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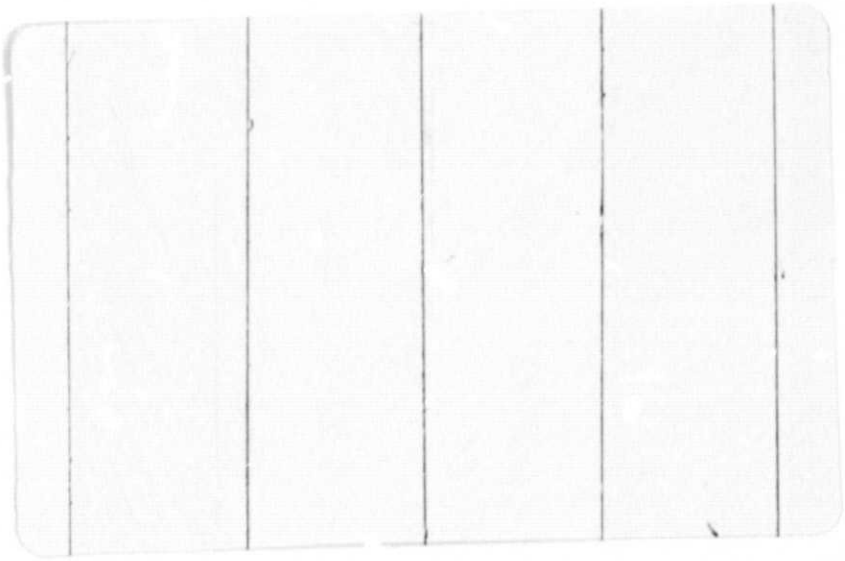

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A Quasi-Newton Approach to Optimization Problems with Probability Density Constraints

by

R. A. Tapia and D. L. Van Rooy
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ABSTRACT:

A quasi-Newton method is presented for minimizing a nonlinear functional while constraining the variables to be nonnegative and sum to one. The nonnegativity constraints are eliminated by working with the squares of the variables and the resulting problem is solved using Tapia's general theory of quasi-Newton methods for constrained optimization. A user's guide for a program implementing this algorithm is provided.

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I. INTRODUCTION

Consider the optimization problem

$$(1) \qquad \min f(x_1, \ldots, x_n) \; ; \; \text{subject to} \quad 1 - \sum_{i=1}^{n} x_i = 0, \quad x_i \geq 0, \; i=1, \ldots, n$$

Problems of the form (1) occur frequently in statistical applications. In these applications, the variables x_i usually represent a discrete probability density function and the functional f represents an optimality criterion, e.g., the negative likelihood or negative log likelihood.

Let us make the change of variables

$$(2) \qquad x_i = \tfrac{1}{2} y_i^2 \quad , \quad i=1, \ldots, n$$

and consider the optimization problem

$$(3) \qquad \min \hat{f}(y_1, \ldots, y_n) \; ; \; \text{subject to} \quad 1 - \sum_{i=1}^{n} \tfrac{1}{2} y_i^2 = 0$$

where

$$(4) \qquad \hat{f}(y_1, \ldots, y_n) \equiv f(\tfrac{1}{2} y_1^2, \ldots, \tfrac{1}{2} y_n^2)$$

Proposition 1.1

If $y = (y_1, \ldots, y_n)^T$ solves problem (3), then $x = (\tfrac{1}{2} y_1^2, \ldots, \tfrac{1}{2} y_n^2)^T$ solves problem (1). Conversely, if $x = (x_1, \ldots, x_n)^T$ solves problem (1), then $y = (\sqrt{2x_1}, \ldots, \sqrt{2x_n})^T$ solves problem (3).

Proof

The proof is not difficult.

Problem (3), in contrast to problem (1), does not involve inequality constraints. The price one pays for this simplification is that problem (3) will have nore critical points than problem (1) and the equality constraint is quadratic instead of linear. We maintain, that according to Proposition 1.1, if one starts sufficiently near the solution, the extraneous critical points will not affect the algorithm. Moreover, when f is nonlinear, the quadratic constraints should not significantly increase the degree of complexity of the problem.

Tapia's approach to quasi-Newton methods for constrained optimization ([1] and [2]) depends heavily on the invertibility of the Hessian of the Lagrangian at the solution. Hence, we are certainly interested in determing the relationship between the invertibility of the Hessian of the Lagrangian for problem (1) and the invertibility of the Hessian of the Lagrangian for problem (3). Toward this end let

$$(5)\quad L(x,\mu,\lambda) = f(x) - \sum_{i=1}^{n} \mu_i x_i + \lambda(1 - \sum x_i)$$

and

$$(6)\quad \hat{L}(y,\lambda) = \hat{f}(y) + \lambda(1 - \sum_{i=1}^{n} \tfrac{1}{2} y_i^2)$$

we use the notation

$$\Lambda = (\lambda, \ldots, \lambda)^T,$$

$$Y = \operatorname{diag}(y_1, \ldots, y_n)$$

and

$$X = \operatorname{diag}(x_1, \ldots, x_n)$$

Straightforward calculations show that

$$(7)\quad \nabla_y \hat{L}(y, \lambda) = Y\left(\nabla f(x) - \Lambda\right) ,$$

$$(8)\quad \nabla_y^2 L(y, \lambda) = Y\, \nabla^2 f(x) Y + \operatorname{diag}\left(\nabla f(x) - \Lambda\right) ,$$

$$(9)\quad \nabla_x L(x, \mu, \lambda) = \nabla f(x) - \Lambda - \mu ,$$

and

$$(10)\quad \nabla_x^2 L(x, \mu, \lambda) = \nabla^2 f(x) .$$

The first order necessary conditions for problem (1) are

$$(11)\qquad \begin{aligned} \nabla f(x) - \Lambda - \mu &= 0 \\ 1 - \sum_{i=1}^{n} x_i &= 0 \\ \mu_i &\geq 0 \\ x_i &\geq 0 \\ \mu_i x_i &= 0 \ , \quad i=1, \ldots, n \ ; \end{aligned}$$

while the first order necessary conditions for problem (3) are

$$(12)\qquad \begin{aligned} Y\left(\nabla f(x) - \Lambda\right) &= 0 \\ 1 - \sum_{i=1}^{n} \tfrac{1}{2} y_i^2 &= 0 \end{aligned}$$

Recall that strict complementarity means that in (11) we do not have $\mu_i = x_i = 0$ for any i.

Proposition 1.2

Let (x, u, λ) be a solution of problem (1) and (y, λ) the corresponding solution of problem (3). Then

(i) we have strict complementarity and $\nabla^2 f(x)$ is positive definite $\Longleftrightarrow \nabla_y^2 \hat{L}(y, \lambda)$ is positive definite

(ii) we have strict complementarity and $\nabla^2 f(x)$ is invertible $\Longleftrightarrow \nabla_y^2 L(y, \lambda)$ is invertible.

Proof

Again the proof is not difficult. One merely works with (8), (10), (11) and (12).

Proposition 1.2 is very satisfying and warns us tha in the algorithm we must guard against the loss of strict complementarity. This will be accomplished by working with the variable

$$(13) \qquad x_i = \frac{1}{E_i} y_i^{E_i}$$

where $E_i = 2$ if $|x_i| + |\mu_i| \neq 0$ and $E_i = 1$ if $|x_i| + |\mu_i| = 0$. Observe that, when $E_i = 1$ in (13), we have effectively ignored the nonnegativity constraint on x_i.

II. THE QUASI-NEWTON ALGORITHM

The algorithm we are about to present is a special case of the approach given by Tapia in [2] applied to problem (3). The reader is referred to that paper for a better understanding of the theory and algorithm. In describing an iterative method, it is convenient to denote the present iterate by x and the subsequent iterate by $\bar{x}$ and similarly for other variables. Also, we let I

denote the identity matrix , $\langle \cdot \rangle$ denotes the Euclidean inner product, $e_1 = (1, 0, \ldots, 0)^T, \ldots, e_n = (0, \ldots, 1)^T$, (a_{ij}) denotes the matrix whose (i,j)-th element is a_{ij} and b_i or $(b)_i$ denotes the i-th element of the vector b.

