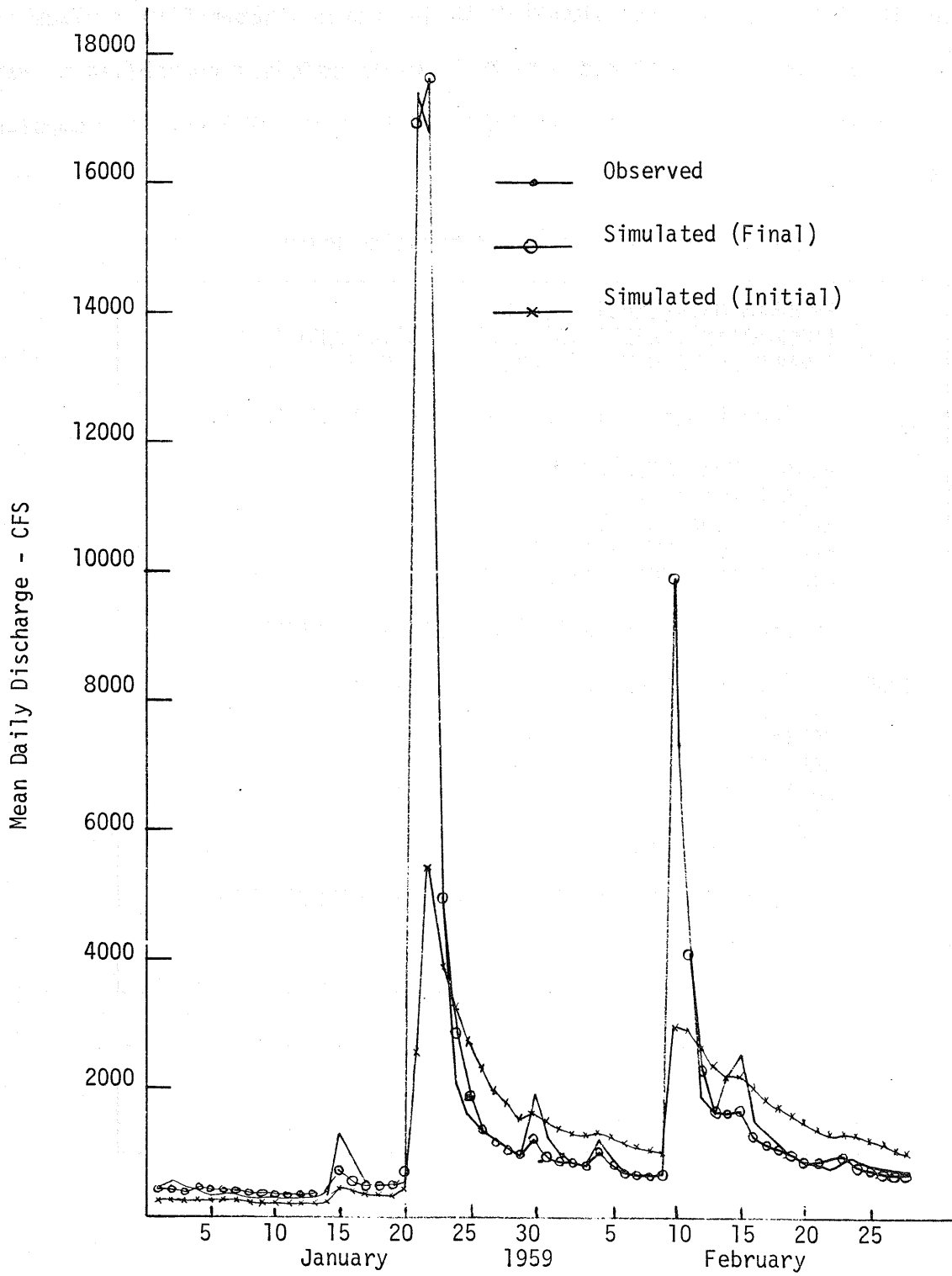


Figure 8.--Selected Portions of the observed streamflow trace for the Mad River Basin, Ohio, the simulated trace using initial coefficient values, and the simulated trace using final values optimized by Pattern Search method.