NOAA Technical Memorandum NOS NGS 29

SUBROUTINE PACKAGE FOR PROCESSING LARGE,
SPARSE, LEAST-SQUARES PROBLEMS

Rockville, Md.
January 1981

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SUBROUTINE PACKAGE FOR PROCESSING LARGE, SPARSE, LEAST-SQUARES PROBLEMS

William H. Dillinger

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ABSTRACT. A package of subroutines has been compiled to
make it relatively easy for application programers to use
several existing subroutines for forming and solving very
large, sparse sets of normal equations. The package provides
a method for reordering, solving, and computing a portion of
the inverse for sparse matrices, including the step of build-
ing the normal equations from the observation equations.

The two sections of the package include (1) reordering the
normal equations and (2) building the normal equations. It
then reduces, solves, and computes the inverse. Although
the two sections can be used independently, they were de-
signed to be used together. Implementing each section
involves three basic steps: (1) initialize some work
space, (2) pass the observation equations to the system,
and (3) call for the needed operation. The number of
parameters passed in each call has been kept to a mini-
mum to make the procedure easy to understand and use.
A simple example demonstrates how quickly the package can
be implemented.

INTRODUCTION

The primary purpose of this software package is to free the application
programer from the complicated details of solving large, sparse systems of
equations. The computer subroutines from which it was assembled involve some
complicated data structures and considerable management for the storage and
retrieval of data. This package takes care of most of these details and
provides a fairly simple procedure for quickly implementing these methods for
solving large systems of equations.

Within the National Geodetic Survey (NGS), this package is routinely used
to solve systems of equations containing up to around 6,000 unknowns. In
fact, the basic assumption for using this package is that the normal equa-
tions are large and sparse. A second assumption inherent in the code is that
limitations on computer memory, coupled with the large size of the problem,
make it necessary or desirable to use techniques for a solution not fully
contained in main memory.

This package has evolved to support the subroutine HERESI (Hanson's
Esoteric Reduction, Solution, and Inversion subroutine). HERESI was devel-
oped by Robert Hanson and is an extension of the work by Poder and Tscherning
(1973). Their record structure and column-oriented approach to the solution
were adopted with changes to compute a modified Cholesky factor and a partial

inverse. The modified Cholesky factor differs from the true Cholesky factor in that each diagonal element D has been replaced by 1/D, in order to use multiplications rather than divisions during the process of computing the Cholesky factor.

This subroutine works with the upper triangular portion of the normals only. In addition, it does not store or process any terms above the "column profile," which is defined as all elements from the first nonzero element to the diagonal in each column. This procedure, when combined with a reorder algorithm, is an efficient method for solving sparse matrices. It works within the space of the original matrix, replacing the original terms with the new terms of the Cholesky factor (or inverse) and the solution vector. The method for computing the inverse within the profile has been found to be exceptionally efficient. In fact, Hanson (1978) shows that even if only the diagonal terms of the inverse are needed, computing all inverse terms within the profile is the method with the fewest operations.

To take proper advantage of the software in the solution package, the unknowns must first be reordered. Reordering unknowns in a sparse set of normal equations can result in a dramatic reduction in the matrix profile. This makes it possible to realize the remarkable savings that can be achieved with the column profile approach used by the solution package. An example of the effects of reordering the unknowns can be seen by comparing figures 1 and 2, which represent a "typical" geodetic network of 416 unknowns. The heavy dots show the initially nonzero elements of the normal equations. The lighter dots indicate elements initially zero but which are required to be stored and processed in this system because they occur beneath the highest nonzero elements of their respective columns. Figure 1 shows the structure of the normal equations when a random input order is used as the order of elimination. After the "banker's" algorithm (Snay 1976) has been used to reorder the unknowns into a new elimination order, the resulting storage requirements are considerably reduced, as can be seen in figure 2. In addition to the reduced storage requirements, the number of computations is reduced even more.

