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SIMMIN - A PROGRAM FOR MINIMIZING FUNCTIONS BY SIMPLEX METHODS FOR IBM PC

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JULY 1987

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**SIMMIN** - A Program for Minimizing Functions by Simplex Methods for IBM PC

**Jerry D. Smith, Miles E. Holloman, William F. Otto**

**16 SUPPLEMENTARY NOTATION**

**19 ABSTRACT (Continue on reverse if necessary and identify by block number)**

SIMMIN is a minicomputer program capable of finding a minimum for any function which can be described using Fortran. A simplex method determines values of coefficients which result in a function local minimum. This document briefly describes the methodology and algorithm originally written by Caceci and Cacheris and modified by Holloman and Otto. It also provides a user's guide for use of the Fortran code (which is included), complete with example cases. Conversion to larger computers is straightforward.
SUMMARY

A computer program, SIMMIN, which is capable of finding a minimum (if one exists) for any function which can be described using Fortran, has been developed and tested on an IBM PC with an 8087 math coprocessor. The program is a modification of a Pascal algorithm written by Cacuci and Cacheris and modified by Holloman and Otto. A simplex method determines values of initially unknown coefficients which result in a local function minimum.

The user can vary initial estimates of the coefficients, step sizes, maximum number of iterations, and the convergence criteria, of which two are available. Final values of the coefficients, an estimate of the function minimum, and the number of iterations required are displayed on screen, while a diagnostic iteration history is recorded on a separate file which can be examined after each execution.

The program can easily be converted for use on larger computers, perhaps allowing the use of single precision. Although divergence is impossible, a price is often paid in more iterations and computing time than with some other traditional minimization methods.
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I. INTRODUCTION

Techniques for minimizing functions include stepwise descent, steepest descent, Newton-Raphson algorithms (and variations), and Marquardt algorithms. However, there are many functions for which these well-known methods are difficult to implement, are computer intensive, and are prone to diverge. Such functions may be nonlinear, partially empirically defined, not continuous in regions of interest, or quite complicated. Inaccurate calculation of derivatives and the lack of good initial estimates for the unknown coefficients are often responsible for the failure of these methods.

The program SIMMIN, the subject of this report, can find a minimum (if one exists) for any function that can be described by the user in Fortran. SIMMIN does this by using a simplex technique to calculate values of initially unknown coefficients which result in a functional minimum. The user should have some familiarity with Fortran so that the subroutine FUNC in the source code shown in the Appendix can be modified for the function of interest. A very simple function has been included for instructional purposes.

II. THE MODEL

The simplex methodology for finding functional minima is used in SIMMIN. The original algorithm was written by Nelder and Mead in 1965 [1] and was implemented in Extended Mercury Autocode on an Orion computer. The starting point for the present study is a Pascal algorithm by Caceci and Cacheris to fit curves to data [2]. Holloman and Otto modified the model by converting to Fortran, introducing a different convergence criterion, to be discussed later, and hard-coding user inputs, such as initial estimates and step sizes, in order to make the model more transparent to the user. They next incorporated their modified model into user-friendly, curve-fitting programs for IBM PC [3,4]. In addition to familiar Fourier, Lagrange and spline methods, data could be fit to any equation selected by the user. The coefficients in the equation were determined by allowing the simplex technique to minimize the nonlinear function sum of squares of residuals as follows:

\[ \text{SSR} = \sum_{i=1}^{N} \left( \text{Y}_{\text{calc}}(X_i, A_1, A_2, \ldots, A_{mm}) - \text{Y}_{\text{exper}}(X_i) \right)^2 \]  

where \( A_1, A_2, \ldots, A_{mm} \) are the unknown coefficients and \( N \) is the number of experimental data points, \( X_i \). Least squares fitting to any equation was done without using derivatives or matrix operations. However, it was noted that for most fitting functions, execution times increased greatly with the number of coefficients, above approximately three.

In the present study, the fitting aspects of the model were removed. User control over most inputs was restored since finding a minimum (or minima) usually requires experimentation with initial estimates, step sizes, the maximum number of iterations, and the convergence criteria, of which two are available.

The user is referred to References 1 and 2 for details of the model, but a short introduction is offered here. A simplex is a geometric figure which has
one more vertex than the space in which it is defined has dimensions. For example, the user will find in the Appendix (the source code for program SIMMIN) a function of the following form defined in line numbers 281-284:

\[ F = (A-1.)^2 + (B-2.)^2 + (C-3.)^2 \]  

The simplex for this function would have four vertices in three-dimensional space. Each vertex is characterized by four values: A,B,C,F. Subroutine SIMPLEX defines the simplex as a two-dimensional array SIMP(I,J), with I being the vertex index and J the dimension index. It should be clear that for our example, values A = 1, B = 2, C = 3 yield the one and only function minimum \( F = 0 \).