Consider the constrained optimization problem

$$(14) \quad \min \ f(x), \quad \text{subject to} \ g(x) = 0 ;$$

where $f, g : R^n \to R^1$. We first describe the quasi-Newton method BFGS given in [2] for problem (14). Let

$$(15) \quad L(x, \lambda) = f(x) + \lambda \, g(x)$$

Quasi-Newton BFGS

Step 1: (Initialization) Determine x and B.

Step 2: (Update x and λ) Let

$$\bar{\lambda} = \frac{g(x) - \langle \nabla g(x), B^{-1} \nabla f(x) \rangle}{\langle \nabla g(x), B^{-1} \nabla g(x) \rangle}$$

$$\bar{x} = x - B^{-1} \nabla_x L(x, \bar{\lambda}) .$$

Step 3: (Update approximate Hessian)

$$\bar{B} = \left(B + \frac{y \, y^T}{\langle y, s \rangle} - \frac{B \, s \, s^T \, B}{\langle s, Bs \rangle} \right)$$

where

$$s = \bar{x} - x$$

and

$$y = \nabla_x L(\bar{x}, \bar{\lambda}) - \nabla_x L(x, \bar{\lambda}) .$$

Step 4: GO TO STEP 2 .

In implementing this algorithm, one would have to make provisions for output and a stopping criterion. In [2], Tapia has demonstrated that the above algorithm is locally superlinearly convergent.

Remark 1:

If the initial B depended on λ, we would make an initial approximation of λ according to the projection formula (see [2]'

$$(16) \qquad \lambda = - \frac{\langle \nabla g(x) , \nabla f(x) \rangle}{\langle \nabla g(x) , \nabla g(x) \rangle}$$

Remark 2:

In updating B in Step 3, it is advantageous to store B factored according to a Cholesky decomposition and then merely update these factors. Moreover, B can be slightly modified so that the resultant matrix is always positive definite. For a detailed description of these modifications, the reader is referred to Gill et al [3], Van Rooy et al [4], Fletcher and Powell [5] and Van Rooy [6]. The quantities $B^{-1} \nabla f(x)$ and $B^{-1} \nabla g(x)$ in Step 2 are then obtained in the standard back-substitution manner.

We now apply the above algorithm for problem (3) with the additional feature of obtaining a discrete Newton approximation to the Hessian every M iterations (where M is an input parameter).

Define the following functions

$$(17) \qquad x_i = \frac{y_i^{E_i}}{E_i}$$

$$(18) \qquad \nabla g_i = - \left[2 - E_i + (E_i - 1)\, y_i \right], \quad i = 1, \ldots, n$$

and

$$(19) \qquad g = 1 - \sum_{i=1}^{n} x_i$$

The quantity ∇g is merely the gradient of g with respect to y and (13) and (17) are the same.

Quasi-Newton Algorithm for Problem (3)

Step 1: (Initialization)

Read CRC (constraint regection criterion)

h (discretization step)

ε (stopping criterion)

DI (descent indicator)

IØUTPUT (output indicator)

M (discrete Hessian indicator)

MAX (maximum number of iterations)

Let

$E_i = 2$

$y_i = \sqrt{\frac{2}{n}}$

$\lambda = \langle \nabla f(x) , x \rangle$

$B = I$

Step 2: Output according to IØUTPUT,
check stopping criterion

IF $\left(\| \nabla_y L(y, \lambda) \| + g^2 < \epsilon \right.$ or

ITERATION > MAX $\left.\right)$ stop

Step 3: Calculate discrete Hessian according to M

$$B = \left(\frac{\nabla_y \hat{L}(y + he_j, \lambda)_i - \nabla_y \hat{L}(y, \lambda)_i}{h} \right)$$

Calculate modified Cholesky decomposition of B.

Step 4: Calculate multiplier correction

$$\Delta\lambda = \frac{g - \langle \nabla g , B^{-1} \nabla_y \hat{L}(y, \lambda) \rangle}{\langle \nabla g , B^{-1} \nabla g \rangle}$$

Step 5: Calculate y-variable correction

$$\Delta y = - B^{-1} \nabla_y \hat{L}(y, \lambda) - \Delta\lambda B^{-1} \nabla g$$

Step 6: Update y according to descent indicator

$$\bar{\lambda} = \lambda + \alpha \Delta\lambda$$

$$\bar{y} = y + \alpha \Delta y$$

where $\alpha = 1$ if descent is not desired, otherwise α is chosen according to the descent principle on $\| \nabla_y \hat{L}(y, -\lambda) \|^2 + g^2$ (see [2]).

Step 7: Update approximate Hessian according to BFGS and modified Cholesky decomposition

$$\bar{B} = B + \frac{Dy\ Dy^T}{\langle Dy, Ds \rangle} - \frac{B\ Ds\ Ds^T\ B}{\langle Ds, B\ Ds \rangle}$$

where $Ds = \bar{x} - x$ and

$$Dy = \nabla_y \hat{L}(\bar{y}, \bar{\lambda}) - \nabla_y \hat{L}(y, \bar{\lambda})$$

Step 8: Update constraint rejection indicators

$$T_0 = a_1 \left[\| \nabla_y \hat{L}(\bar{y}, \bar{\lambda}) \|^2 + \left(1 - \sum_{i=1}^{n} x_i \right)^2 \right]^{a_2},$$

$$T_1 = \min \left(\frac{1}{4n}, T_0 \right),$$

$$T_2 = \min (CRC, T_0)$$

If $\left(|\bar{x}_i| < T_1 \text{ and } \left| \frac{\partial f}{\partial x_i} - \lambda \right| < T_2 \right)$, let $E_i = 1$

If E_i has changed, reset $\bar{y}_i$ $\quad i = 1, \ldots, n$

Step 9: GO TO STEP 2 .

III. USER'S GUIDE

The above algorithm has been implemented in a set of FORTRAN subroutines whose entry point is the subroutine CONOPT. In this section, we shall describe how to use this program, provide a description of the workings of the program, and illustrate its use with examples. A listing of the program is given in the appendix. This program runs on an IBM 370/155 using the FORTRAN G , G1 , or H compilers. All computations are done in double precision. Unit 6 is used for output, if requested.

To utilize this program, the user supplies several parameters and two subprograms which calculate the function value and its gradient at a specified point. The program will then attempt to minimize the function subject to the constraints and return the argument at the minimum.

The calling sequence of the program is CALL CONOPT (N, DELF, FUNCT, X, WKA, MITER, STC, CRC, IDN, DH, IØUT, DSNT, A, RSTRT, USELAM, XLAM).

These parameters are described below:

N - integer variable indicating the dimension of the problem.

DELF - a user supplied subroutine which calculates the gradient of the function. The calling sequence is CALL DELF (DF, X, N) , where X is the N dimensional argument and DELF returns the gradient in the vector DF . Note that DF and X are both double precision variables.

FUNCT - a user supplied double precision function subprogram which calculates the function value at a specified point. The calling sequence is F = FUNCT (X, N) where X is the (double precision) argument of length N . Though the function value is not required by the algorithm, CONOPT will output it in the convergence test step if the user requests output. (It is called only when output is requested.) If, for any reason, the user is not interested in this value, he may just supply a function subprogram that sets the function value to zero and returns. [N.B. The two programs DELF and FUNCT must be declared external in the calling program. The two programs may have other entry points, with different arguments, referred to by the user's calling program prior to his calling CONOPT in order to make other variables or their addresses available to either or these subprograms.]

