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FUNCTION OPTIMIZATION PACKAGE

VERSION FLOPT1

J.W. Bandler and W.Y. Chu

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FACULTY OF ENGINEERING  
McMASTER UNIVERSITY  
HAMILTON, ONTARIO, CANADA





# FUNCTION OPTIMIZATION PACKAGE:

## VERSION FLOPT1

J.W. Bandler and W.Y. Chu

Abstract The program developed solves unconstrained optimization problems by the Fletcher method. It is adaptable to solving constrained problems by using sequential unconstrained minimization techniques. The program is available for batch processing as well as on the time-sharing system INTERCOM of McMaster's CDC 6400.

### I. INTRODUCTION

The package FLOPT1 is a modified and more concise version of GRADMIN [1] to be used for optimizing any well-behaved once continuously differentiable unconstrained objective function of the form

$U = U(x_1, x_2, \dots, x_n)$ , where  $x_1, x_2, \dots, x_n$  are independent variables. By applying the Fiacco-McCormick method [2], objective functions subject to equality and/or inequality constraints can readily be optimized.

Three options are available for the package FLOPT1. The user can access the package for batch processing or he can use the package on the time-sharing system INTERCOM. Except for using the demonstration program, the user has to supply the main program and a subroutine called FUNCT which defines the objective function, the constraint functions (if applicable) and all first-order partial derivatives.

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The authors are with the Group on Simulation, Optimization and Control, and Department of Electrical Engineering, McMaster University, Hamilton, Ontario, Canada.

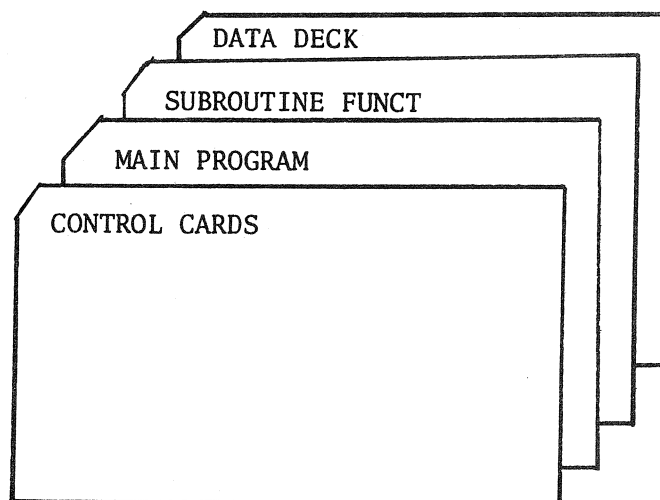
## II. USAGE

The three options of the package FLOPT1 are stored on permanent files; each has its own filename. They are called:

1. FLOPT1B [for batch processing]
2. FLOPT1I [for INTERCOM]
3. FLOPT1D [for the demonstration program on INTERCOM]

### A. Batch processing

1. Set up the input deck as follows:



### 2. CONTROL CARDS

A typical set of control cards is:

```

ABCD.                                USER NAME
ATTACH, &fn, FLOPT1B, ID = *****, MR = 1.†
FTN.
LOAD (&fn)
LGO.
END OF RECORD
PROGRAM TST(INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT)
3. MAIN PROGRAM

```

Write the main program as indicated below:

(a) Dimension the following arrays

$$X(N), G(N), EPS(N), H(K)$$

where  $N$  = The number of independent variables

$$K = N*(N+7)/2$$

(b) Supply the values of the following parameters.

$N$  = The number of independent variables

$$K = N*(N+7)/2$$

$M = 1$  if data deck is to be read

$= 0$  if data deck is not to be read.

Always set  $M$  equal to 1 for the first call of FLOPT1.

(c) Call subroutine FLOPT1 as follows:

$$\text{CALL FLOPT1}(N, K, M, X, G, H, EPS)$$

(d) Add STOP and END cards.

---

<sup>†</sup> &fn stands for logical filename of no more than 7 characters.  
Appropriate identification parameter ID should be inserted in \*\*\*\*\*,.

## 4. SUBROUTINE FUNCT

This subroutine defines the objective function, the constraints (where applicable) and all first-order partial derivatives. It is to be written as follows:

```
SUBROUTINE FUNCT(X, G, U)
```

```
  DIMENSION X(N), G(N)
```

where N = The number of independent variables (to be entered explicitly in the dimension statement)

Define the objective function

$$U = U(x_1, x_2, \dots, x_n)$$

Define the gradients of the objective function

$$G(1) = \frac{\partial U}{\partial x_1}$$

$$G(2) = \frac{\partial U}{\partial x_2}$$

$$\vdots$$

$$G(N) = \frac{\partial U}{\partial x_n}$$

Add RETURN and END cards.

If other statements are required for defining the function or the gradients, they may be added to this subroutine, e.g., function U may be defined in another subprogram which may then be called by subroutine FUNCT. Additional statements are also required if the problem is subject to constraints (See Appendix A).

## 5. DATA DECK

Parameters to be supplied as input data are defined below.

MAX        Maximum number of iterations allowed

IPT        Intermediate output is printed out every IPT iterations;  
it should be 0 if no intermediate output is desired

ID         Input data is printed out when ID=1; it should be 0 if  
input data is not to be printed

EST        Minimum estimated value of the objective function

X(I),      Starting values for the variables

I=1,N       $x_1, x_2, \dots, x_n$

EPS(I),    Test quantities used by Fletcher method  
I=1,N

Recommended values for some of the parameters are

MAX = 100

EST = 0.0

EPS(I), I=1,N Each = 1.E-6

## 6. ARRANGEMENT OF THE DATA DECK

| CARD NO.               | FORMAT | PARAMETERS    |
|------------------------|--------|---------------|
| 1                      | 3I5    | MAX, IPT, ID  |
| 2                      | E16.8  | EST           |
| As many as<br>required | 5E16.8 | X(I), I=1,N   |
| As many as<br>required | 5E16.8 | EPS(I), I=1,N |

## B. Time-sharing system INTERCOM

On the time-sharing system INTERCOM, the user may either access the standard package or the demonstration program. To use the standard package:

1. The user should access the file by typing the command  
ATTACH, lfn, FLOPT1I, ID = \*\*\*\*\*†
2. The user then gets into the EDITOR mode to create the main program and subroutine FUNCT required by the package. This can be done by typing the commands

EDITOR.