As a result of the reordering, the matrix elements are stored and the unknowns are eliminated in an order different from the input order defined by the application program. This new order is completely transparent to the applications program when this package is used in a manner similar to the example shown in the appendix. The new elimination order and the profile structure of the resulting matrix are determined by the reorder subroutines and passed to the solution package without the need of any interaction by the applications program. Even for an iterated solution, this step needs to be done only once.

Three different reorder algorithms have been provided in the package. The simplest is the reverse Cuthill-McKee (1969) algorithm. The algorithm which has, in general, been found to produce the best column profile for horizontal geodetic networks is the banker's algorithm developed by Snay (1976). The other algorithm available was published by King (1970).
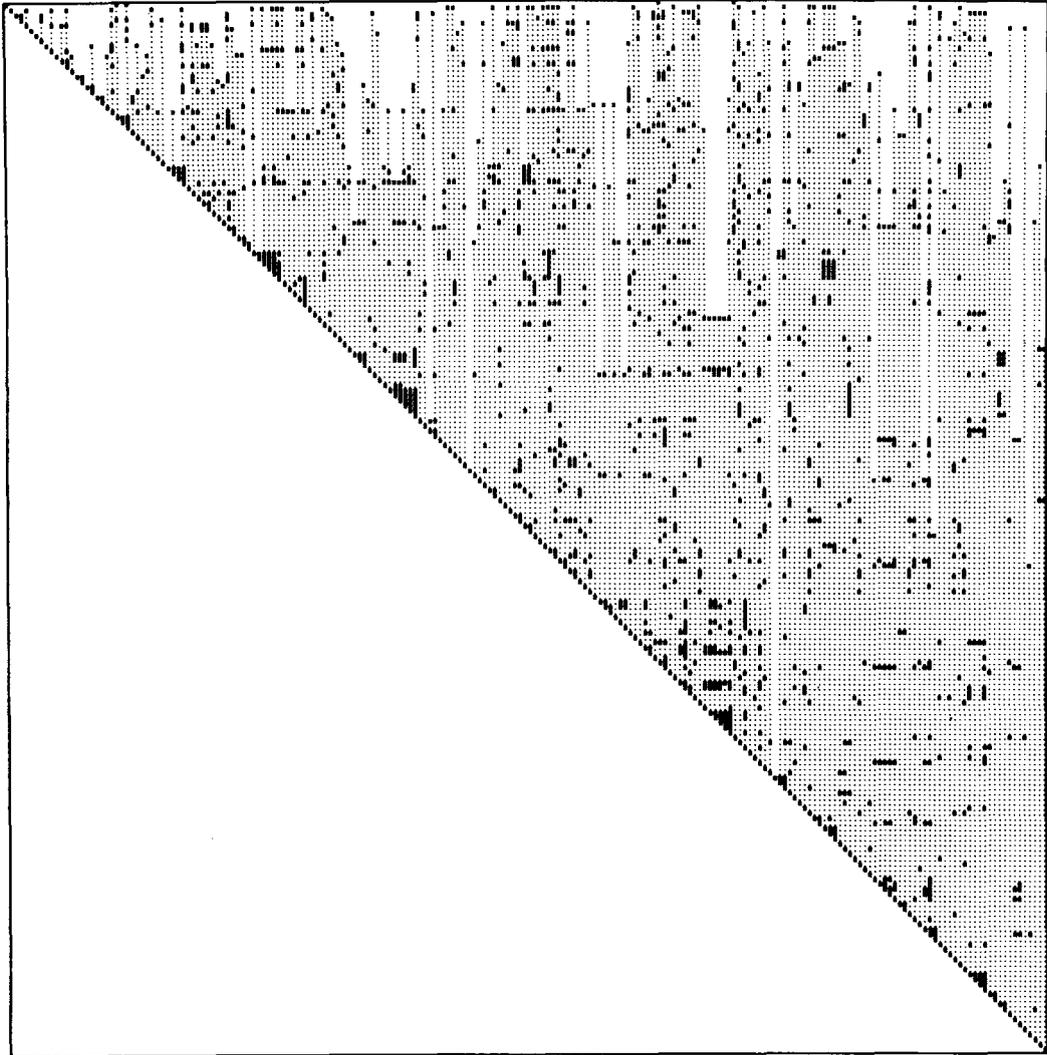
Figure 1.--Unreordered normal equation system.