The principal of the simplex method is to move and reshape the simplex in ways resulting in decreased values of the response function as iterations proceed. Each iteration involves combinations of reflection, expansion, contraction, and shrinkage of the vertices according to logical rules, and then testing the newly calculated function value against the previous value. If the new value is better (meaning lower) than the previous one, then the vertices are accepted and the simplex proceeds in the same general direction. If not, then the vertex changing logic proceeds in an orderly, efficient search or a new direction.

III. COMPUTER IMPLEMENTATION

The present study was done on an IBM PC equipped with an 8087 coprocessor using Ryan-McFarland Fortran (V2.11). This Fortran creates very efficient executable code at the expense of longer compilation times. Double precision was used for all reals by appropriately placed implicit double precision statements. The user can easily remove the double precision if SIMMIN is used on fast computers with large word size, where large numbers of iterations and truncation/round-off errors are not likely to cause problems using single precision.

The primary modification the user will make is to substitute a function of interest for the demonstration function in subroutine FUNC (see the Appendix, Lines 272-287). The program requires that the coefficients enter the subroutine as an array COEF(I), I = 1,...,MM, where MM is the number of coefficients to be determined. The user is then free to convert to a more convenient notation. Perhaps the function to be minimized is available as a function subprogram or a subroutine which would then be called from within subroutine FUNC. The calculated value of the function must be returned from FUNC as COEF(MM+1).

Constraints can be added in the form of Fortran statements directing the program flow to statement 999 in FUNC, often in the form of IF statements restricting the coefficients or function to certain regions. Note what happens then: the function value COEF(MM+1) is returned as the previous value plus a very large number 1.D30. Most calls of subroutine FUNC from within subroutine SIMPLEX are followed by IF tests to determine if the new trial function value RNEXT(MM+1) is less than the previous value, referred to in subroutine simplex as SIMP(MM+1,IH(MM+1)). It certainly will not be if a constraint condition has been exceeded and the logic will guide the simplex away from this region.
An important additional word about constraints: the user may well have them without being aware of them for awhile. The simplex moves about in hyperspace without regard to such problems as attempting to take logarithms of zero or of negative numbers, dividing by zero, or attempting to evaluate functions (such as factorials, gamma functions, etc.) in regions leading to computer underflow or overflow. The user should protect against all such possibilities by adding appropriate statements to direct the program to statement 999, or to do the equivalent action described after statement 999 somewhere else.

A. Input Parameters

Values supplied by the user during interactive operation of SIMMIN are shown within boxes in Figures 1, 2, and 3.

1. MM - The number of coefficients to be calculated, 3 for the example in Equation (2).

2. MAXITR - The maximum number of iterations allowed. This may be only approximate since the program now counts every trial set of vertices as an iteration, regardless of whether the function value increases or decreases. Therefore, the number of iterations shown as part of the results could slightly exceed MAXITR.

3. Initial Estimates of the Coefficients - The user must insure that their order conforms to the definition of coefficients in subroutine FUNC. One should always experiment with these initial estimates to see the effect on results.

4. Convergence Criterion Option

ICON = 1 -- The program compares relative errors of calculated coefficients with a limit entered by the user, typically between 1.D-05 and 1.D-04. If every relative error is less than the limit, then convergence is obtained. Before defining this error, recall for Equation (2) that there are four vertices for the simplex: A, B, C, F, and that each vertex is characterized by four values: A, B, C, F. The simplex is defined as a two-dimensional array SIMP(I,J), with I being the vertex index and J being the dimension index. The error is defined as follows (Appendix, Line 231):

\[
\text{ERROR} (I) = \frac{\text{SIMP}(I, \text{IH}(I)) - \text{SIMP}(I, \text{L}(I)))}{\text{SIMP}(I, \text{IH}(I))}
\]

(3)

subroutine ORDER has provided IH(I) and L(I), the indices of the highest and lowest values, respectively, currently associated with vertex I. The value of ERROR(MM+1), the function error, does not seem to decrease to nearly as small as the coefficient errors ERROR(I), I=1,MM even though inspection of latter iterations in file ITER.OUT shows a minimum is close to being found, by either convergence criterion. Therefore, the error comparisons were restricted to the coefficients only.

ICON = 2 -- This convergence option allows the program to keep a count of the number of consecutive times that new trial vertices have been calculated without reducing the value of the function. If this count exceeds (MM+1)*3 then convergence is obtained. It was arrived at through experience
with nonlinear functions in fitting applications, and relieves the user from choosing acceptable limits for errors [3,4]. The simplex has usually found a minimum. However, it may be trapped near some unusual topological feature, perhaps moving up and down a valley where coefficient values change but the function value does not. When dealing with new, unfamiliar, complicated functions, it is always advisable to experiment with initial estimates and step sizes and to examine at least the latter iterations in file ITER.OUT.