CREATE

The main program and subroutine FUNCT should be written in the same manner as described in the previous section. However, there are some minor adjustments. In the main program, the dimension statement should be

```
DIMENSION X(N), G(N), EPS(N), H(K), XS(N)
```

and the CALL statement should be

```
CALL FLOPT1 (N, K, M, X, G, H, EPS, XS, JOPT)
```

The parameter JOPT, which specifies the mode of optimization, has to be defined. For unconstrained optimization, JOPT should be set to 0; for constrained optimization, JOPT has to be set to 1.

After typing the main program and subroutine FUNCT, the user may leave the EDITOR mode by typing the commands

SAVE, filename

BYE



3. The program just written has to be compiled. The user should type the command

FTN, I = filename.

4. To execute the program with the package FLOPT1, the necessary commands are

CONNECT, INPUT, OUTPUT.

XEQ.

LOAD = LGO, &fn<sup>†</sup>.

EXECUTE

5. The input data required is the same as in batch processing. However, in the interactive mode, the user will be instructed to enter the required data. Input format is arbitrary. The user may separate each value by a comma, a blank, a few blanks or by typing the RETURN key. If a line cannot accommodate a specific input string, the user may go to the next line by typing the LINE FEED key. Unless specified, questions are expected to be answered by YES or NO. The user is also allowed to modify his data after he has entered all the data.

At the end of the run, the computer will await an instruction to stop execution or to rerun the program with different input data.

To use the demonstration program, the user simply types the following commands:

ATTACH, &fn, FLOPT1D, ID = \*\*\*\*\*.

CONNECT, INPUT, OUTPUT.

XEQ, &fn.

---

<sup>†</sup> &fn stands for logical filename of no more than 7 characters. It should be the same in the ATTACH command and in the LOAD command.

The main program and subroutine FUNCT for a specific problem will be printed out. The user is then asked to enter the data and the program is executed.

### III. COMMENTS

The user will find much flexibility when using the package on INTERCOM. However, for a long subroutine FUNCT, it is advisable to store the created program on permanent file. The user can subsequently call back his program for execution.

In all the three options, by choosing appropriate values of IPT and ID, the user may or may not print out the input data and the intermediate output. Problems with constraints may be solved using the Fiacco-McCormick techniques as illustrated in Appendix C. In Appendix A, instructions for using the package to solve problems with constraints are given. Results for some of the problems solved using this package have been included in Appendix B and C. Appendix D shows the general structure of the package.

### REFERENCES

- [1] J.W. Bandler and V.K. Jha, "GRADMIN - a package for function minimization using efficient gradient methods", Department of Electrical Engineering, McMaster University, Hamilton, Ontario, Canada, 1972, internal report.

- [2] A.V. Fiacco and G.P. McCormick, "Computational algorithm for the sequential unconstrained minimization technique for nonlinear programming", Management Science, vol. 10, pp. 601-617, July 1964.
- [3] R. Fletcher, "A new approach to variable metric algorithms", Computer J., vol. 13, pp. 317-322, Aug. 1970.

## APPENDIX A

The program package is primarily written to solve unconstrained optimization problems. By using the Fiacco-McCormick [2] techniques, a constrained problem can readily be transformed into an unconstrained one. The technique is basically to add the constraints as penalties to the unconstrained objective function. For example, to minimize with respect to  $\underset{\sim}{\phi}$

$$U = U(\underset{\sim}{\phi}) \quad (\text{A.1})$$

subject to inequality constraints

$$\underset{\sim}{g}(\underset{\sim}{\phi}) \geq \underset{\sim}{0} \quad (\text{A.2})$$

and equality constraints

$$\underset{\sim}{h}(\underset{\sim}{\phi}) = \underset{\sim}{0} \quad (\text{A.3})$$

A new objective function is defined

$$P(\underset{\sim}{\phi}, r) = U(\underset{\sim}{\phi}) + r \left[ \sum_{i=1}^m \frac{1}{g_i(\underset{\sim}{\phi})} \right] + \frac{1}{\sqrt{r}} \left[ \sum_{j=1}^s h_j^2(\underset{\sim}{\phi}) \right] \quad (\text{A.4})$$

to be minimized instead of  $U(\underset{\sim}{\phi})$ . By reducing the parameter  $r$ , the effect of the penalty is reduced and under suitable conditions, a constrained minimum will be obtained.

A typical way of implementing the Fiacco-McCormick method is as follows

1. In subroutine FUNCT, define the penalty function as described above.

To avoid possible confusion, define the unconstrained objective function as  $F$  and the new objective function as  $U$  (function  $P$  in Eq. A.4). The constraint functions, their gradients and the gradients of the new objective function have to be defined. Appropriate adjustment in the dimension statement is expected.

2. In the main program, define the parameter  $r$  (the value of  $r$  should be available to the subroutine FUNCT and this can easily be done by using a COMMON statement) and put the subroutine FLOPT1 in a DO loop. In the batch processing option, the user has to pre-determine the number of calls of subroutine FLOPT1. In the interactive processing option, there is no such restriction.

Samples of the main program required when solving constrained problems are shown below:

For batch processing option FLOPT1B

```

DIMENSION X(N), G(N), EPS(N), H(K)

COMMON/SS/R

M = 1

R = 1.0

DO 1 I = 1, 5

CALL FLOPT1 (N, K, M, X, G, H, EPS)

M = 0

R = 0.01*R

1 CONTINUE

STOP

END

```

For interactive processing option FLOPT1I

```
DIMENSION X(N), G(N), EPS(N), H(K), XS(N)
COMMON/SS/R
M = 1
R = 1.0
JOPT = 1
1 CALL FLOPT1 (N, K, M, X, G, H, EPS, XS, JOPT)
M = 0
R = 0.01*R
GO TO 1
END
```

## APPENDIX B

To minimize

$$U = 100(x_1^2 - x_2)^2 + (1 - x_1)^2$$

with the starting point:

$$x_1 = 0.0$$

$$x_2 = 0.0$$

A suitable listing of the input deck, a printout of the input data and some final results (using the batch-processing option) are given in Figs. 1-3.

```

HSRO.
ATTACH,TAPE,FLOPT1R,ID=HSROBNLER,MR=1.
FTN.
LOAD(TAPE)
LGO.
I      6400 END OF RECORD
      PROGRAM TST (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION X(2),G(2),H(9),FPS(2)
      CALL FLOPT1(2,9,1,X,G,H,FPS)
      STOP
      END

C
      SUBROUTINE FUNCT(X,G,U)
      DIMENSION X(2),G(2)
      A=X(1)*X(1)
      B=A-X(2)
      C=1.0-X(1)
C THE OBJECTIVE FUNCTION
      U=100.*B*B+C*C
C GRADIENTS OF THE OBJECTIVE FUNCTION WITH RESPECT TO THE VARIABLE
C PARAMETERS
      G(1)=400.0*(X(1)*A-X(1)*X(2))-2.0*C
      G(2)=-200.0*B
      RETURN
      END

I      6400 END OF RECORD
      100      1      1
      0.0
      0.0      0.0
      1.E-      61.E-      6
I      END OF FILE

```

Fig. 1 Main program and subroutine FUNCT for the example of Appendix B. Input data is also shown.