   Deciding upon which algorithm to use will depend on the nature of the network being reordered. In general, the banker's algorithm takes longer to run than the others. In many problems, however, the improvement in profile storage and solution time provided by Snay's algorithm is likely to offset the increased time for reordering. This will depend on the type of problem, but was decidedly true in the gravity adjustment program currently being used by NGS (Chin 1980). None of the algorithms guarantees the smallest possible matrix profile. Any evaluation of the true computer cost will involve reorder time, solution time, storage, and time for reading and writing mass storage records.
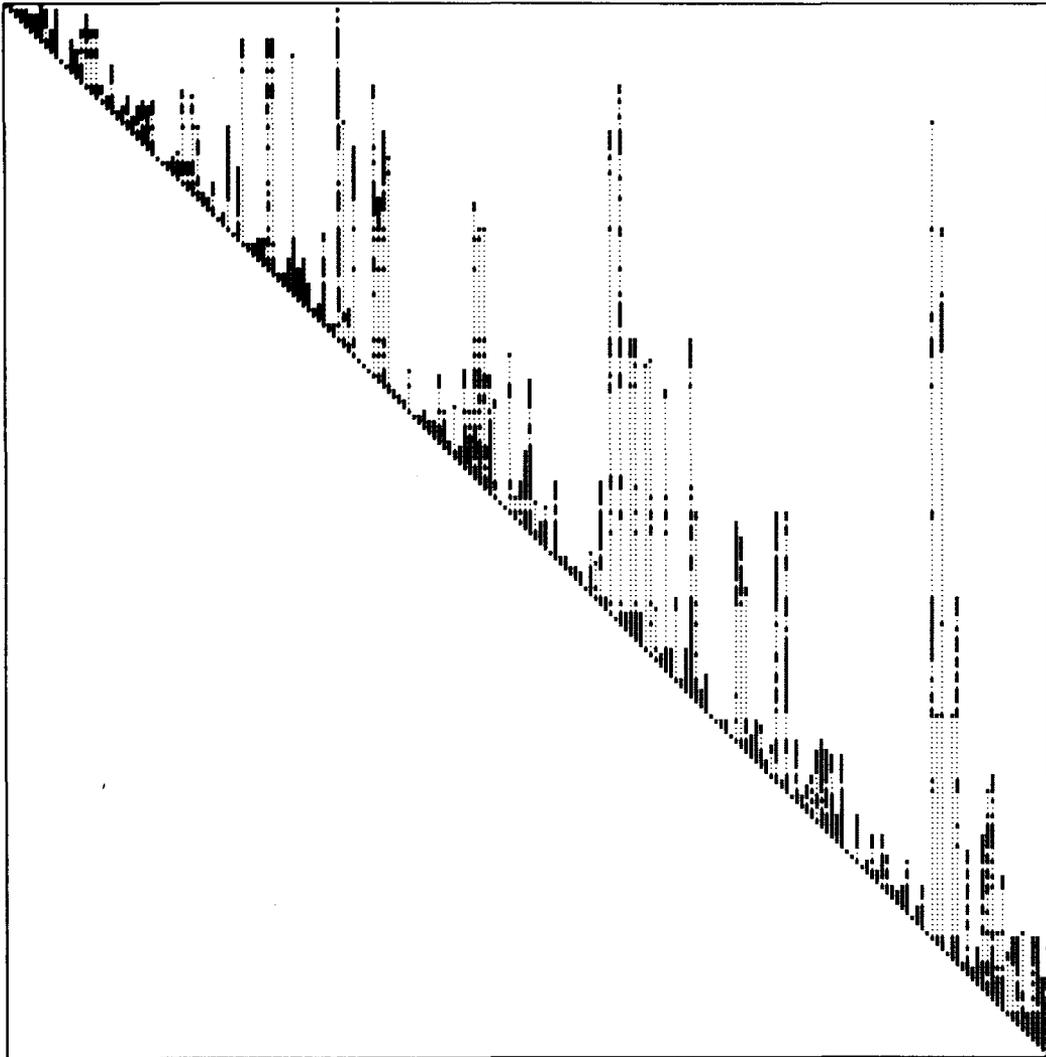
Figure 2.--A reordered normal equation matrix.