B. Results

In Figures 1, 2, and 3, test results begin after the lines "*****CALCULATING SIMPLEX*****". Tables 1 and 2 show the latter iterations from iteration history file ITER.OUT produced by executing the cases shown in Figures 1 and 2, respectively. After each execution, this file can be examined, printed, or renamed, but file ITER.OUT is destroyed and recreated near the beginning of each execution.

Figure 1 shows convergence criterion 1 being satisfied with 74 iterations for a selected error limit of 1.D-05. Table 1 shows that all coefficient relative errors are indeed less than 1.D-05 at iteration 74. This table also shows the construction of this diagnostic file, with results labeled for iteration number 69.

Figure 2 shows the same case as Figure 1 except that convergence criterion 2 was selected. Note that the final value of the function (0.414162E-24) is lower, and the number of iterations (224) is higher. Criterion 2 is often more stringent than criterion 1.

Table 2 shows iterations 211-224 from file ITER.OUT. Notice that beginning with iteration 213, the relative errors develop a pattern as iterations proceed: the first and third ones switch back and forth between pairs of values, and the second remains constant. This continues for 3*(MM+1)=12 iterations, and then criterion 2 is satisfied. This type of error behavior is common when the simplex has locked in to a minimum. Given the logical rules for changing vertex values and the truncation/round-off limits in the computer's arithmetics, the program is unable to find a change which results in a lower function value. Without the logic for criterion 2, iterations would have proceeded until the iteration limit was exceeded.

The case in Figure 3 is the same as that in Figure 2 except the initial estimates were 200, 300, 400 instead of 2, 3, 4, which were much closer to the correct answers 1, 2, 3. Using convergence criterion 2, 268 iterations were required. Approximate wall clock execution time was 30 seconds for Figure 3 and 26 seconds for Figure 2 (224 iterations). For comparison, using single precision, the execution times were approximately 16 and 12 seconds, respectively. However, the estimation of the true function minimum of 0.0 was about 10^{-12} - 10^{13} using single precision, while double precision improved it to approximately 10^{29} - 10^{30}.

IV. CONCLUSIONS

The computer program SIMMIN is capable of finding a minimum (if one exists) for any function which can be described using Fortran. It was tested on an IBM PC with an 8087 math coprocessor using Ryan-McFarland Fortran. This
simplex method determines values of initially unknown coefficients which result in a local function minimum.

The user can vary initial estimates of the coefficients, step sizes, maximum number of iterations, and the convergence criteria, of which two are available. Final values for the coefficients, an estimate of the function minimum, and the number of iterations required are displayed on the screen. A diagnostic iteration history is recorded on a separate file which can be examined after each execution.

The program can easily be converted for use on larger computers with larger word sizes, perhaps allowing the use of single precision. Although divergence is impossible using this simplex method, a price is often paid in more iterations and computing time than with some other traditional minimization methods, such as those mentioned in the introduction.

The user is cautioned against drawing overly optimistic conclusions from the test results. A very simple test function was used. Actual functions encountered in research and development - analytical, empirical, or hybrids - which cause problems when using minimization methods such as those mentioned in the introduction could require care when using simplex techniques as well.

Here are a few advantages simplex methods such as those in SIMMIN offer over other methods:

1. No derivatives of any kind are calculated.
2. Divergence is impossible.
3. Initial estimates for the coefficients can be poor, but this will slow down convergence, depending upon step size.
4. Simplex logic insures economical calculation of the response function.
5. No matrix operations are involved.
6. Constraint conditions which can be stated in Fortran can be added very easily.

Here are a few disadvantages of simplex compared with other methods:

1. More iterations and computing time can be required. SIMMIN is recommended for larger computers, especially when the function is complicated, when other methods have proved unsatisfactory or need to be verified, or when the user has little knowledge of the functional behavior.

2. The following can cause computational problems: very large initial estimates coupled with small steps, insensitivity of the function to one or more coefficients, too large an acceptable error when using an error comparison convergence criterion. These and other problem areas are discussed in much more detail in Reference 2.
REFERENCES


ENTER MM, NUMBER OF PARAMETERS TO BE CALCULATED -3

ENTER MAXITR, MAXIMUM NO. OF ITERATIONS, TYPICALLY SEVERAL HUNDRED. PROGRAM USUALLY CONVERGES WITHIN 20*(MM**2) ITERATIONS. - 200

ENTER MM INITIAL ESTIMATES OF PARAMETERS. BE SURE THE ENTRY ORDER CONFORMS WITH YOUR DEFINITION OF PARAMETERS COEF(I) IN SUBROUTINE FUNC. ESTIMATES USUALLY CAN BE QUITE INACCURATE. - 2, 3, 4