X - on output, this will contain the N-dimensional double precision argument last calculated by the program (at the minimum if the program converged). On input, the program will set each element of X to the value 1/N , unless the user has specified restart (see description of the variable RSTRT below), in which case

the supplied values of X will be used as the starting point.

WKA - a double precision working storage array of length $\geq \frac{1}{2} N^2 + (23N + 7) / 2$. If a restart has been specified, the first N (2-byte integer) locations should contain the desired constraint rejection indicators. However, if these variables do not contain either 1's or 2's, the program will set them to 2. The final constraint rejection indicators will be in these locations.

MITER - an integer variable indicating the maximum number of iterations to perform. If the user sets this to 0, the program will reset it to max (30, 2 * N).

STC - a real variable specifying the stopping criterion on the norm squared of the gradient of the Lagrangian plus the constraint, i.e. $\| \nabla L \|^2 + \left(1 - \sum_{i=1}^{n} x_i\right)^2$. If 0 is specified, the program will set STC = 10^{-8}.

CRC - a real variable specifying the constraint rejection criterion. See the algorithm description section for a precise definition of its use. If 0, is specified, the program will set CRC = 10^{-2}.

IDN - an integer variable specifying the frequency of calculation of the discrete approximation to the Hessian, i.e., this finite difference Hessian is calculated every IDN iterations. If 0 is specified, this approximation is never used.

If a negative value is specified, the program sets IDN = min (10, N).

DH - a real variable specifying the step size to be used in calculating the finite difference Hessian (see the algorithm description for a detailed definition). If 0 is specified, the program will set DH = 10^{-2} .

IØUT - an integer variable specifying the frequency of output; i.e., the program will output various computed quantities every IØUT iterations. If 0 is specified, no output will be produced. If a negative value is specified, the program sets IØUT = 1 .

DSNT - a one-byte logical variable indicating whether the program should implement descent in its search at each iteration.

A - a two-word real vector containing respectively the multiplier and exponent for DNORM $\left(= \| \nabla L \|^2 + \left(1 - \sum_{i=1}^{n} x_i \right)^2 \right)$ for use in the constraint rejection test; i.e., the appropriate quantity is A(1) * DNORM * * A(2) . The defaults for A(1) and A(2) are 1. and .2 respectively. If the user wishes to set A(2) = 0., he should set A(1) to the negative of what he wants for A(1) and then a value of zero will be used for A(2) .

RSTRT - a one-byte logical variable indicating whether the user is supplying an initial value for X (as in a restart case). If RSTRT = .TRUE., the first 2N bytes of WKA should contain the vector ICR (see description of WKS and the algorithm description—the E_i's).

USELAM - a one-byte logical variable used if RESTR = .TRUE. to indicate if the user is supplying a value for XLAM . If RESTR = .TRUE. and USELAM = .FALSE. , the value $< \nabla f , x >$ is used for XLAM .

XLAM - the Langrange multiplier for the equality constraint. Used on input only if USELAM = RSTRT = .TRUE.

The default values for the above parameters have been chosen so that many problems will converge; thus, the only input parameters with which the user need concern himself in many cases is N, IØUT, DSNT and RSTRT (usually = .FALSE.)

The subprograms used and a brief description of their function is given below:

CONOPT - main driver subroutine

DIMS - computes base addresses for various working arrays used throughout the calculations.

INPT - sets default values for parameters and outputs the parameters used.

INIT initializes y, x, ICR, H and λ . Also fetches values of ∇f and ∇L .

CHKSTP - checks the stopping criterion and outputs quantities if requested.

DHESS - calculates a finite difference approximation to the Hessian and its modified Cholesky decomposition, if requested. The Hessian is forced to be positive definite.

DELAMY - computes the update terms $\nabla \lambda$ and ∇y.

NEWY - updates y and λ based optionally on descent of $\| \nabla L \|^2 + \left(1 - \sum_{i=1}^{n} x_i \right)^2$.

UPDTH - updates the approximate Hessian using the Broyden-Fletcher-Goldfarb-Shannon (BFGS) update technique. (Really the MCD of it is updated.) Here again the Hessian is forced to be positive definite.

CONSTR - updates the constraint rejection indicators and, if necessary, y and ∇L.

GRADL - computes ∇L given ∇f, λ, y, and ICR.

SUM - a function subprogram that performs various utility functions $\left(\sum_{i=1}^{n} x_i , \sum_{i=1}^{n} x_i^2 , \sum_{i=1}^{n} x_i y_i \right)$.

MCHLSK - computes the modified Cholesky decomposition (MCD) of a matrix. If the matrix is not positive definite, the MCD is modified to represent a matrix that is (see e.g. ref 4).

PDSOLV - solves $Ax = y$ where A contains the MCD of a matrix.

COMPT - computes a rank one update of an MCD using the composite-t method (see refs. 5 and 6).

LDMUL - multiply a vector by a matrix whose MCD is supplied.

Examples:

The following quadratic programming (i.e., min $\| Ax - b \|^2$ s. t. $x_i \geq 0$ and $\sum x_i = 1$) examples were run using all the default options:

1. $$A = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad b = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$x = (.11112108,\ .44443959,\ .44443959)^T$$

congerged in 5 iterations. Exact answer = $(1/9,\ 4/9,\ 4/9)^T$

The robustness of the algorithm is exemplified by the following two examples for which the algorithm, theoretically, should not converge since the Hessian is singular at the solution.

2. $$A = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \\ 2 & 1 & 2 \end{pmatrix} \qquad b = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}$$

$$x = (.50000019,\ 0.,\ .50000004)^T$$

converged in 14 iterations. Exact answer = $(\frac{1}{2},\ 0,\ \frac{1}{2})^T$.

The constraint for x_2 is not active in this case.

3.
$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad b = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$x = (0,\ 0,\ 1)^T$$

congerged in 11 iterations. The constraints for x_1 and x_2 are not active in this case.

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[5] Fletcher, R. and Powell, M.J.O., "On the Modification of LDL^T Factorizations," Math. Comp., 28 (1974), pp. 1067-1087.