INPUT DATA

```

NUMBER OF INDEPENDENT VARIABLES.....N = 2
-----
MAXIMUM NUMBER OF ALLOWABLE ITERATIONS.....MAX = 100
INTERMEDIATE PRINTOUT AT EVERY IPT ITERATIONS.....IPT = 1
-----
STARTING VALUE FOR VECTOR X(I).....X( 1) = 0.
                                         X( 2) = 0.
TEST QUANTITIES TO BE USED.....EPS( 1) = .100000E-05
                                         EPS( 2) = .100000E-05
-----
ESTIMATE OF LOWER BOUND OF FUNCTION TO BE MINIMIZED..EST = 0.

```

Fig. 2 Input data for the example of Appendix B.

```

IFXIT = 1
CRITERION FOR OPTIMUM (CHANGE IN VECTOR X .LT. EPS) HAS BEEN SATISFIED

```

OPTIMAL SOLUTION FOUND BY FLETCHER METHOD

```

U = .534187E-13
X( 1) = .100000E+01      G( 1) = .856057E-05
X( 2) = .100000E+01      G( 2) = -.475743E-05
NUMBER OF FUNCTION EVALUATIONS = 30
EXECUTION TIME IN SECONDS = .243

```

Fig. 3 Results for the example of Appendix B.

## APPENDIX C

To minimize

$$F = x_1^2 + 4x_2^2$$

subject to the following equality constraint

$$h = x_1 + 2x_2 - 1$$

The unconstrained function for this problem using the Fiacco-McCormick technique is

$$U = F + h^2/\sqrt{r}$$

The starting point used is

$$x_1 = 0.0$$

$$x_2 = 0.0$$

Commands to enter the EDITOR mode, a listing of the main program and subroutine FUNCT, commands to compile the program, access the option FLOPT11 and execute the program, instructions for entering data, a record of the input data and some final results are given in Figs. 4-8.

```
MCMASTER UNIV INTERCOM 4.1
DATE 08/15/73
TIME 21.36.54.
```

```
PLEASE LOGIN
LOGIN.
ENTER USER NAME- HSBJ
XXXXXXXXXXXXXXXXX ENTER PASSWORD-
```

```
08/15/73  LOGGED IN AT 21.38.09.
          WITH USER-ID BR
          EQUIP/PORT 70/12
COMMAND- EDITOR.
..CREATE
```

Fig. 4 Commands for entering the EDITOR mode.

```

100=      PROGRAM TST(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
110=      COMMON/SS/R
120=      DIMENSION X(2),G(2),H(9),EPS(2),XS(2)
130=      R=1.0
140=      M=1
150=1     CALL FLOPT1(2,9,M,X,G,H,EPS,XS,1)
160=      M=0
170=      R=R*.01
180=      GO TO 1
190=      END
200=      SUBROUTINE FUNCT(X,G,U)
210=      COMMON/SS/R
220=      DIMENSION X(2),G(2),GF(2),GC(2)
230=      A=2.*X(2)
235=C     THE OBJECTIVE FUNCTION
240=      F=X(1)*X(1)+A*A
245=C     GRADIENTS OF THE OBJECTIVE FUNCTION
250=      GF(1)=2.*X(1)
260=      GF(2)=4.*A
265=C     THE EQUALITY CONSTRAINT
270=      C=X(1)+A-1.
275=C     GRADIENTS OF THE CONSTRAINT
280=      GC(1)=1.
290=      GC(2)=2.
292=C     THE UNCONSTRAINED OBJECTIVE FUNCTION USING FIACCO-MCCORMICK
293=C     TECHNIQUE
295=      U=F+(C*C)/SQRT(R)
300=      AB=2.*C/SQRT(R)
305=C     GRADIENTS OF THE OBJECTIVE FUNCTION U
310=      G(1)=GF(1)+AB*GC(1)
320=      G(2)=GF(2)+AB*GC(2)
330=      RETURN
340=      END
..SAVE,A
..BYE
COMMAND- FTN,I=A.
          .323 CP SECONDS COMPILATION TIME
COMMAND- ATTACH,XX,FLOPT1I, ID=HSBOBNLER.
PF CYCLE NO. = 006
COMMAND- CONNECT,INPUT,OUTPUT.
COMMAND- XEQ.
OPTION=LOAD=LGO,XX.
OPTION=EXECUTE

```

Fig. 5 A listing of the main program and subroutine FUNCT of the example of Appendix C. Commands for compiling and executing the program with option FLOPT1I are also shown.

YOU ARE WELCOME TO USE THE PACKAGE " F L O P T 1 ".  
 PLEASE SUPPLY DATA WHEN ASKED FOR. YOU CAN ENTER YOUR DATA IN ANY  
 FORMAT, HOWEVER, BE REASONABLE. PLEASE SEPARATE EACH VALUE BY A  
 COMMA, A BLANK OR TYPING THE RETURN KEY. THANK YOU.

SPECIFY THE MAXIMUM NUMBER OF ITERATIONS ALLOWED.

1+ 100

ENTER AN INTEGER SO THAT INTERMEDIATE OUTPUT WILL BE PRINTED AFTER  
 EVERY SPECIFIED NUMBER OF ITERATIONS. ENTER 0 IF YOU DON'T WANT  
 ANY INTERMEDIATE OUTPUT.

2+ 0

ENTER 1 IF YOU WANT TO HAVE A RECORD OF YOUR INPUT DATA, OTHERWISE  
 ENTER 0.

3+ 1

SPECIFY A MINIMUM ESTIMATED VALUE OF THE OBJECTIVE FUNCTION.

4+ 0.0

ENTER STARTING VALUES FOR THE VARIABLE PARAMETERS.

5+ 0.0 0.0

ENTER SMALL VALUES FOR TESTING CONVERGENCE.

6+ 1.E-6,1.E-6

ANY MODIFICATION

# YES

WHICH ENTRY

# 1

SPECIFY THE MAXIMUM NUMBER OF ITERATIONS ALLOWED.