The subroutine HERESI uses a special random access mass storage record structure to hold partitions of the normal equations. The procedure for setting up this record structure and then accumulating the normal equations can be complicated. An efficient procedure for creating the HERESI records and accumulating the normal equation elements has been implemented in three subroutines by John Isner. These subroutines optimize storage for the minimum number of records in the space available and determine which columns belong in each record. They set up skeleton records, and then accumulate observation equations into the normal matrix. When the entire normal equation system will not fit in core, the subroutine queues partial normal equation elements in a linked buffer area for those HERESI records not in core. When the buffer becomes full, it then exchanges records and accumulates the queued

elements into the new record. The techniques used here have been discussed more completely by Schwarz (1978); the mathematics and procedures in HERESI are discussed by both Hanson (1978) and Schwarz (1978).

This package was written to make the efficient strategy of the HERESI subroutine available to a wide class of programers handling different applications. The space available in memory is allocated differently in the various stages of building the normals and in solving the equations. The memory allocation and the calls to the subroutines previously mentioned are fairly complicated. The package takes care of many of these procedures for the applications programer, thus making it considerably easier to use these programs. In doing so, some simplifying assumptions have been made which remove some of the flexibility of the subroutine HERESI. However, the other options are fairly sophisticated. Any programer expecting to use these features will, of necessity, have to become more knowledgeable about HERESI than is required for using this package.

MATHEMATICAL CONVENTIONS

In its simplest form, this package may be thought of as handling only observation equations and normal equations. The normal equations are defined and solved according to the following conventions. The observation equation can be written as

$$AX = L + V,$$

where A is a matrix containing the coefficients of the observation equations, X is the vector of unknowns, L is the vector of observed quantities, and V is the vector of residuals. Thus the ith observation equation would be

$$\sum_{j=1,n} A_{ij} X_i = L_i + V_i, \text{ where n is number of unknowns.}$$

Given the diagonal weight matrix P, the diagonal terms are defined as $1/\sigma^2$, where σ^2 is the variance of the ith observation.

The normal equations are formed as

$$A^t PAX = A^t PL$$

or alternatively

$$NX = U.$$

Within the context of this package, U is referred to as the right-hand side of the equations. For any problem set up differently, the sign of the resulting solution vector must be changed. In practice, the right-hand side, U, of the normal equation is appended to the normal equation matrix. Thus, given n unknowns, it becomes column n+1.

The basic assumption for this subroutine package is that the observation equations and the resulting normal equations will be sparse. It is not necessary to store or work with an observation equation containing coefficients for all unknowns, since most of these are not defined in any given measurement and are, therefore, zero. Thus, for the purposes of the subroutine package, the observation equation is defined by two arrays in the following way. Given the ith observation equation

$$\sum_{j=1,n} A_{ij} X_i = L_i + V_i,$$

and the number of nonzero terms in the ith observation equation (LOBSEQ), define FORTRAN arrays

$$IU(K) = j$$

$$C(K) = A_{ij}.$$

Here K varies from 1 to LOBSEQ. Also define the FORTRAN variables

$$WT = P_{ii}$$

$$R = L_i.$$

Then for each observation equation the subroutine package must first be given the array IU. The unknowns are then reordered. In a second pass the arrays IU and C, and the variables LOBSEQ, R, and WT are passed to the package for the solution phase.