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APPENDIX

Program Listings of CONOPT

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              SUBROUTINE CONOPT(N,DELF,FUNCT,X,WKA,TMITER,TSTC,TCRC,TIDN,TDH,
                     1 TIOUT,TDSNT,A,RSTRT,USELAM,XLAM)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                C
                C     THIS ROUTINE MINIMIZES F(X) S.T. X(I).GE.0 & SUM(X(I))=1.
                C     FOR A DETAILED DESCRIPTION OF THE PROGRAM SEE ICSA TECHNICAL
                C     REPORT NO. 275-025-029, RICE UNIV.,HOUSTON,TEX. JUNE, 1976.
                C
                C     FUNCT IS A FUNCTION WHICH RETURNS F(X), ITS ARGUMENTS ARE X,N
                C     DELF IS A SUBROUTINE WHICH COMPUTES THE GRADIENT OF F(X).   ITS
                C     ARGUMENTS ARE DF (THE GRAD), X, & N
                C     DELF & FUNCT MUST BE DECLARED EXTERNAL IN THE MAIN PROGRAM.
                C     WKA IS A WORK AREA OF LENGTH .GE. .5*N**2+(23*N+7)/2
                C     X ON RETURN IS THE ARGUMENT AT THE MINIMUM
                C     N IS THE DIMENSION OF X
                C     A(1) & A(2) ARE USED IN THE CONSTRAINT REJECTION TEST. AS
                C     A(1)*DNORM**A(2)  DEFAULTS ARE A(1)=1. & A(2)=.2 . IF THE USER
                C     WISHES A(2) TO =0, HE SHOULD SET A(1) TO THE NEGATIVE OF WHAT HE
                C     WANTS FOR A(1).
                C     RSTRT - A LOGICAL VARIABLE INDICATING WHETHER THE USER IS
                C     RESTARTING.  IF SO, THE X'S MUST BE SUPPLIED & THE CONSTRAINT
                C     REJECTION INDICATORS AS INTEGER*2 VARIABLES SHOULD BE IN THE FIRST
                C     N LOCATIONS OF WKA
                C     USELAM - A LOGICAL VARIABLE INDICATING WHETHER OR NOT THE USER
                C     IS SUPPLYING A VALUE FOR XLAM IN THE CASE OF A RESTART.
                C     XLAM - THE LAGRANGE MULTIPLIER FOR THE EQUALITY CONSTRAINT.
                C
ISN 0004              REAL*8 X(N),WKA(1)
ISN 0005              REAL*4 TSTC,TCRC,TDH
ISN 0006              REAL*4 STC,CRC,DH
ISN 0007              REAL*4 A(2)
ISN 0008              INTEGER*4 TMITER,TIDN,TIOUT
ISN 0009              LOGICAL*1 DSNT,       TDSNT,RSTR,USELAM
ISN 0010              COMMON /INPUT/ MITER,STC,CRC,IDN,DH,IOUT,DSNT
ISN 0011              EXTERNAL DELF,FUNCT
ISN 0012              COMMON /ARANGE/ IICR,IY,IH,IDF,IGL,     IGL2,IDY,IWK,IGY,IYSAV,
                     1 IHGL,IHGY,IDLY,IDS
                C
                C     COMPUTE THE STARTING ADDRESSES OF VARIOUS WORKING ARRRYS.
                C
ISN 0013              CALL DIMS(N)
                C
                C     SET DEFAULT VALUES & OUTPUT (STEP 1)
                C
ISN 0014              CALL INPT(TMITER,TSTC,TCRC,TIDN, TDH,TIOUT,TDSNT,N,A,RSTRT)
                C
                C     INITIALIZE VARIABLES
                C
ISN 0015              CALL INIT(X,WKA(IDF),WKA(IY),WKA(IH),WKA(IGL),WKA(IICR),XLAM,
                     1 NITER,N,DELF,RSTRT,USELAM)
                C
                C     STEP 2 - CHECK STOPPING CRITERION & OUTPUT IF REQUESTED
                C
ISN 0016         100 CALL CHKSTP (X,N,G,DNORM,NITER,XLAM,WKA(IGL),
                    1          FUNCT,     &200)
                C
```

```
C       STEP 3 - CALCULATE DISCRETE HESSIAN (OPTIONAL)
C
ISN 0017      CALL DHESS (    NITER,WKA(IH),          WKA(IWK),WKA(IGL),
     1  WKA(IGL2),  DELF,  XLAM,WKA(IICR),WKA(IY),N,X)
C
C       STEPS 4 & 5 - CALCULATE MULTIPLIER & Y-VARIABLE CORRECTIONS
C
ISN 0018      CALL DELAMY (WKA(IGY),WKA(IH),WKA(IGL),N,WKA(IHGL),WKA(IHGY),
     1  DLAM,WKA(IDLY),G,WKA(IY),WKA(IICR))
C
C       STEP 6 - CALCULATE NEW Y BASED ON (OPTIONAL ) D%SCENT
C
ISN 0019      CALL NEWY (DNORM,XLAM,WKA(IY),N,DLAM,WKA(IDLY),G,NITER,WKA(IICR),
     1  WKA(IYSAV),X,WKA(IDF),DELF,WKA(IDY),WKA(IGL))
C
C       STEP 7 - UPDATE APPROXIMATE INVERSE HESSIAN
C
ISN 0020      CALL UPDTH(NITER,WKA(IYSAV),N,          WKA(IGL),XLAM,WKA(IICR),
     1  WKA(IY),WKA(IH),          WKA(IGL2),WKA(IDY),WKA(IDS!),WKA(IWK))
C
C       STEP 8 - UPDATE CONSTRAINT REJECTION INDICATORS
C
ISN 0021      CALL CONSTR(WKA(IDF),X,N,WKA(IICR),XLAM,DELF,WKA(IGL),WKA(IY),
     1          WKA(IYSAV),DNORM,A)
ISN 0022      GO TO 100
ISN 0023    200 RETURN
ISN 0024      END
```

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                         SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              SUBROUTINE DIMS(N)
                    C
                    C     COMPUTE STARTING POINTS OF WORKING ARRAYS USED.  THE ORDER IS ICR,
                    C      Y,H, DF,GL,GL2,DY, & WK
                    C
ISN 0003              INTEGER*4 IDM(8)
ISN 0004              COMMON /ARANGE/ IDM,IGY,IYSAV,IHGL,IHGY,IDLY,IDS
ISN 0005              IDM(1)=1
ISN 0006              IDM(2)=(N+1)/2
ISN 0007              IDM(3)=N
ISN 0008              IDM(4)=N*(N+1)/2
ISN 0009              IDM(5)=N
ISN 0010              IDM(6)=N
ISN 0011              IDM(7)=N
ISN 0012              IDM(8)=N
ISN 0013              DO 10 I=2,8
ISN 0014           10 IDM(I)=IDM(I)+IDM(I-1)
ISN 0015              IGY=IDM(8)
ISN 0016              IYSAV=IGY+N
ISN 0017              IHGL=IYSAV+N
ISN 0018              IHGY=IHGL+N
ISN 0019              IDLY=IHGY+N
ISN 0020              IDS=IDLY+N
ISN 0021              RETURN
ISN 0022              END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
  ISN 0002              SUBROUTINE INPT (TMITER,TSTC,TCRC,TIDN,TDH,TIOUT,TDSNT,N,A,RSTRT)
                C
                C       SET DEFAULT VALUES FOR PARAMETERS USED.
                C
  ISN 0003              LOGICAL*1 DSNT,TDSNT,RSTRT
  ISN 0004              INTEGER*4 TMITER,TIDN,TIOUT
  ISN 0005              REAL*4 A(2)
  ISN 0006              REAL*4 TSTC,TCRC,TDH
  ISN 0007              REAL*4 STC,CRC,DH
  ISN 0008              COMMON /INPUT/ MITER,STC,CRC,IDN,DH,IOUT,DSNT
  ISN 0009              NAMELIST /IN/ MITER,STC,CRC,IDN,DH,IOUT,DSNT
  ISN 0010              EPS=1.E-20
  ISN 0011              MITER=MAX0(30,2*N)
  ISN 0012              IF (TMITER.GT.0) MITER=TMITER
  ISN 0014              STC=1.E-8
  ISN 0015              IF (TSTC.GT.EPS) STC=TSTC
  ISN 0017              CRC=.01
  ISN 0018              IF (TCRC.GT.EPS) CRC=TCRC
  ISN 0020              IDN=MIN0(10,N)
  ISN 0021              IF (TIDN.GE.0) IDN=TIDN
  ISN 0023              DH=.01
  ISN 0024              IF (TDH.GT.EPS) DH=TDH
  ISN 0026              IOUT=1
  ISN 0027              IF (TIOUT.GE.0) IOUT=TIOUT
  ISN 0029              DSNT=TDSNT
  ISN 0030              IF (A(2) .LE.EPS) A(2)=.2
  ISN 0032              IF (A(1).LT.0.) A(2)=0.
  ISN 0034              A(1)=ABS(A(1))
  ISN 0035              IF (A(1).LE.EPS) A(1)=1.
  ISN 0037              WRITE (6,11)
  ISN 0038           11 FORMAT ('1 PARAMETERS USED')
  ISN 0039              WRITE (6,IN)
  ISN 0040              WRITE (6,12) A
  ISN 0041           12 FORMAT (' A(1)=',G16.8,' A(2)=',G16.8)
  ISN 0042              WRITE (6,13) RSTRT
  ISN 0043           13 FORMAT (' RSTRT=',L8)
  ISN 0044              RETURN
  ISN 0045              END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              SUBROUTINE INIT(X,DF,Y,H,GL,ICR,XLAM,NITER,N,DELF,RSTRT,USELAM)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                C
                C     THIS ROUTINE INITIALIZES SEVERAL VARIABLES USED IN THE OPTIMIZATION
                C
ISN 0004              LOGICAL*1 USELAM
ISN 0005              LOGICAL*1 RSTRT
ISN 0006              INTEGER*2 ICR(N)
ISN 0007              REAL*8 X(N),DF(N),Y(N),GL(N),H(1)
ISN 0008              IF (RSTRT) GO TO 5
ISN 0010              SN=SQRT(2./N)
ISN 0011              DO 10 I=1,N
ISN 0012              ICR(I)=2
ISN 0013              Y(I)=SN
ISN 0014           10 X(I)=1./N
ISN 0015              GO TO 15
ISN 0016            5 DO 40 I=1,N
ISN 0017              Y(I)=X(I)
ISN 0018              IF (ICR(I).EQ.1) GO TO 40
ISN 0020              ICR(I)=2
ISN 0021              Y(I)=DSQRT(2.*X(I))
ISN 0022           40 CONTINUE
ISN 0023           15 CONTINUE
                C
                C     DF IS THE GRADIENT OF F
                C
ISN 0024              CALL DELF(DF,X,N)
                C
                C     SET H TO THE IDENTITY MATRIX
                C
ISN 0025              N2=N*(N+1)/2
ISN 0026              DO 20 K=1,N2
ISN 0027           20 H(K)=0.
ISN 0028              I=0
ISN 0029              DO 30 K=1,N
ISN 0030              I=I+K
ISN 0031           30 H(I)=1.
ISN 0032              IF (.NOT.USELAM) XLAM=DOT(DF,X,N)
ISN 0034              NITER=0
                C
                C     GL IS THE GRADIENT OF THE LAGRANGIAN
                C
ISN 0035              CALL GRADL(GL,DF,XLAM,ICR,Y,N)
ISN 0036              RETURN
ISN 0037              END
```