ENTER MULTIPLIER IN STEP CALCS., APPROX. RANGE FROM 0.1 TO 0.5. (STEP = ESTIMATE * MULTIPLIER) - 2

ENTER CONVERGENCE CRITERION OPTION -
1, FOR COMPARISON OF RELATIVE ERRORS WITH INPUT LIMIT.
2, FOR THE CONDITION THAT THE NUMBER OF UNSUCCESSFUL ATTEMPTS TO DECREASE THE FUNCTION EXceeds 3*(MM+1) - 1

ENTER LIMIT ON RELATIVE ERRORS, THE SAME FOR ALL COEFFICIENTS.
RECOMMENDED RANGE 1.D-06 TO 1.D-04. - 1.D-05

***** CALCULATING SIMPLEX*****
FINAL VALUES OF COEFFICIENTS -
1.00000 2.00000 3.00000
FINAL VALUE (MINIMUM) OF FUNCTION = 0.417040E-10
NUMBER OF ITERATIONS = 74
Execution terminated: OK

Figure 1. Screen input and results for a typical execution of SIMMIN.
Convergence criterion 1 was selected.
**TABLE 1. Latter Contents of Iteration History File ITER.OUT Produced During Execution With Input Parameters Shown in Figure 1.**

<table>
<thead>
<tr>
<th>Iteration number</th>
<th>Current values of coefficients</th>
<th>Estimate of function value, printed only when the iteration led to a better (lower) function value.</th>
<th>Estimates of relative errors for the coefficients, MM = 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.000</td>
<td>0.1210E-09</td>
<td>1.48453975763265370E-05 7.86123165807031016E-06 7.56428230863572653E-06</td>
<td></td>
</tr>
<tr>
<td>2.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7947E-10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0000</td>
<td>1.48453976763265370E-05</td>
<td>4.89503933556161228E-06 7.56428230863572653E-06</td>
<td></td>
</tr>
<tr>
<td>2.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7947E-10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0000</td>
<td>1.44438985795023159E-05</td>
<td>4.89503933556161228E-06 7.56428230863572653E-06</td>
<td></td>
</tr>
<tr>
<td>2.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.0000</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>0.7947E-10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0000</td>
<td>1.20481762607656796E-05</td>
<td>3.12815572995717666E-06 5.2012188225269973E-06</td>
<td></td>
</tr>
<tr>
<td>2.0000</td>
<td></td>
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</tr>
<tr>
<td>0.7947E-10</td>
<td></td>
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</tr>
<tr>
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<td>3.12815572995717666E-06 2.91527801458411470E-06</td>
<td></td>
</tr>
<tr>
<td>2.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7947E-10</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

All relative errors < 1.0E-05. Option 1 convergence (ICON = 1) obtained.
ENTER MM, NUMBER OF PARAMETERS TO BE CALCULATED - [3]

ENTER MAXITR, MAXIMUM NO. OF ITERATIONS, TYPICALLY SEVERAL HUNDRED. PROGRAM USUALLY CONVERGES WITHIN 20*(MM**2) ITERATIONS. - [300]

ENTER MM INITIAL ESTIMATES OF PARAMETERS. BE SURE THE ENTRY ORDER CONFORMS WITH YOUR DEFINITION OF PARAMETERS COEF(I) IN SUBROUTINE FUNC. ESTIMATES USUALLY CAN BE QUITE INACCURATE. - [2, 3, 4]

ENTER MULTIPLIER IN STEP CALCS., APPROX. RANGE FROM 0.1 to 0.5. (STEP = ESTIMATE * MULTIPLIER) - [0.2]

ENTER CONVERGENCE CRITERION OPTION -
1, FOR COMPARISON OF RELATIVE ERRORS WITH INPUT LIMIT.
2, FOR THE CONDITION THAT THE NUMBER OF UNSUCCESSFUL ATTEMPTS TO DECREASE THE FUNCTION EXCEEDS 3*(MM+1) - [2]

***** CALCULATING SIMPLEX*****
FINAL VALUES OF COEFFICIENTS -
1.00000 2.00000 3.00000
FINAL VALUE (MINIMUM) OF FUNCTION = 0.414162E-29
NUMBER OF ITERATIONS = 224
Execution terminated : OK

Figure 2. Screen input and results for a typical execution of SIMMIN. Convergence criterion 2 was selected.
TABLE 2. Latter Contents of File ITER.OUT Produced by Input Parameters in Figure 2. Repetitive Pattern in Coefficient Errors Begins at Iteration 213.