1+ 50

ANY MODIFICATION

# NO

YOUR DATA IS NOW BEING PROCESSED. IT MAY TAKE SOME TIME BEFORE  
 RESULTS ARE AVAILABLE. PLEASE BE PATIENT.

Fig. 6 Instructions for entering data for the example of Appendix C.

## INPUT DATA

```

-----
NUMBER OF INDEPENDENT VARIABLES.....N = 2
MAXIMUM NUMBER OF ALLOWABLE ITERATIONS.....MAX = 50
INTERMEDIATE PRINTOUT AT EVERY IPT ITERATIONS.....IPT = 0
STARTING VALUE FOR VECTOR X(I)
    X( 1) = 0.
    X( 2) = 0.
TEST QUANTITIES TO BE USED
    EPS( 1) = .100000E-05
    EPS( 2) = .100000E-05
ESTIMATE OF LOWER BOUND OF FUNCTION TO BE MINIMIZED..EST = 0.

```

Fig. 7 Input data for the example of Appendix C.

```

IEXIT = 1
CRITERION FOR OPTIMUM (CHANGE IN VECTOR X .LT. EPS) HAS BEEN SATISFIED

```

## OPTIMAL SOLUTION FOUND BY FLETCHER METHOD

```

-----
    U = .499975E+00
X( 1) = .499975E+00      G( 1) = -.335586E-09
X( 2) = .249988E+00      G( 2) = -.672216E-09

```

```

    NUMBER OF FUNCTION EVALUATIONS = 7
    EXECUTION TIME IN SECONDS = .014

```

```

DO YOU WANT TO TERMINATE THE PROGRAM
#      YES

```

```

    TOTAL NO. OF FUNCTION EVALUATIONS = 33
    TOTAL EXECUTION TIME IN SECONDS = .072

```

```

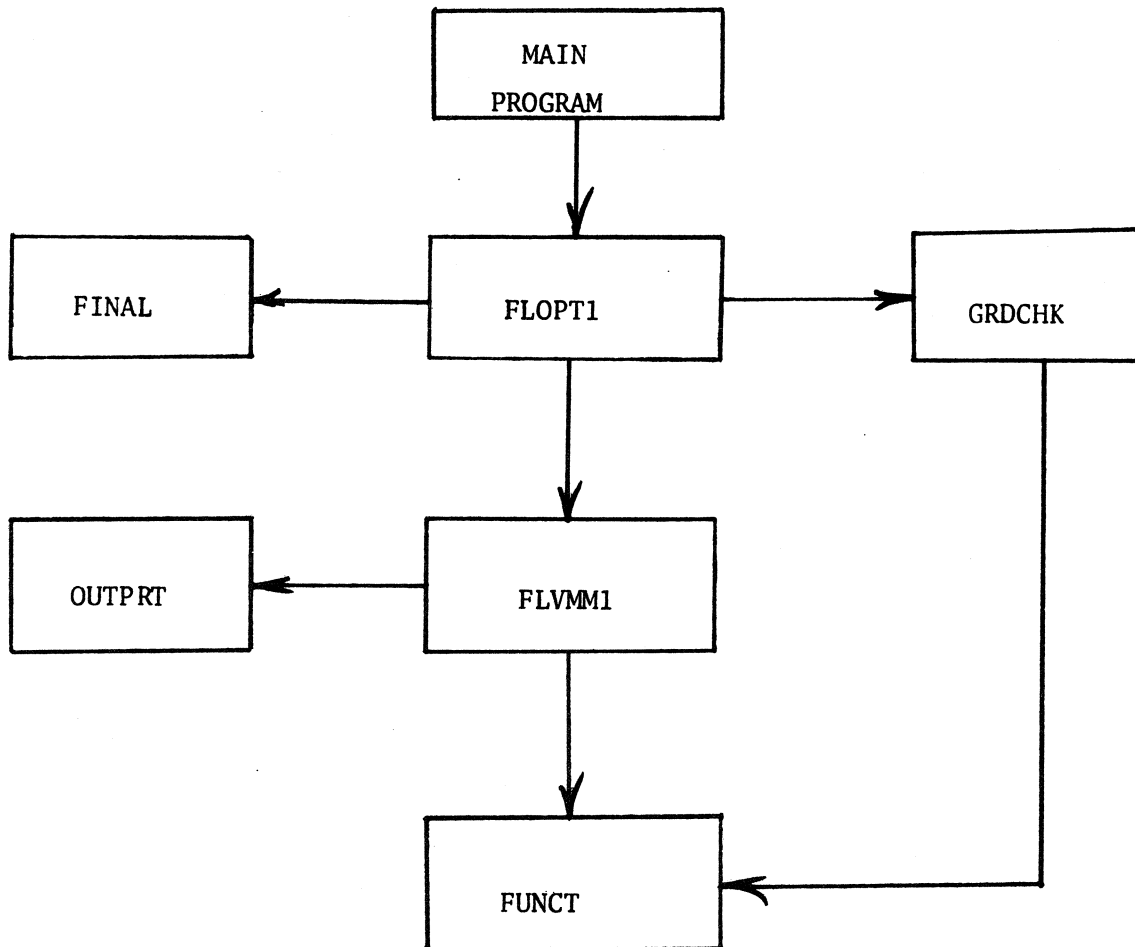
EXIT

```

Fig. 8 Results for the example of Appendix C.

## APPENDIX D

The general structure of the package is



Attached is the complete FORTRAN listing of the package - option FLOPT1I.