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                        SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              SUBROUTINE CHKSTP(X,N,G,DNORM,NITER,XLAM,GL,          FUNCT,
                     1*)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004              REAL*8 SUM,SUM2
ISN 0005              REAL*8 X(N),GL(N)
ISN 0006              REAL*4 STC,CRC,DH
ISN 0007              COMMON /INPUT/ MITER,STC,CRC,IDN,DH,IOUT
                C
                C     EVALUATE THE NORM OF GRAD(L) + THE NORM OF THE EQUALITY CONSTRAINT, G.
                C
ISN 0008              G=1.D0-SUM(X,N)
ISN 0009              DNORM=G*G+SUM2(GL,N)
ISN 0010              IF (DNORM.GE.STC.AND.NITER.LT.MITER) GO TO 15
ISN 0012              IF (IOUT.EQ.0) RETURN 1
ISN 0014              F=FUNCT(X,N)
ISN 0015              WRITE (6,11) NITER,DNORM,G,XLAM,F,(X(I),I=1,N)
ISN 0016           11 FORMAT (//' NITER,DNORM,G,LAM,F,& X',I10,4G16.8,(/8G16.8))
ISN 0017              RETUR' 1
                C
                C     INTERMEDIATE OUTPUT IF DESIRED
                C
ISN 0018           15 IF (IOUT.EQ.0) GO TO 25
ISN 0020              IF (NITER/IOUT*IOUT.NE.NITER) GO TO 25
ISN 0022              F=FUNCT(X,N)
ISN 0023              WRITE (6,11) NITER,DNORM,G,XLAM,F,(X(I),I=1,N)
ISN 0024           25 NITER=NITER+1
ISN 0025              RETURN
ISN 0026              END
```