The results available after computation will be the solution vector X and, if requested, the elements of N^{-1} (the inverse of the normal equations) which are stored beneath the profile. Remembering that the vector U was appended to the normal matrix as column n+1, and defining a Fortran variable NUNK = n, the results can be extracted using the Fortran function ELEM. Because it is a function, ELEM can be viewed as a large matrix where

$$ELEM\ (I,J,FLAG) = N^{-1}_{ij}$$

$$ELEM\ (I,NUNK+1,FLAG) = X_i.$$

While ELEM can be viewed as a large matrix containing those quantities shown above, not all elements of N^{-1} are available because the zero terms of the normal equations above the profile are not processed. Therefore, the logical variable FLAG has been provided to check whether an element is available. The variable FLAG is returned .TRUE. if N^{-1}_{ij} is available; otherwise FLAG is returned .FALSE.

RESOURCES

The working space used by the solution package must be allocated by the calling program and should be as large a scratch array as is practical considering the computer memory available. The length of this array will determine, to a large extent, the number of accesses to the mass storage device. This may vary considerably from one system to another. If the working scratch array is too small, it can cause excessive "reads" and "writes" to mass storage, which may be detrimental to the performance of the system. Much of this scratch array can be used by the calling program when not actually being used for the solution process.

The internal communication between the various subroutines is handled in several ways. Part of the information is saved in the first part of the large scratch array that must be provided for working space. A second method uses the labeled common block, NABIBB. Consequently, the name of the common block, NABIBB, must not be used in any conflicting manner. In some applications it may be useful to declare common NABIBB in the calling program, as it contains some information related to the solution process.

This package requires the use of two mass storage units. One is a sequential FORTRAN unit used as scratch space during the building of the neighbor list prior to reordering the unknowns. This sequential scratch unit is no longer needed after the call to subroutine NEWORD, which generates the new order of elimination of the unknowns. The other unit is a random access unit. The random access unit is used for the neighbor list during the reorder phase. It is then reopened and used for the normal equation records during the reduction and the solution.

The subroutine HERESI was originally coded for the CDC 6600 computer and uses variable length random access disk records. The software to simulate and perform the same function on the IBM 360/195 and the UNIVAC 1140 was coded by Charles Schwarz. This package could not be expected to run on a computer other than those mentioned here, unless the same facility could be simulated in some way. The random access software should not be too difficult to provide, but is necessary unless major changes are made to this package. The subroutines needed are OPENMS, READMS, WRITMS. These same routines are also used for reading the neighbor list.

OPTIONAL FEATURES

This paper is intended to provide interested users with an introduction to this package and a method for quick and easy implementation. Therefore, not all active or planned options have been covered. However, in putting this package together an attempt has been made to provide more flexibility

than is discussed in the appendix. Some of the additional options are as follows:

●The package has the capability to solve repeated solution vectors for any given normal equation coefficient matrix.

●The normal equations, Cholesky factor, or inverse can be printed easily if desired.

●An option is available to create a check column automatically as one means of investigating the roundoff error in reducing the matrix.

●Entry points are available to give access to the neighbor list records either before or after the actual reordering of the unknowns.

●Much of the large scratch array provided as working space can be made available to the calling program for additional scratch space when it is not being used in the solution step. (In the future all of this space may be available.)

●The normal equation matrix can optionally be filled one element at a time rather than by using the observation equations shown in the appendix.

In the future, it is expected that this package will be extended to provide an interface to a system for blocking the normal equations (Dillinger and Hanson 1976, Dillinger 1978) so that even larger problems can be solved routinely.

When the entry ADOBS is used to add observation equations to the normal equations, the sum of weighted squares of the misclosures is also accumulated. After reduction, the sum of weighted squares of the linearized residuals can be retrieved by the call SUM = ELEM (NUNK+1,NUNK+1,FLAG).

OUTLINE FOR IMPLEMENTATION

The same variable names are used in the appendix as in the following outline:

(1) Determine the number of unknowns to be solved.