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Values</th>
<th>Coefficient Errors</th>
</tr>
</thead>
<tbody>
<tr>
<td>211</td>
<td>1.000 2.000 3.000 0.4930E-31</td>
<td></td>
</tr>
<tr>
<td>212</td>
<td>1.0000 2.000 3.000</td>
<td></td>
</tr>
<tr>
<td>213</td>
<td>1.0000 2.000 3.000</td>
<td></td>
</tr>
<tr>
<td>214</td>
<td>1.99840144432528138E-15</td>
<td>6.66133814775093530E-16</td>
</tr>
<tr>
<td>215</td>
<td>1.0000 2.000 3.000</td>
<td></td>
</tr>
<tr>
<td>216</td>
<td>1.99840144432528138E-15</td>
<td>6.66133814775093530E-16</td>
</tr>
<tr>
<td>217</td>
<td>1.0000 2.000 3.000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.99840144432528138E-15</td>
<td>6.6613381477593530E-16</td>
</tr>
<tr>
<td>------------</td>
<td>------------------------</td>
<td>----------------------</td>
</tr>
<tr>
<td>1.000</td>
<td>2.000</td>
<td>3.000</td>
</tr>
<tr>
<td>2.2204604925031111E-15</td>
<td>6.6613381477593530E-16</td>
<td>5.92118946466750122E-16</td>
</tr>
<tr>
<td>1.0000</td>
<td>2.000</td>
<td>3.000</td>
</tr>
<tr>
<td>2.2204604425093530E-16</td>
<td>6.6613381477593530E-16</td>
<td>5.92118946466750122E-16</td>
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<tr>
<td>1.0000</td>
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<td>5.92118946466750122E-16</td>
</tr>
<tr>
<td>1.000</td>
<td>2.000</td>
<td>3.000</td>
</tr>
<tr>
<td>2.2204604925031111E-15</td>
<td>6.6613381477593530E-16</td>
<td>5.92118946466750122E-16</td>
</tr>
<tr>
<td>1.000</td>
<td>2.000</td>
<td>3.000</td>
</tr>
<tr>
<td>2.2204604432528138E-15</td>
<td>6.6613381477593530E-16</td>
<td>5.92118946466750122E-16</td>
</tr>
<tr>
<td>1.000</td>
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<td>3.000</td>
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<td>6.6613381477593530E-16</td>
<td>5.92118946466750122E-16</td>
</tr>
</tbody>
</table>
ENTER MM, NUMBER OF PARAMETERS TO BE CALCULATED - [3]

ENTER MAXITR, MAXIMUM NO. OF ITERATIONS, TYPICALLY SEVERAL HUNDRED. PROGRAM USUALLY CONVERGES WITHIN 20*(MM**2) ITERATIONS. - [300]

ENTER MM INITIAL ESTIMATES OF PARAMETERS. BE SURE THE ENTRY ORDER CONFORMS WITH YOUR DEFINITION OF PARAMETERS COEF(1) IN SUBROUTINE FUNC. ESTIMATES USUALLY CAN BE QUITE INACCURATE. - [200,300,400]

ENTER MULTIPLIER IN STEP CALCS., APPROX. RANGE FROM 0.1 to 0.5. (STEP = ESTIMATE * MULTIPLIER) - [2]

ENTER CONVERGENCE CRITERION OPTION - 1, FOR COMPARISON OF RELATIVE ERRORS WITH INPUT LIMIT. 2, FOR THE CONDITION THAT THE NUMBER OF UNSUCCESSFUL ATTEMPTS TO DECREASE THE FUNCTION EXCEEDS 3*(MM+1) - [2]

***** CALCULATING SIMPLEX*****
FINAL VALUES OF COEFFICIENTS - 1.00000 2.00000 3.00000
FINAL VALUE (MINIMUM) OF FUNCTION = 0.246519E-30
NUMBER OF ITERATIONS = 268
Execution terminated : OK

Figure 3. Screen input and results for a typical execution of SIMMIN.
Initial coefficient estimates were 100, 200, 300.
Convergence criterion 2 was selected.
APPENDIX