```
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      COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                         SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              SUBROUTINE DHESS(    NITER,H,    WK,GL,GL2,DELF, XLAM,ICR,Y,N,X)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                C
                C     CALCULATE DISCRETE APPROX. TO THE HESSIAN IF DESIRED
                C
ISN 0004              REAL*8 WK(1),H(1),          GL(N),GL2(N),      Y(N),X(N)
ISN 0005              INTEGER*2 ICR(N)
ISN 0006              REAL*4 STC,CRC,DH
ISN 0007              COMMON /INPUT/ MITER,STC,CRC,IDN,DH
ISN 0008              IF (IDN.EQ.0) RETURN
ISN 0010              IF ((NITER-1)/IDN*IDN.NE.NITER-1) RETURN
                C
                C     COMPUTE THE HESSIAN
                C
ISN 0012              K=0
ISN 0013              DO 10 J=1,N
ISN 0014              YT=Y(J)
ISN 0015              Y(J)=Y(J)+DH
ISN 0016              XT=X(J)
ISN 0017              X(J)=Y(J)**ICR(J)/ICR(J)
ISN 0018              CALL DELF(WK,X,N)
ISN 0019              X(J)=XT
ISN 0020              CALL GRADL(GL2,WK,XLAM,ICR,Y,N)
ISN 0021              Y(J)=YT
ISN 0022              DO 10 I=1,J
ISN 0023              K=K+1
ISN 0024              H (K)  =(GL2(I)-GL(I))/DH
ISN 0025           10 CONTINUE
                C
                C     COMPUTE THE MODIFIED CHOLESKY DECOMP. OF H & STORE IN H
                C
ISN 0026              CALL MCHLSK(H,N,WK)
ISN 0027              RETURN
ISN 0028              END
```

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                        SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              SUBROUTINE DELAMY(GY,H,GL,N,HGL,HGY,DLAM,DLY,G,Y,ICR)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                    C
                    C     COMPUTE DELTA=LAMBDA & DELTA=Y
                    C
ISN 0004              REAL*8 GY(N),H(1),  GL(N),HGL(N),HGY(N),DLY(N),Y(N)
ISN 0005              INTEGER*2 ICR(N)
ISN 0006              DO 10 I=1,N
ISN 0007              GY(I)=-Y(I)
ISN 0008           10 IF (ICR(I).NE.2) GY(I)=-1.
ISN 0010              CALL PDSOLV(H,HGL,GL,N)
ISN 0011              CALL PDSOLV(H,HGY,GY,N)
ISN 0012              DLAM=(G-DOT(GY,HGL,N))/DOT(GY,HGY,N)
ISN 0013              DO 20 I=1,N
ISN 0014           20 DLY(I)=-HGL(I)-DLAM*HGY(I)
ISN 0015              RETURN
ISN 0016              END
```

```
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        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
 ISN 0002              SUBROUTINE NEWY (DNORM,XLAM,Y,N,DLAM,DELY,G,NITER,ICR,YSAV,X,
                      1 DF,DELF,DFSAV,GL)
 ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                C
                C     COMPUTE A NEW VALUE OF Y BASED (OPTIONALLY) ON THE DESCENT OF THE
                C     NORM OF GRAD(L) + NORM OF G.
                C
 ISN 0004              REAL*8 SUM2
 ISN 0005              REAL*8 SUM
 ISN 0006              LOGICAL*1 DSNT,DSNT2
 ISN 0007              REAL*8 GL(N),DFSAV(N)
 ISN 0008              REAL*8 Y(N),DELY(N),YSAV(N),X(N),DF(N)
 ISN 0009              REAL*4 STC,CRC,DH
 ISN 0010              INTEGER*2 ICR(N)
 ISN 0011              COMMON /INPUT/ NITER,STC,CRC,IDN,DH,IOUT,DSNT
 ISN 0012              DSNT2=DSNT
 ISN 0013              ALP=1.
 ISN 0014              DNSAVE=DNORM
 ISN 0015              XLSAV=XLAM
 ISN 0016              DO 10 I=1,N
 ISN 0017              DFSAV(I)=DF(I)
 ISN 0018           10 YSAV(I)=Y(I)
 ISN 0019           15 DO 20 I=1,10
 ISN 0020              XLAM=XLSAV+ALP*DLAM
 ISN 0021              DO 30 J=1,N
 ISN 0022              Y(J)=YSAV(J)+ALP*DELY(J)
 ISN 0023              IF (ICR(J).EQ.1.AND.Y(J).LT.0.) Y(J)=0.
 ISN 0025              X(J)=Y(J)**ICR(J)/ICR(J)
 ISN 0026           30 CONTINUE
 ISN 0027              CALL DELF(DF,X,N)
                C
                C     DESCEND IF DESIRED
                C
 ISN 0028              G=1.D0-SUM(X,N)
 ISN 0029              CALL GRADL(GL,DF,XLAM,ICR,Y,N)
 ISN 0030              IF (.NOT.DSNT2) RETURN
 ISN 0032              DNORM=G*G+SUM2(GL,N)
 ISN 0033              IF (DNORM.LT.DNSAVE) RETURN
 ISN 0035           20 ALP=ALP/2.
 ISN 0036              IF (ALP.LT.0.) GO TO 25
                C
                C     TRY OTHER DIRECTION
                C
 ISN 0038              ALP=-1.
 ISN 0039              GO TO 15
 ISN 0040           25 WRITE (6,11) NITER
 ISN 0041           11 FORMAT (' *ON ITER',I5,' DESCENT COULD NOT BE IMPLEMENTED, STEP LE
                      1NGTH SET TO 1')
 ISN 0042              ALP=1.
 ISN 0043              DSNT2=.FALSE.
 ISN 0044              GO TO15
 ISN 0045              RETURN
 ISN 0046              END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              SUBROUTINE UPDTH(NITER,YSAV,N,     GL,XLAM,ICR,Y,H,   GL2,DY,DS,T)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                    C
                    C     UPDATE APPROX. INVERSE HESSIAN
                    C
ISN 0004              REAL*8 H(1),          YSAV(N),          GL(N),Y(N)
ISN 0005              REAL*8 GL2(N),DY(N),DS(N)
ISN 0006              REAL*8 T(1)
ISN 0007              REAL*4 STC,CRC
ISN 0008              INTEGER*2 ICR(N)
ISN 0009              COMMON /INPUT/ MITER,STC,CRC,IDN
ISN 0010              IF (IDN.EQ.0) GO TO 15
ISN 0012              IF (NITER/IDN*IDN.EQ.NITER) RETURN
                    C
                    C     CALCULATE INTERMEDIATE QUANTITIES
                    C
ISN 0014           15 CONTINUE
ISN 0015              E1=1.E-16
ISN 0016              E2=.1
ISN 0017              CALL GRADL(GL2,DY,XLAM,ICR,YSAV,N)
ISN 0018              DO 10 I=1,N
ISN 0019              DY(I)=GL(I)-GL2(I)
ISN 0020              DS(I)=Y(I)-YSAV(I)
ISN 0021           10 CONTINUE
ISN 0022              D=DOT(DY,DS,N)
ISN 0023              IF (DABS(D) .GT.E1) GO TO 25
ISN 0025              WRITE (6,12)
ISN 0026           12 FORMAT (' D NEAR 0 IN UPDTH')
ISN 0027              RETURN
ISN 0028           25 CONTINUE
                    C
                    C     COMPUTE THE PRODUCT H*DS & STORE IN GL2
                    C
ISN 0029              CALL LDMUL(H,DS,GL2, T,N)
                    C
                    C     UPDATE H
                    C
ISN 0030              TX=-DOT(DS,GL2,N)
ISN 0031              T(1)=D
ISN 0032              CALL COMPT(H,T,DY,N,T(N+2),T(2*N+2))
ISN 0033              T(1)=TX
ISN 0034              CALL COMPT(H,T,GL2,N,T(N+2),T(2*N+2))
                    C
                    C     INSURE THAT H IS POS. DEFN.
                    C
ISN 0035              II=0
ISN 0036              DO 20 I=1,N
ISN 0037              II=II+I
ISN 0038              IF (H(II).LE.E1) H(II)=E2
ISN 0040           20 CONTINUE
ISN 0041              RETURN
ISN 0042              END
```

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          COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
  ISN 0002              SUBROUTINE CONSTR(DF,X,N,ICR,XLAM,DELF,GL,Y,      YSAV,DNORM,A)
  ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                C
                C       CHECK FOR REDUNDANT CONSTRAINTS & RESET CONSTRAINT INDICATORS
                C
  ISN 0004              INTEGER*2 ICR(N)
  ISN 0005              REAL*8 YSAV(N)
  ISN 0006              REAL*8 DF(N),X(N)
  ISN 0007              REAL*8 GL(N),Y(N)
  ISN 0008              REAL*4 STC,CRC,DH
  ISN 0009              REAL*4 A(2)
  ISN 0010              LOGICAL*1 IND
  ISN 0011              COMMON /INPUT/ MITER,STC,CRC,IDN,DH,IOUT
  ISN 0012              XML=1.
  ISN 0013              SN=SQRT(FLOAT(N))
  ISN 0014              EPS=.25
  ISN 0015              IND=.FALSE.
                C
                C       TESTING & RESETTING LOOP
                C
  ISN 0016              DO 10 I=1,N
  ISN 0017              T=DF(I)*XLAM
  ISN 0018              TS=A(1)*DNORM**A(2)
  ISN 0019              CR=EPS/N
  ISN 0020              CR=DMIN1(CR,TS)
  ISN 0021              IF (DABS(X(I)).GE.CR) GO TO 12
  ISN 0023              CR=DMIN1(CRC/SN,TS)
  ISN 0024              IF (DABS(T).GE.CR) GO TO 12
  ISN 0026              IF (ICR(I).NE.1) IND=.TRUE.
  ISN 0028              ICR(I)=1
  ISN 0029              GO TO 10
  ISN 0030           12 CONTINUE
  ISN 0031              IF (ICR(I).NE.2) IND=.TRUE.
  ISN 0033              ICR(I)=2
  ISN 0034           10 CONTINUE
  ISN 0035           15 CONTINUE
  ISN 0036              IF (IOUT.EQ.0) GO TO 25
  ISN 0038              IF (IOUT*(NITER/IOUT).EQ.NITER) WRITE (6,21) (ICR(I),I=1,N)
  ISN 0040           21 FORMAT (' ICR',20I5)
  ISN 0041           25 CONTINUE
  ISN 0042              IF (.NOT.IND) RETURN
  ISN 0044              DO 30 I=1,N
  ISN 0045              Y(I)=X(I)
  ISN 0046              IF (ICR(I).NE.2) GO TO 30
  ISN 0048              Y(I)=0.
  ISN 0049              IF (X(I).GT.0.) Y(I)=DSQRT(2.*X(I))
  ISN 0051           30 CONTINUE
  ISN 0052              CALL GRADL(GL,DF,XLAM,ICR,Y,N)
  ISN 0053              RETURN
  ISN 0054              END
```

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          COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                             SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
  ISN 0002              SUBROUTINE GRADL(GL,DF,XLAM,ICR,Y,N)
  ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                C
                C       COMPUTE THE GRADIENT OF THE LAGRANGIAN
                C
  ISN 0004              REAL*8 GL(N),DF(N),Y(N)
  ISN 0005              INTEGER*2 ICR(N)
  ISN 0006              DO 10 I=1,N
  ISN 0007              GY=-Y(I)
  ISN 0008              IF (ICR(I).NE.2) GY=-1.
  ISN 0010           10 GL(I)=-(DF(I)-XLAM)*GY
  ISN 0011              RETURN
  ISN 0012              END
```