|   |   |   |    |
|---|---|---|----|
|   | SUBROUTINE FLOPT1 (N,K,M,X,G,H,FPS,XS,JOPT) | A | 1  |
|   | COMMON /PLK/ KO                             | A | 2  |
|   | COMMON /BLK1/ NF                            | A | 3  |
|   | LOGICAL UNITH                               | A | 4  |
|   | DIMENSION X(N), G(N), FPS(N), H(K), XS(N)   | A | 5  |
|   | DATA D/2HNO/                                | A | 6  |
|   | UNITH=.TRUE.                                | A | 7  |
|   | IF (M.FQ.0) GO TO 9                         | A | 8  |
|   | TIMET=0.0                                   | A | 9  |
|   | NFT=0                                       | A | 10 |
|   | WRITE (6,24)                                | A | 11 |
|   | WRITE (6,25)                                | A | 12 |
|   | READ (5,*) MAX                              | A | 13 |
|   | WRITE (6,26)                                | A | 14 |
|   | READ (5,*) IPT                              | A | 15 |
|   | WRITE (6,27)                                | A | 16 |
|   | READ (5,*) ID                               | A | 17 |
|   | WRITE (6,28)                                | A | 18 |
|   | READ (5,*) EST                              | A | 19 |
|   | WRITE (6,29)                                | A | 20 |
|   | READ (5,*) X                                | A | 21 |
|   | WRITE (6,30)                                | A | 22 |
|   | READ (5,*) FPS                              | A | 23 |
| 1 | WRITE (6,17)                                | A | 24 |
|   | READ (5,18) ANS                             | A | 25 |
|   | IF (ANS.FQ.0) GO TO 8                       | A | 26 |
|   | WRITE (6,19)                                | A | 27 |
|   | READ (5,*) NN                               | A | 28 |
|   | GO TO (2,3,4,5,6,7), NN                     | A | 29 |
| 2 | WRITE (6,25)                                | A | 30 |
|   | READ (5,*) MAX                              | A | 31 |
|   | GO TO 1                                     | A | 32 |
| 3 | WRITE (6,26)                                | A | 33 |
|   | READ (5,*) IPT                              | A | 34 |
|   | GO TO 1                                     | A | 35 |
| 4 | WRITE (6,27)                                | A | 36 |
|   | READ (5,*) ID                               | A | 37 |
|   | GO TO 1                                     | A | 38 |
| 5 | WRITE (6,28)                                | A | 39 |
|   | READ (5,*) EST                              | A | 40 |
|   | GO TO 1                                     | A | 41 |
| 6 | WRITE (6,29)                                | A | 42 |
|   | READ (5,*) X                                | A | 43 |
|   | GO TO 1                                     | A | 44 |
| 7 | WRITE (6,30)                                | A | 45 |
|   | READ (5,*) FPS                              | A | 46 |
|   | GO TO 1                                     | A | 47 |
| 8 | WRITE (6,31)                                | A | 48 |
|   | IF (ID.FQ.0) GO TO 9                        | A | 49 |
|   | WRITE (6,32)                                | A | 50 |
|   | WRITE (6,33) N                              | A | 51 |
|   | WRITE (6,34) MAX                            | A | 52 |
|   | WRITE (6,35) IPT                            | A | 53 |
|   | WRITE (6,36)                                | A | 54 |
|   | WRITE (6,37) (I,X(I),I=1,N)                 | A | 55 |
|   | WRITE (6,38)                                | A | 56 |
|   | WRITE (6,39) (I,FPS(I),I=1,N)               | A | 57 |
|   | WRITE (6,40) EST                            | A | 58 |
| 9 | CONTINUE                                    | A | 59 |



|    |   |   |     |
|----|---|---|-----|
|    | IF (JOPT.EQ.1) GO TO 11   | A | 60  |
|    | DO 10 I=1,N   | A | 61  |
|    | XS(I)=X(I)  | A | 62  |
| 10 | CONTINUE  | A | 63  |
| 11 | MF=1  | A | 64  |
|    | CALL GRDCHK (N,X,G)   | A | 65  |
|    | IF (IPT.EQ.0) GO TO 12  | A | 66  |
|    | WRITE (6,41)  | A | 67  |
|    | WRITE (6,42)  | A | 68  |
|    | WRITE (6,43)  | A | 69  |
| 12 | CALL SECOND (T1)  | A | 70  |
|    | CALL FLVMM1 (N,K,X,U,G,H,UNITH,FST,FPS,MAX,IPT)                     | A | 71  |
|    | CALL SECOND (T2)  | A | 72  |
|    | CALL FINAL (N,X,U,G)  | A | 73  |
|    | T=T2-T1   | A | 74  |
|    | WRITE (6,44) T  | A | 75  |
|    | TIMET=TIMET+T   | A | 76  |
|    | NFT=NFT+MF  | A | 77  |
|    | WRITE (6,20)  | A | 78  |
|    | READ (5,18) ANS   | A | 79  |
|    | IF (JOPT.EQ.1) GO TO 13   | A | 80  |
|    | GO TO 14  | A | 81  |
| 1  | IF (ANS.EQ.0) GO TO 16  | A | 82  |
|    | WRITE (6,21) NFT  | A | 83  |
|    | WRITE (6,22) TIMET  | A | 84  |
|    | CALL EXIT   | A | 85  |
| 14 | IF (ANS.NE.0) GO TO 16  | A | 86  |
|    | WRITE (6,23)  | A | 87  |
|    | READ (5,18) ANS   | A | 88  |
|    | IF (ANS.EQ.0) GO TO 1   | A | 89  |
|    | DO 15 I=1,N   | A | 90  |
|    | X(I)=XS(I)  | A | 91  |
| 15 | CONTINUE  | A | 92  |
|    | GO TO 1   | A | 93  |
| 16 | RETURN  | A | 94  |
|    |   | A | 95  |
|    |   | A | 96  |
| 17 | FORMAT (1H0,*ANY MODIFICATION*/* , *)                               | A | 97  |
| 18 | FORMAT (A10)  | A | 98  |
| 19 | FORMAT (1H ,*WHICH ENTRY*/* , *)                                    | A | 99  |
| 20 | FORMAT (1H0/1H ,*DO YOU WANT TO TERMINATE THE PROGRAM*/* , *)       | A | 100 |
| 21 | FORMAT (1H0,1X,*TOTAL NO. OF FUNCTION EVALUATIONS =*,I5)            | A | 101 |
| 22 | FORMAT (1H0,3X,*TOTAL EXECUTION TIME IN SECONDS =*,F7.3/)           | A | 102 |
| 23 | FORMAT (1H ,*SHALL I RETAIN THE STARTING VALUES OF THE VARIABLE PA  | A | 103 |
|    | RAMETERS*/* , *)  | A | 104 |
| 24 | FORMAT (1H1,*YOU ARE WELCOME TO USE THE PACKAGE ' F L O P T 1 '.* / | A | 105 |
|    | 1* PLEASE SUPPLY DATA WHEN ASKED FOR. YOU CAN ENTER YOUR DATA IN A  | A | 106 |
|    | 2NY*/* FORMAT, HOWEVER, BE REASONABLE. PLEASE SEPARATE EACH VALUE   | A | 107 |
|    | 2RY A*/* COMMA, A BLANK OR TYPING THE RETURN KEY. THANK YOU.* /)    | A | 108 |
| 25 | FORMAT (1H ,*SPECIFY THE MAXIMUM NUMBER OF ITERATIONS ALLOWED.* /*  | A | 109 |
|    | 11( *)  | A | 110 |
| 26 | FORMAT (1H ,*ENTER AN INTEGER SO THAT INTERMEDIATE OUTPUT WILL BE   | A | 111 |
|    | 1PRINTED AFTER*/* EVERY SPECIFIED NUMBER OF ITERATIONS. ENTER 0 IF  | A | 112 |
|    | 2 YOU DON'T WANT*/* ANY INTERMEDIATE OUTPUT.* /*                    | A | 113 |
| 27 | FORMAT (1H ,*ENTER 1 IF YOU WANT TO HAVE A RECORD OF YOUR INPUT DA  | A | 114 |
|    | 1TA, OTHERWISE*/* ENTER 0.* /*                                      | A | 115 |
| 28 | FORMAT (1H ,*SPECIFY A MINIMUM ESTIMATED VALUE OF THE OBJECTIVE FU  | A | 116 |
|    | 1NCTION.* /*  | A | 117 |
| 29 | FORMAT (1H ,*ENTER STARTING VALUES FOR THE VARIABLE PARAMETERS.* /* | A | 118 |