FORTRAN SOURCE CODE FOR SIMMIN

A-1/(A-2 Blank)
PROGRAM SIMMIN

PROGRAM SIMMIN CAN FIND A MINIMUM (IF ONE EXISTS) FOR ANY FUNCTION DEFINED BY THE USER IN SUBROUTINE FUNC. THE FUNCTION CAN BE LINEAR OR NONLINEAR, PARTIALLY EMPIRICALLY DEFINED, AND NEED NOT BE CONTINUOUS. SIMMIN DOES THIS BY USING SIMPLEX TECHNIQUES TO CALCULATE THE VALUES OF INITIALLY UNKNOWN COEFFICIENTS THAT YIELD THE MINIMUM. PROGRAM IS BASED ON A PASCAL ALGORITHM IN "FITTING CURVES TO DATA", BYTE, MAY 1964, WHICH WAS CONVERTED TO FORTRAN77 AND MODIFIED FOR USE IN GENERAL PC CURVE FITTING PROGRAMS BY MILES HOLLOMK AND BILL OTTO. DIRECTED ENERGY DIRECTORATE, NICOH. FURTHER MODIFICATIONS RESULTED IN THIS INITIAL VERSION OF SIMMIN BY JERRY D. SMITH, OF THE SAME DIRECTORATE. USER SHOULD BE FAMILIAR ENOUGH WITH FORTRAN TO MODIFY SUBROUTINE FUNC AS REQUIRED, CONVERGENCE CRITERIONS IF DESIRED (SEE COMMENTS WITHIN SUBROUTINE SIMPLX), AND PERHAPS MINOR FORMAT CHANGES IF MANY UNKNOWN COEFFICIENTS COEF(I) OCCUR IN THE FUNCTION. CURRENT MAX. NO. = 10. NOTE --- EXECUTION TIMES INCREASE GREATLY WITH NUMBER OF COEFFICIENTS, ABOVE THREE. AFTER EXECUTION FILE ITER. OUT WILL CONTAIN A HISTORY OF THE ITERATION RESULTS: COEFFICIENT AND FUNCTION VALUES, AND RELATIVE ERROR VALUES FOR THE COEFFICIENTS. USER CAN EXAMINE AFTER EXECUTION IF DESIRED. IT IS DESTROYED AND RECREATED DURING THE NEXT EXECUTION.

ADVANTAGES OVER OTHER NONLINEAR METHODS:
1. NO DERIVATIVES ARE CALCULATED.
2. DIVERGENCE IS IMPOSSIBLE.
3. INITIAL ESTIMATES FOR COEFFICIENTS CAN BE QUITE POOR, ALTHOUGH THIS WILL SLOW DOWN CONVERGENCE.
4. SIMPLEX LOGIC INSURES ECONOMICAL CALCULATIONS OF RESPONSE FUNCTION.
5. NO MATRIX OPERATION IS INVOLVED.
6. CONSTRAINTS CAN BE ADDED VERY EASILY. (SEE SUBROUTINE FUNC.)

DISADVANTAGES OVER OTHER NONLINEAR METHODS:
1. MORE ITERATIONS AND COMPUTING TIME ARE OFTEN REQUIRED. SIMMIN RECOMMENDED FOR FAST PC'S, AND NUMBER-CRUNCHERS, ESPECIALLY WHEN THE FUNCTION TO BE MINIMIZED IS COMPLICATED AND USER HAS VERY LITTLE IF ANY KNOWLEDGE OF THE FUNCTIONAL BEHAVIOR.
2. FOLLOWING CAN CAUSE COMPUTATIONAL PROBLEMS, AND RESULT IN INACCURATE ANSWERS: VERY LARGE INITIAL GUESSES, VERY SMALL INITIAL INCREMENTS, INSENSITIVITY OF FUNCTION TO ONE OR MORE COEFFICIENTS, TOO LARGE A ACCEPTABLE ERROR (WHEN USING CONVERGENCE OPTION ICON=).  JERRY D. SMITH 11 MAY 87

COMMON FINAL(11), SIMP(11,11), STEP(11), MM, LUG, MAXITR, NITER, ICON, RX

IMPLICIT DOUBLE PRECISION (A-H,O-Z)
LUO=7
OPEN UNIT=LUO,FILE='ITER.OUT',STATUS='UNKNOWN')
CLOSE(UNIT=LUO,STATUS='DELETE')
OPEN(UNIT=LUO,FILE='ITER.OUT',STATUS='NEW')

E2 WRITE(*,1600)
1600 FORMAT(1HI,'ENTER MM, NUMBER OF PARAMETERS TO BE CALCULATED - ')
READ(*,*) MM
WRITE(*,1601)
1601 FORMAT(1X,'ENTER MAXITR, MAXIMUM NO. OF ITERATIONS, TYPICALLY SEVER
XAL HUNDRED',/,' PROGRAM USUALLY CONVERGES WITHIN 20*(MM**2) ITERAT
XIONS. - ')
READ(*,*) MAXITR
MM=MM+1
WRITE(*,1602)
1602 FORMAT(1X,'ENTER MM INITIAL ESTIMATES OF PARAMETERS. BE SURE
X,/', THE ENTRY ORDER CONFGRNS WITH YOUR DEFINITION OF PARAMETERS'
X,/', COEF(I) IN SUBROUTINE FUNC. ESTIMATES USUALLY CAN BE QUITE'
X,/', INACCURATE - '/)
READ(*,*) (SIMP(I,I),I=1,MM)
WRITE(*,1603)
1603 FORMAT(1X,'ENTER MULTIPLIER IN STEP CALCULS, APPROX. RANGE FROM 0.1
X*, TO 0.5. (STEP=ESTIMATE * MULTIPLIER; - ')
READ(*,*) SMULT
DO 10 J=1,MM
10 SIMP(J,J)*SMULT
WRITE(*,1604)
1604 FORMAT(1X,'ENTER CONvergence CRITERION OPTION - ',/1X, '1, FOR COM
XPARISON OF RELATIVE ERRORS WITH INPUT LIMIT',/1X, '2, FOR THE CON
XITION THAT THE NUMBER OF UNSUCCESSFUL ATTEMPTS TO',/1X, 'DECRE
XASE THE FUNCTION EXCEEDS 3*(MM+1) - ')
READ(*,*) ICON
IF(ICON.EQ.1) THEN
PRINT 1610
1610 FORMAT(1X,'ENTER LIMIT ON RELATIVE ERRORS, THE SAME FOR ALL COEFF
XICIENTS . ',/1X, 'RECOMMENDED RANGE 1.0-05 TO 1.0-04 - ')
READ(*,*) RX
ENDIF
7 CALL SIMPLEX
PRINT 1612
WRITE(*,1612) (FINAL(I),I=1,MM)
1614 FORMAT(1X,'FINAL VALUES OF COEFFICIENTS - ',/2X, 6E12.6)
PRINT 1606, FINAL(MM)
1606 FORMAT(1X, 'FINAL VALUE (MINIMUM) OF FUNCTION = ', 6E12.6)
PRINT 1608, NITER
1608 FORMAT(1X,'NUMBER OF ITERATIONS = ', I4)
STOP 'OK'
END
SUBROUTINE SIMPLEX