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                         SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              REAL FUNCTION SUM*8 (X,N)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                    C
                    C     PERFORM UTILITY FUNCTIONS
                    C
ISN 0004              REAL*8 X(N),Y(N)
ISN 0005              REAL*8 S,SUM2
ISN 0006              S=0.D0
ISN 0007              DO 20 I=1,N
ISN 0008           20 S=S+X(I)
ISN 0009              SUM=S
ISN 0010              RETURN
ISN 0011              ENTRY SUM2(X,N)
ISN 0012              S=0.D0
ISN 0013              DO 30 I=1,N
ISN 0014           30 S=S+X(I)*X(I)
ISN 0015              SUM2=S
ISN 0016              RETURN
ISN 0017              ENTRY DOT(X,Y,N)
ISN 0018              S=0.D0
ISN 0019              DO 40 I=1,N
ISN 0020           40 S=S+X(I)*Y(I)
ISN 0021              DOT=S
ISN 0022              RETURN
ISN 0023              END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002            SUBROUTINE MCHLSK(KK,NV,DUM)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
                    C                                                              DVR04770
                    C  ************************************************************DVR04780
                    C        THIS ROUTINE COMPUTES THE MODIFIED CHOLESKY DECOMPOSITION
                    C     (MCD) OF A SYMMETRIC MATRIX STORED IN SYM. STORAGE MODE.  THE
                    C     DECOMPOSITION OVERLAYS THE ELEMENTS OF THE MATRIX.  IF THE MATRIX
                    C     IS NOT POSITIVE DEFINITE, THE MCD REPRESENTS A MODIFIED MATRIX
                    C     WHICH IS.  THIS IS DONE BY SETTING THE APPROPRIATE ELEMENTS OF
                    C     D TO 1.
                    C     SEE E.G. 'THE USE OF THE MODIFIED CHOLESKY DECOMPOSITION IN
                    C     DIVERGENCE AND CLASSIFICATION CALCULATIONS',BY D.L. VAN ROOY,
                    C     M.S. LYNN, & C.H. SNUDER, ICSA TECH. RPT. 275-025-008, RICE
                    C     UNIV., HOUSTON,TX, MAY,1973.
                    C  ************************************************************DVR04830
                    C                                                              DVR04840
                    C        KK = THE COVARIANCE MATRIX STORED IN SYMMETRIC STORAGE MODE.   DVR04850
                    C        KK=L D L*                                             DVR04820
                    C           WHERRE L IS UNIT LOWER TRIANGULAR & D DIAGONAL WITH POS.
                    C           ENTRIES.
                    C        NV = THE NUMBER OF CHANNELS USED                      DVR04860
                    C        DUM = A DOUBLE PRECISION WORK AREA OF SIZE NV=1
                    C                                                              DVR04890
ISN 0004            REAL*8 KK(1)
ISN 0005            REAL*8 DUM(1)
ISN 0006            REAL*8 R,R1,T1,TF
ISN 0007            LOGICAL*1 JE1                                                  DVR04910
ISN 0008            JE1=.TRUE.                                                     DVR04920
ISN 0009            EPS=.1
ISN 0010            J1=0                                                           DVR04930
ISN 0011            JD=0                                                           DVR04940
                    C                                                              DVR04960
                    C        LOOP OVER ALL DIMENSIONS
                    C                                                              DVR04980
ISN 0012            DO 10 J=1,NV                                                   DVR04990
ISN 0013            KL=J-1                                                         DVR05000
ISN 0014            L=J+1                                                          DVR05010
ISN 0015            JD=J1                                                          DVR05020
ISN 0016            J1=J1+J                                                        DVR05030
ISN 0017            TF=0.D0
ISN 0018            IF (JE1) GO TO 12                                              DVR05050
ISN 0020            K1=0                                                           DVR05060
                    C                                                              DVR05070
                    C        COMPUTE THE DIAGONAL ELEMENTS OF D AND STORE IN KK    DVR05080
                    C        TEMPORARILY STORE THE PEODUCT KK(I,I)*KK(J,I) IN DUM(I)  DVR05090
                    C                                                              DVR05100
ISN 0021            DO 15 I=1,KL                                                   DVR05110
ISN 0022            R=KK(JD+I)                                                     DVR05120
ISN 0023            K1=K1+I                                                        DVR05130
ISN 0024            R1=KK(K1)*R                                                    DVR05140
ISN 0025            TF=TF-R1*R                                                     DVR05150
ISN 0026            DUM(I)=R1                                                      DVR05160
ISN 0027         15 CONTINUE                                                       DVR05170
ISN 0028         12 CONTINUE                                                       DVR05190
ISN 0029            TF=TF+KK(J1)
                    C
```

```
                C       IF K IS NOT POS. DEF. , MAKE IT SO
                C
ISN 0030                IF (TF.LT.0.) TF=EPS
ISN 0032                KK(J1      )=TF                                          DVR05180
ISN 0033                IF (L.GT.NV) GO TO 10                                    DVR05210
ISN 0035                IRD=J1-L+1                                               DVR05220
                C                                                                DVR05230
                C          COMPUTE THE R,J-TH ELEMENT OF L USING T1               DVR05240
                C                                                                DVR05250
ISN 0036                DO 20 IR=L,NV                                            DVR05260
ISN 0037                IRD=IRD+IR-1                                             DVR05270
ISN 0038                T1=0.D0
ISN 0039                IF (JE1) GO TO 16                                        DVR05290
ISN 0041                DO 25 I=1,KL                                             DVR05300
ISN 0042                T1=T1-DUM(I)*KK(IRD+I)                                   DVR05310
ISN 0043             25 CONTINUE                                                 DVR05320
ISN 0044             16 KK(IRD+J)=(T1+KK(IRD+J))/TF
ISN 0045             20 CONTINUE                                                 DVR05340
ISN 0046                JE1=.FALSE.                                              DVR05350
ISN 0047             10 CONTINUE                                                 DVR05360
ISN 0048                RETURN
ISN 0049                END                                                      DVR05460
```

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LEVEL 21.8 ( JUN 74 )                    OS/360  FORTRAN H                    DATE

         COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                            SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002                SUBROUTINE PDSOLV(A,X,Y,N)
ISN 0003                IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004                REAL*8 A(1),X(N),Y(N)
ISN 0005                REAL*8 S
                C
                C       SOLVE A*X=Y WHERE A IS A SYMMETRICALLY STORED MATRIX CONTAINING
                C       THE MODIFIED CHOLESKY DECOMPOSITION OF  ANOTHER MATRIX.
                C
ISN 0006                ISB(J,I)=J*(J-1)/2+I
                C
                C       SOLVE L*Z=Y & PUT RESULT IN X
                C
ISN 0007                K=0
ISN 0008                DO 10 I=1,N
ISN 0009                S=Y(I)
ISN 0010                IF (I.EQ.1) GO TO 15
ISN 0012                I1=I-1
ISN 0013                DO 20 J=1,I1
ISN 0014                K=K+1
ISN 0015             20 S=S-A(K)*X(J)
ISN 0016             15 K=K+1
ISN 0017             10 X(I)=S
                C
                C       SOLVE D*B=Z FOLLOWDO BY L-TRANSPOSE * X=B & OVERWRITE RESULT ON X
                C
ISN 0018                LL=N*(N+1)/2
ISN 0019                X(N)=X(N)/A(LL)
ISN 0020                IF (N.LE.1) RETURN
ISN 0022                DO 30 II=2,N
ISN 0023                I=N-II+1
ISN 0024                LL=LL-I-1
ISN 0025                X(I)=X(I)/A(LL)
ISN 0026                I1=I+1
ISN 0027                S=X(I)
ISN 0028                DO 40 J=I1,N
ISN 0029                L=ISB(J,I)
ISN 0030             40 S=S-A(L)*X(J)
ISN 0031             30 X(I)=S
ISN 0032                RETURN
ISN 0033                END
```