|    |   |   |     |
|----|---|---|-----|
| 1  | 5( *)   | A | 119 |
| 20 | FORMAT (1H ,*ENTER SMALL VALUES FOR TESTING CONVERGENCE.*/* 6( *)       | A | 120 |
| 21 | FORMAT (//,* YOUR DATA IS NOW BEING PROCESSED. IT MAY TAKE SOME T       | A | 121 |
|    | IME BEFORE*/* RESULTS ARE AVAILABLE. PLEASE BE PATIENT.*)               | A | 122 |
| 22 | FORMAT (1H1,*INPUT DATA*/,1H ,10(*-*))                                  | A | 123 |
| 22 | FORMAT (1H0,*NUMBER OF INDEPENDENT VARIABLES*,24(*.*),*N =*,I4)         | A | 124 |
| 24 | FORMAT (1H ,*MAXIMUM NUMBER OF ALLOWABLE ITERATIONS*,15(*.*),*MAX       | A | 125 |
|    | 1=*,I4)   | A | 126 |
| 25 | FORMAT (1H ,*INTERMEDIATE PRINTOUT AT EVERY IPT ITERATIONS*,8(*.*)      | A | 127 |
|    | 1,*IPT =*,I4)   | A | 128 |
| 26 | FORMAT (1H ,*STARTING VALUE FOR VECTOR X(I)*)                           | A | 129 |
| 27 | FORMAT (1H ,5X,*X(*,I2,*) =*,E14.6)                                     | A | 130 |
| 28 | FORMAT (1H ,*TEST QUANTITIES TO BE USED*)                               | A | 131 |
| 29 | FORMAT (1H ,3X,*EPS(*,I2,*) =*,F14.6)                                   | A | 132 |
| 40 | FORMAT (1H ,*ESTIMATE OF LOWER BOUND OF FUNCTION TO BE MINIMIZED*,      | A | 133 |
|    | 12(*.*),*FST =*,F14.6)  | A | 134 |
| 41 | FORMAT (1H1)  | A | 135 |
| 42 | FORMAT (1H ,*OPTIMIZATION BY FLTCHER METHOD*/,1H ,31(*-*))              | A | 136 |
| 4  | FORMAT (1H0,*ITER.* ,2X,*FUNCT.* ,5X,*TIME(SEC)* ,5X,*OBJECTIVE* ,6X,*  | A | 137 |
|    | 1VARIABLE* ,7X,*GRADIENT*/1H ,1X,*NO.* ,3X,*EVALU.* ,6X,*ELAPSED* ,6X,* | A | 138 |
|    | 2FUNCTION* ,6X,*VECTOR X(I)* ,4X,*VECTOR G(I)* ,/)                      | A | 139 |
| 44 | FORMAT (1H0,9X,*EXECUTION TIME IN SECONDS =*,F7.3)                      | A | 140 |
|    | END   | A | 141 |

|   |   |   |    |
|---|---|---|----|
|   | SUBROUTINE FLVMM1 (N,K,X,U,G,H,UNITH,FST,EPS,MAX,IPT) | R | 1  |
|   | DIMENSION X(N), G(N), EPS(N), H(K)                    | B | 2  |
|   | COMMON /BLK1/ NF                                      | B | 3  |
|   | COMMON /BLK/ KO                                       | B | 4  |
|   | LOGICAL CONV,UNITH                                    | R | 5  |
|   | CALL SECONDD (T3)                                     | R | 6  |
|   | KO=0  | R | 7  |
|   | CALL FUNCT (X,G,U)                                    | B | 8  |
|   | IF (U.LT.FST) GO TO 23                                | R | 9  |
|   | ITN=1   | R | 10 |
|   | STEP=1.0  | B | 11 |
|   | ID=N+N  | B | 12 |
|   | IH=ID+N   | B | 13 |
|   | IF (.NOT.UNITH) GO TO 2                               | B | 14 |
|   | IJ=IH+1   | R | 15 |
|   | DO 1 I=1,N  | B | 16 |
|   | DO 1 J=I,N  | B | 17 |
|   | H(IJ)=0.0   | B | 18 |
|   | IF (I.FQ.J) H(IJ)=1.0                                 | B | 19 |
| 1 | IJ=IJ+1   | B | 20 |
| 2 | CONV=.TRUE.   | B | 21 |
|   | GDX=0.0   | R | 22 |
|   | DO 6 I=1,N  | R | 23 |
|   | Z=0.0   | R | 24 |
|   | IJ=IH+I   | R | 25 |
|   | IF (I.FO.1) GO TO 4                                   | R | 26 |
|   | L=I-1   | B | 27 |
|   | DO 3 J=1,L  | B | 28 |
|   | Z=Z-H(IJ)*G(J)  | B | 29 |
|   | IJ=IJ+N-J   | R | 30 |
| 3 | CONTINUE  | B | 31 |
| 4 | DO 5 J=I,N  | R | 32 |
|   | Z=Z-H(IJ)*G(J)  | R | 33 |
|   | IJ=IJ+1   | B | 34 |
| 5 | CONTINUE  | R | 35 |
|   | IF (ABS(Z).GT.EPS(I)) CONV=.FALSE.                    | R | 36 |
|   | H(N+I)=Z  | B | 37 |
|   | GDX=GDX+G(I)*Z  | R | 38 |
| 6 | CONTINUE  | R | 39 |
|   | IF (IPT.FO.0) GO TO 7                                 | R | 40 |
|   | IF (MOD(ITN,IPT).NF.0) GO TO 7                        | R | 41 |
|   | CALL SECONDD (T4)                                     | B | 42 |
|   | TIME=T4-T3  | B | 43 |
|   | CALL OUTPRT (X,N,G,U,NF,ITN,TIME)                     | R | 44 |
| 7 | IFEXIT=1  | B | 45 |
|   | IF (CONV) GO TO 24                                    | R | 46 |
|   | IFEXIT=2  | R | 47 |
|   | IF (GDX.GF.0.0) GO TO 24                              | R | 48 |
|   | Z=1.0   | B | 49 |
|   | IF (ITN.LT.N.AND.UNITH) Z=STEP                        | R | 50 |
|   | W=2.*(FST-U)/GDX                                      | R | 51 |
|   | IF (W.LT.Z) Z=W                                       | R | 52 |
|   | STEP=Z  | B | 53 |
| 8 | GDX=GDX*Z   | B | 54 |
|   | DO 9 I=1,N  | B | 55 |
|   | H(N+I)=H(N+I)*Z                                       | B | 56 |
|   | X(I)=X(I)+H(N+I)                                      | R | 57 |
| 9 | CONTINUE  | B | 58 |
|   | NF=NF+1   | B | 59 |