LOGICAL DONE,EQ
COMMON FINAL(11),SIMP(1,11),STEP(11),MM,LUX,MAXITR,NITER,ICON,RX
DIMENSION CENTER(11),ERROR(I1),RMAXER(I1),PS(I1),Q(I1),IH(11)

IMPLICIT DOUBLE PRECISION (A-H,O-Z)

DLOW=1.0D+38
DLWL=1.0D+38
LCNT=0
PRINT 1030 FORMAT(********* CALCULATING SIMPLEX *********)

C

DO 1060 I=1,MM
1060  SIMP(J,1)=SIMP(J,1)+Q(J)
1070  CONTINUE

DO 1090 I=1,MM
1090  IH(I)=1
1100  CALL ORDER(MM1,SIMP,L.IH.
1110  NITER=0
1120  DONE=.TRUE.
1130  NITER=NITER+1

COMPUTE CENTROID OF THE SIMPLEX.

DO 1110 I=1,MM
1110  CENTER(I)=0.0
1120  DO 1130 J=1,MM
1130  IF(I.EQ.IH(MM1)) GO TO 1130
1140  CENTER(J)=CENTER(J)+SIMP(J,1)

CALL FUCNC(SIMP',1,11),MM1
DO 1060 I=1,MM
SIMP(J,1)=SIMP(J,1)+(PS(I)/MM*ROOT2)
Q(I)=STEP(I)*((SORT(PNN)+MM-I)/(MM*ROOT2))
CONTINUE

CALL ORDER(MM1,SIMP,L.IH.

DONE=.TRUE.
NITER=0
IH(I)=1
CALL ORDER(MM1,SIMP,L.IH.
CONTINUE
CONTINUE
DO 140 I=1,MM
CENTER(I)=CENTER(I)/MM
RNEXT(I)=(1.0+ALFA)*CENTER(I)-ALFA*SIMP(I,IMM(I))
CONTINUE
CALL FUNC(RNEXT,MMI)
IF(RNEXT(MMI),LE,SIMP(MMI,IMM(I))) GO TO 1150
GO TO 1170
CALL NEWVR(MMI,SIMP,RNEXT,IMM(I))
CONTINUE
CALL FUNC(RNEXT,MM1I)
IF(RNEXT(MMI),LE,SIMP(MMI,IMM(I))) GO TO 1180
GO TO 1190
CALL NEWVR(MMI,SIMP,RNEXT,IMM(I))
GO TO 1250
CONTINUE
DO 140 I=1,MM
RNEXT(I)=GAMMA*SIMP(I,IMM(I)+1.0-GAMMA)*CENTER(I)
CALL FUNC(RNEXT,MMI)
IF(RNEXT(MMI),LE,SIMP(MMI,IMM(I))) GO TO 1210
GO TO 1220
CALL NEWVR(MMI,SIMP,RNEXT,IMM(I))
GO TO 1250
DO 140 I=1,MM
RNEXT(I)=BETA*SIMP(I,IMM(I)+(1.0-BETA)*CENTER(I)
CALL FUNC(RNEXT,MMI)
IF(RNEXT(MMI),LE,SIMP(MMI,IMM(I))) GO TO 1240
GO TO 1250
CALL NEWVR(MMI,SIMP,RNEXT,IMM(I))
GO TO 1250
DO 140 I=1,MM
SIMP(J,I)=SIMP(J,I)+SIMP(J,IMM(I))*BETA
CALL FUNC(RNEXT,MMI)
CONTINUE
FORMAT(14/)}
IF(LEQO,LCNT=LCNT+1
IF(.NOT.LEQO,LCNT=0
DLOWL=DLow
WRITE(LOU,1270) NITER