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                       SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002              SUBROUTINE COMPT (LD,T,Z,N,  V,TMP)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
                C
                C     THIS ROUTINE IS AN IMPLEMENTATION OF THE COMPOSITE - T ALGORITHM
                C     TO PRRFORM A RANK 1 UPDATE OF THE MCD STORED IN ARRAY LD(I.E.
                C     K=L*D*L-TRANS & WE WISH TO COMPUTE L' &D' S.T.K'=K+Z*Z-TRANS/T(1)
                C     & K'=L'*D'*L'-TRANS).
                C     THE COMPOSITE-T ALGORITHM WAS DEVELOPED BY FLETCHER & POWELL
                C     SEE 'ON THE COMPUTATION & UPDATING OF THE MODIFIED CHOLESKY
                C     DECOMPOSITION OF A COVARIANCE MATRIX,' BY D.L. VAN ROOY, ICSA
                C     TECH.RPT. 275-025-024,RICE UNIV., HOUSTON, TX. MAY, 1976.
                C
ISN 0004              REAL*8 LD(1),Z(N)
ISN 0005              REAL*8 T(1),     V(N)
ISN 0006              REAL*8 TMP(N)
ISN 0007              REAL*8 S
ISN 0008              LOGICAL*1  TPOS,RNDERR,LALP
                C
                C     LD - ARRAY CONTAINING L & D STORED IN SYM.STORAGE MODE
                C     T - AN N+1 VECTOR WHOSE FIRST ELEMENT IS AS ABOVE
                C     Z - VECTOR OF THE UPDAEE AS ABOVE
                C     N - THE DIMENSION
                C     V - WORKING STORAGE OF LENGTH .GE. N
                C     TMP - DOUBLE PRECISION WORKING STORAGE OF LENGTH .GE. N
                C
ISN 0009              TPOS=T(1).GT.0.
ISN 0010              IF (TPOS) GO TO 35
                C
                C     A POINT IS TO BE DELETED
                C
ISN 0012              EPS=5.97E-8
                C
                C     SOLVE L*V=Z FOR V
                C
ISN 0013              K=1
ISN 0014              V(1)=Z(1)
ISN 0015              DO 10 I=2,N
ISN 0016              IJ=I-1
ISN 0017              S=0.D0
ISN 0018              DO 15 J=1,IJ
ISN 0019              K=K+1
ISN 0020           15 S=S+LD(K)*V(J)
ISN 0021              K=K+1
ISN 0022              V(I)=Z(I)-S
ISN 0023           10 CONTINUE
                C
                C     COMPUTE THE T(I'S)
                C
ISN 0024              K=0
ISN 0025              RNDERR=.FALSE.
ISN 0026              DO 20 I=1,N
ISN 0027              K=K+I
ISN 0028              TMP(I)=V(I)*V(I)/LD(K)
ISN 0029              T(I+1)=T(I)+TMP(I)
ISN 0030              IF (T(I+1).GE.0.) RNDERR=.TRUE.
ISN 0032           20 CONTINUE
```

```
ISN 0033            IF (.NOT.RNDERR) GO TO 35
                C
                C     ROUNDING ERROR HAS MADE A T(I+1).GE.0. SO CORRECT FOR THIS
                C
ISN 0035            T(N+1)=EPS*T(1)
ISN 0036            DO 30 J=1,N
ISN 0037            I=N-J+1
ISN 0038            T(I)=T(I+1)-TMP(I)
ISN 0039         30 CONTINUE
ISN 0040         35 CONTINUE
ISN 0041            IJ=0
ISN 0042            DO 40 I=1,N
ISN 0043            I1=I+1
ISN 0044            IJ=IJ+I
ISN 0045            V(I)=Z(I)
ISN 0046            DI=LD(IJ)
ISN 0047            IF (DI.GT.0.) GO TO 44
                C
                C     D(I) =0. SO RANK OF D WILL EITHER INCREASE OR REMAIN UNCHANGED.
                C
ISN 0049            IF (DABS(V(I)).GT.1.E-30) GO TO 42
                C
                C     RANK OF D WILL REMAIN UNCHANGED
                C
ISN 0051            T(I+1)=T(I)
ISN 0052            GO TO 40
                C
                C     RANK OF D WILL INCREASE BY 1
                C
ISN 0053         42 LD(IJ)=V(I)*V(I)/T(I)
ISN 0054            IF (I.EQ.N) RETURN
ISN 0056            K=IJ
ISN 0057            DO 45 J=I1,N
ISN 0058            K=K+J-1
ISN 0059            LD(K)=Z(J)/V(I)
ISN 0060         45 CONTINUE
ISN 0061            RETURN
ISN 0062         44 CONTINUE
                C
                C     UPDATE D
                C
ISN 0063            IF (TPOS) T(I+1)=T(I)+V(I)*V(I)/DI
ISN 0065            ALP=T(I+1)/T(I)
ISN 0066            LD(IJ)=DI*ALP
ISN 0067            IF (I.EQ.N) RETURN
                C
                C     UPDATE L & MODIFY Z ACCORDINGLY
                C
ISN 0069            BETA=(V(I)/DI)/T(I+1)
ISN 0070            LALP=.FALSE.
ISN 0071            IF (ALP.LE.4.) GO TO 52
                C
                C     THIS METHOD USED TO INSURE STABILITY IF ALPHA GT. 4
ISN 0073            LALP=.TRUE.
ISN 0074            GAM=T(I)/T(I+1)
ISN 0075            K=IJ
ISN 0076            DO 50 J=I1,N
ISN 0077            K=K+J-1
```

```
ISN 0078              XX=GAM*LD(K)+BETA*Z(J)
ISN 0079              Z(J)=Z(J)-V(I)*LD(K)
ISN 0080              LD(K)=XX
ISN 0081           50 CONTINUE
ISN 0082              GO TO 40
ISN 0083           52 K=IJ
ISN 0084              DO 60 J=I1,N
ISN 0085              K=K+J-1
ISN 0086              Z(J)=Z(J)-V(I)*LD(K)
ISN 0087              LD(K)=LD(K)+BETA*Z(J)
ISN 0088           60 CONTINUE
ISN 0089           40 CONTINUE
ISN 0090              RETURN
ISN 0091              END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002                SUBROUTINE LDMUL ( H,S,R,T,N)
ISN 0003                IMPLICIT REAL*8 (A-H,O-Z)
                C
                C       MULTIPLY THE MATRIX WHOSE MCD IS STORED IN  H (IN SYM. STORAGE
                C       MODE) BY S & STORE THE RESULT IN R
                C       T IS WORKING STORAGE OF LENGTH .GE.N-1
                C
ISN 0004                REAL*8  H(1),S(N),R(N),T(N)
ISN 0005                REAL*8 SK
ISN 0006                II=1
ISN 0007                DO 10 I=1,N
                C
                C       MULTIPLY BY L-TRANSPOSE
                C
ISN 0008                IS=II
ISN 0009                SK= S(I)
ISN 0010                IF (I.GE.N) GO TO 25
ISN 0012                IP1=I+1
ISN 0013                DO 20 J=IP1,N
ISN 0014                IS=IS+J-1
ISN 0015             20 SK=SK+S(J)*H(IS)
                C
                C       MULTIPLY BY D
                C
ISN 0016             25 SK=SK*H(II)
ISN 0017                T(I)=SK
                C
                C       MULTIPLY BY L
                C
ISN 0018                IF (I.LE.1) GO TO 35
ISN 0020                IM1=I-1
ISN 0021                IJ=II-I
ISN 0022                DO 30 J=1,IM1
ISN 0023                IJ=IJ+1
ISN 0024             30 SK=SK+T(J)*H(IJ)
ISN 0025             35 R(I)=SK
ISN 0026                II=II+I+1
ISN 0027             10 CONTINUE
ISN 0028                RETURN
ISN 0029                END
```