|    |  |   |     |
|----|--|---|-----|
|    | CALL FUNCT (X,H,FP)  | R | 60  |
|    | IF (FP.LT.FST) GO TO 23  | B | 61  |
|    | IFEXIT=2   | R | 62  |
|    | IF (ITN.EQ.MAX) GO TO 24   | B | 63  |
|    | GPD <sub>X</sub> =0.0  | R | 64  |
|    | DO 10 I=1,N  | R | 65  |
|    | H(ID+I)=H(I)-G(I)  | R | 66  |
|    | GPD <sub>X</sub> =GPD <sub>X</sub> +H(I)*H(N+I)                          | R | 67  |
| 10 | CONTINUE   | R | 68  |
|    | DGD <sub>X</sub> =GPD <sub>X</sub> -GDX                                  | R | 69  |
|    | IF (U.GT.FP-0.0001*GDX) GO TO 12   | R | 70  |
|    | IFEXIT=4   | R | 71  |
|    | IF (GPD <sub>X</sub> .LT.0.0.AND.ITN.GT.N) GO TO 24                      | R | 72  |
|    | Z=2.*(U-FP)+GPD <sub>X</sub> +GDX  | R | 73  |
|    | W=SQRT(1.0-GDX/Z*GPD <sub>X</sub> /Z)*ABS(Z)                             | R | 74  |
|    | Z=1.0-(GPD <sub>X</sub> +W-Z)/(DGD <sub>X</sub> +2.0*W)                  | R | 75  |
|    | IF (Z.LT.0.1) Z=0.1  | R | 76  |
|    | DO 11 I=1,N  | R | 77  |
|    | X(I)=X(I)-H(N+I)   | R | 78  |
| 11 | CONTINUE   | R | 79  |
|    | GO TO 14   | R | 80  |
| 12 | U=FP   | R | 81  |
|    | DO 13 I=1,N  | R | 82  |
|    | G(I)=H(I)  | R | 83  |
| 1  | CONTINUE   | R | 84  |
|    | IF (DGD <sub>X</sub> .GT.0.0) GO TO 15                                   | R | 85  |
|    | GDX=GPD <sub>X</sub>   | R | 86  |
|    | Z=4.0  | R | 87  |
| 14 | STEP=Z*STEP  | R | 88  |
|    | GO TO 8  | R | 89  |
| 15 | IF (GPD <sub>X</sub> .LT.0.5*GDX) STEP=2.0*STEP                          | R | 90  |
|    | DGH <sub>DG</sub> =0.0   | R | 91  |
|    | DO 19 I=1,N  | R | 92  |
|    | Z=0.0  | R | 93  |
|    | IJ=IH+I  | R | 94  |
|    | IF (I.EQ.1) GO TO 17   | R | 95  |
|    | L=I-1  | R | 96  |
|    | DO 16 J=1,L  | R | 97  |
|    | Z=Z+H(IJ)*H(ID+J)  | R | 98  |
|    | IJ=IJ+N-J  | R | 99  |
| 16 | CONTINUE   | R | 100 |
| 17 | DO 18 J=I,N  | R | 101 |
|    | Z=Z+H(IJ)*H(ID+J)  | R | 102 |
|    | IJ=IJ+1  | R | 103 |
| 18 | CONTINUE   | R | 104 |
|    | DGH <sub>DG</sub> =DGH <sub>DG</sub> +Z*H(ID+I)                          | R | 105 |
|    | H(I)=Z   | R | 106 |
| 19 | CONTINUE   | R | 107 |
|    | IF (DGH <sub>DG</sub> .LT.0.0) DGH <sub>DG</sub> =DGD <sub>X</sub> *0.01 | R | 108 |
|    | IF (DGD <sub>X</sub> .LT.DGH <sub>DG</sub> ) GO TO 21                    | R | 109 |
|    | W=1.0+DGH <sub>DG</sub> /DGD <sub>X</sub>                                | R | 110 |
|    | DO 20 I=1,N  | R | 111 |
|    | H(N+I)=W*H(N+I)-H(I)   | R | 112 |
| 20 | CONTINUE   | R | 113 |
|    | DGD <sub>X</sub> =DGD <sub>X</sub> +DGH <sub>DG</sub>                    | R | 114 |
|    | DGH <sub>DG</sub> =DGD <sub>X</sub>                                      | R | 115 |
| 21 | IJ=IH  | R | 116 |
|    | DO 22 I=1,N  | R | 117 |
|    | W=H(N+I)/DGD <sub>X</sub>  | R | 118 |