A-6
DO 1308 I=1,MM
IF(I.NE.MM) WRITE(LUO,1280) RNEXT(I)
IF(I.EQ.MM,AND.RNEXT(MM).LT.DLOW) WRITE(LUO,1280) RNEXT(I)
1308 FINAL(I)=RNEXT(I)
WRITE(LUO,1420)
1305 LEN=(DLOW,EN.DLOW)
CALL ORDER(MM,SIMP,L,IN)
1320 CONTINUE
WRITE(LUO,*)(ERROR(J),J=1,MM)

FOLLOWING IS PRESENT AUTHORS' CRITERION FOR CONVERGENCE,
BASED ON EXPERIENCE WITH NONLINEAR FUNCTIONS IN FITTING
APPLICATIONS. ESSENTIALLY, THIS CRITERION SAYS THAT IF NUMBER OF
CONSECUTIVE UNSUCCESSFUL ATTEMPTS TO FIND A NEW DIRECTION AND
SHAPE TO DECREASE THE VALUE OF THE FUNCTION REACHES MM+3,
THEN CALL IT A GAME AND RETURN TO MAIN PROGRAM. THE SIMPLEX HAS
EITHER FOUND A MINIMUM AND IS SPINNING ITS WHEELS, OR IT IS EATING
UP TIME DUE TO POORLY CHOSEN INPUTS. TRY AGAIN WITH DIFFERENT
INITIAL ESTIMATES AND STEP SIZES, IF USER SUSPECTS SOMETHING
UNUSUAL. IN FACT, IT IS ALWAYS GOOD PROCEDURE TO VERIFY
RESULTS BY RE-RUNNING WITH DIFFERENT INPUTS, AND TO INSPECT
ITERATION HISTORY FILE ITER.OUT.

IF(ICON.EQ.0,.AND. LCNT.GE.MM+3) GO TO 1350
1350 CONTINUE
WRITE(LUO,1420)
RETURN
SUBROUTINE FUNC(COEF,MM1)

A SIMPLE TEST FUNCTION, WITH THREE UNKNOWN COEFFICIENTS
COEF(J), J=1,3, IS TO BE MINIMIZED. NOTE THE CURRENT FUNCTION
VALUE (THE MM+1 th VERTEX OF THE SIMPLEX) IS STORED IN COEF(MM+1)

DIMENSION COEF(II)
IMPLICIT DOUBLE PRECISION (A-H.O-Z)

TERM1=COEF(1)-1.0
TERM2=COEF(2)-2.0
TERM3=COEF(3)-3.0
COEF(MM1)=TERM1**2 + TERM2**2 + TERM3**2
RETURN

CONSTRAINT CONDITION EXCEEDED - SEND BACK A MESSAGE TO
SUBROUTINE SIMPLX, BY TAGGING ON A LARGE VALUE TO THE FUNCTION.
NOTE ---- USER MUST PROTECT AGAINST SUCH OCCURRENCES AS TRYING
TO TAKE LOGARITHMS OF 0 OR NEGATIVE NUMBERS, ETC. TREAT THEM
AS CONSTRAINTS, AND DIRECT PROGRAM TO STATEMENT 999, WHEN
NECESSARY.

CONTINUE
COEF(MM1)=COEF(MM1)+1.030
RETURN
END
SUBROUTINE NEWVP(MM1,SIMP,RNEXT,IH)

THIS SUBROUTINE STORES THE NEW CHOICES FOR VERTICES, WHICH HAVE
RESULTED IN A DECREASE IN THE VALUE OF THE RESPONSE FUNCTION.

DIMENSION SIMP(I,I),RNEXT(I),IH(I)

IMPLICIT DOUBLE PRECISION (A-H,O-Z)

DO 3010 I=1,MM1
SIMP(I,I/MM1)=RNEXT(I)
CONTINUE
RETURN
END
SUBROUTINE ORDER(MM1),SIMP,L,IH)

THIS SUBROUTINE DETERMINES CURRENT LOWEST AND HIGHEST VERTEXES, AND STORES ORDER INFORMATION USING SECOND INDEX OF SIMP(J,I).

THIS WILL BE USED BY SUBROUTINE SIMPLEX IN DETERMINING THE NEXT TRIAL SHAPE AND LOCATION OF THE SIMPLEX.

DIMENSION SIMP(11,1),L(11),IH(1)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)

DO 4010 J=1,MM1
   DO 4010 I=1,MM1
      IF (SIMP(J,I).LT.SIMP(J,L(I))) L(I)=I
      IF (SIMP(J,I).GT.SIMP(J,IH(I))) IH(I)=I
   4010 CONTINUE
4020 CONTINUE
RETURN
END
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