|    |  |        |
|----|--|--------|
|    | Z=H(I)/DGHDC   | R 119  |
|    | DO 22 J=I,N  | R 120  |
|    | IJ=IJ+1  | B 121  |
| 22 | H(IJ)=H(IJ)+W*H(N+J)-Z*H(J)  | B 122  |
|    | ITN=ITN+1  | B 123  |
|    | GO TO 2  | B 124  |
| 23 | IFXIT=5  | B 125  |
| 24 | IF (IFXIT.EQ.1) KO=1   | R 126  |
|    | GO TO (25,26,27,26,28), IEXIT  | R 127  |
| 25 | WRITE (6,30) IEXIT   | B 128  |
|    | GO TO 29   | B 129  |
| 26 | WRITE (6,31) IEXIT   | R 130  |
|    | GO TO 29   | B 131  |
| 27 | WRITE (6,32) IEXIT   | R 132  |
|    | GO TO 29   | B 133  |
| 28 | WRITE (6,33) IEXIT   | R 134  |
| 29 | CONTINUE   | R 135  |
|    | RETURN   | B 136  |
| C  |  | B 137  |
| C  |  | B 138  |
| 30 | FORMAT (1H1,*IEXIT =*,I2,/1H ,*CRITERION FOR OPTIMUM (CHANGE IN VE<br>CTOR X .LT. EPS) HAS BEEN SATISFIED*)  | R 139  |
| 31 | FORMAT (1H1,*IEXIT =*,I2,/1H ,*EITHER OF THE FOLLOWING THINGS HAS<br>1HAPPENED*,/10X,*1. EPS CHOSEN IS TOO SMALL*,/10X,*2. GRADIENTS ARE<br>2 NOT CORRECT*,/10X,*3. MATRIX H GOES SINGULAR*) | R 141  |
| 32 | FORMAT (1H1,*IEXIT =*,I2,/1H ,*MAXIMUM NUMBER OF ALLOWABLE ITERATI<br>ON HAS BEEN EXCEEDED*)   | R 142  |
| 33 | FORMAT (1H1,*IEXIT =*,I2,/1H ,*FUNCTION VALUE LESS THAN MINIMUM ES<br>TIMATED HAS BEEN DETECTED*)  | R 144  |
|    | END  | R 145  |
|    |  | R 146  |
|    |  | R 147  |
|    |  | B 148- |

|   |  |   |    |
|---|--|---|----|
|   | SUBROUTINE GRDCHK (N,X,G)  | C | 1  |
|   | DIMENSION X(N), G(N), T(100)                                       | C | 2  |
|   | IC=0   | C | 3  |
|   | CALL FUNCT (X,G,U)   | C | 4  |
|   | WRITE (6,3)  | C | 5  |
|   | WRITE (6,4)  | C | 6  |
|   | DO 1 I=1,N   | C | 7  |
|   | DX=1.E-4*X(I)  | C | 8  |
|   | IF (ABS(DX).LT.1.E-10) DX=1.E-10                                   | C | 9  |
|   | X(I)=X(I)+DX   | C | 10 |
|   | CALL FUNCT (X,T,F2)  | C | 11 |
|   | X(I)=X(I)-2.0*DX   | C | 12 |
|   | CALL FUNCT (X,T,F1)  | C | 13 |
|   | Y=0.5*(F2-F1)/DX   | C | 14 |
|   | X(I)=X(I)+DX   | C | 15 |
|   | IF (ABS(Y).LT.1.E-14) Y=1.E-14                                     | C | 16 |
|   | IF (ABS(G(I)).LT.1.E-14) G(I)=1.E-14                               | C | 17 |
|   | YP=ABS((Y-G(I))/Y)*100.0   | C | 18 |
|   | WRITE (6,5) G(I),Y,YP  | C | 19 |
|   | IF (YP.GT.10.0) IC=1   | C | 20 |
| 1 | CONTINUE   | C | 21 |
|   | IF (IC.EQ.1) GO TO 2   | C | 22 |
|   | WRITE (6,6)  | C | 23 |
|   | RETURN   | C | 24 |
| 2 | WRITE (6,7)  | C | 25 |
|   | CALL EXIT  | C | 26 |
| C |  | C | 27 |
| C |  | C | 28 |
| 3 | FORMAT (1H1,*GRADIENT CHECK AT STARTING POINT*/1H ,32(*-*))        | C | 29 |
| 4 | FORMAT (1H0,5X,*ANALYTICAL GRADIENTS*,5X,*NUMERICAL GRADIENTS*,5X, | C | 30 |
|   | 1*PERCENTAGE ERROR*)   | C | 31 |
| 5 | FORMAT (1H ,8X,F14.6,10X,F14.6,8X,F14.6)                           | C | 32 |
| 6 | FORMAT (1H0,*GRADIENTS ARE O.K.*)                                  | C | 33 |
| 7 | FORMAT (1H0,*YOUR PROGRAM HAS BEEN TERMINATED BECAUSE GRADIENTS AR | C | 34 |
|   | IF INCORRECT*/1H ,*PLEASE CHECK IT AGAIN*)                         | C | 35 |
|   | END  | C | 36 |

```
SUBROUTINE OUTPRT (X,N,G,U,NE,ITN,TIME)
```

```
DIMENSION X(N), G(N)
```

```
WRITE (6,1) ITN,NE,TIME,U,((X(I),G(I)),I=1,N)
```

```
RETURN
```

```
1) FORMAT (1H ,I3,5X,I3,6X,F10.3,1X,F14.6,1X,80(F14.6,1X,F14.6,/,44X)
```

```
1)
```

```
END
```

```
D 1  
D 2  
D 3  
D 4  
D 5  
D 6  
D 7  
D 8  
D 9-
```

|   |  |   |     |
|---|--|---|-----|
|   | SUBROUTINE FINAL (N,X,U,G)   | E | 1   |
|   | DIMENSION X(N), G(N)   | E | 2   |
|   | COMMON /BLK/ KO  | E | 3   |
|   | COMMON /BLK1/ NF   | F | 4   |
|   | IF (KO.EQ.0) GO TO 1   | F | 5   |
|   | WRITE (6,3)  | F | 6   |
|   | GO TO 2  | E | 7   |
| 1 | WRITE (6,4)  | E | 8   |
| 2 | CONTINUE   | E | 9   |
|   | WRITE (6,5) U  | E | 10  |
|   | WRITE (6,6) (I,X(I),I,G(I),I=1,N)                                  | F | 11  |
|   | WRITE (6,7) NF   | F | 12  |
|   | RETURN   | F | 13  |
| C |  | E | 14  |
| C |  | E | 15  |
| 3 | FORMAT (1H0,/1H0,*OPTIMAL SOLUTION FOUND BY FLETCHER METHOD*/1H ,4 | F | 16  |
|   | 11(*-*))   | E | 17  |
| 4 | FORMAT (1H0,/1H0,*RESULTS FOUND BY FLETCHER METHOD AT LAST ITERATI | E | 18  |
|   | ON*/1H ,50(*-*))   | E | 19  |
| 5 | FORMAT (1H0,4X,*U =*,F14.6/)                                       | F | 20  |
| 6 | FORMAT (1H ,*X(*,I2,*) =*,F14.6,2X,*G(*,I2,*) =*,F14.6)            | F | 21  |
| 7 | FORMAT (1H0,4X,*NUMBER OF FUNCTION EVALUATIONS =*,I5)              | E | 22  |
|   | END  | F | 23- |