NUNK = number of unknowns.

(2) Define a large working array for use in the solution.

IW = working array.

(3) Determine the length of IW available for the solution. This array should be as large as practical.

ISPACE = dimension of IW available for the solution process.

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(4) Determine scratch FORTRAN random access units to be used.

IS = sequential scratch unit number .

IH = random access scratch unit.

(5) Allocate working space in the array IW and initialize the reorder procedure.

CALL NABGEN (IW, ISPACE, NUNK, IS, IH)

(6) For each observation equation, pass the associated unknown numbers for addition to the neighbor list. (See page 6.)

CALL ADCON (IU,LOBSEQ)

IU = array of unknown numbers associated with the observation equation.

LOBSEQ = Length of the observation equation (i.e., the number of elements stored in the IU array).

(7) The following call signals all connections have been passed and the unknowns are to be reordered. The parameter IREO is set equal to 1, 2, or 3 for the reverse Cuthill-McKee, King, or Snay algorithm, respectively. The new order of the unknowns and the profile structure of the normal equation matrix are returned in the array IW to be passed on to the subroutine BIBB in the solution process. In the procedure outlined here, it is not necessary for the applications program to use either of these arrays. For an iterated solution, steps 4, 5, 6, and 7 need to be done only once.

CALL NEWORD (IREO)

(8) For an iterated solution, IT is the iteration count. The first time BIBB is called, IT must equal 0. Before each subsequent iteration, BIBB is called with IT greater than or equal to 1. This call allocates working space within the array IW for the solution phase.

CALL BIBB (ISPACE, IW, NUNK, IT)

(9) For each observation equation, pass the observation equation for addition to the normal equations.

CALL ADOBS (IU, C, LOBSEQ, R, WT)

IU = array of unknown numbers associated with this observation equation (same as step 6).

C = array of coefficients of the observation equation.

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LOBSEQ = length of observation equation (i.e., arrays IU, C).

R = constant term in the observation equation in the sense "observed minus computed."

WT = weight of this observation (i.e., $1/\sigma^2$).

An alternative to the above would be to pass partial normal equation elements specifying the element to be accumulated and the associated unknown numbers. For example:

CALL FILL1(I,J,VALUE)

(10) Specify the tolerance TOL. If TOL = 0 is specified, a default value of 9×10^{-10} is used. The Googe Number (Schwarz 1978), defined as the ratio of the reduced diagonal element to the original diagonal element in each column, is compared to the tolerance. It is assumed that a Googe Number which is less than the tolerance indicates a numeric singularity in the normal equations. No solution can be obtained for an unknown corresponding to a column for which the tolerance test fails. The HERESI subroutine continues the solution as though the indicated unknown had been constrained to zero.

(11) The following call will perform the forward reduction that computes a modified Cholesky factor, and then does a back substitution to determine the solution vector.

CALL SOLVE (NE, IERR, TOL, KEEP)

NE = number of singularities found during the forward solution.

IERR = beginning location in array IW where the column numbers of the unknown that failed the tolerance test are stored.

TOL = tolerance used in the test for singularities.

KEEP = the amount of space in array IW needed after the solution is computed for accessing the results. Space beyond KEEP can be reused for some other purpose if desired.

(12) Test NE for the number of errors. If NE is greater than zero, then IERR gives the location in array IW where a list of identifiers (column numbers) of unknowns that failed the tolerance test is stored. These identifiers are thus found in array IW from location IERR to location IERR+NE-1.

(13) Extract the solution vector and any needed inverse elements. Only inverse elements within the column profile are available.

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The variable KEEP informs the calling program how much of the
array IW is needed for use in retrieving elements of the
inverse or the solution vector.

Space beyond IW(KEEP) is no longer needed unless another
call to BIBB is to be done. It can then be used as temporary
scratch space between iterations.

Elements of the solution vector are stored in column (NUNK+1).
Any element of the inverse or the solution vector can be
retrieved with the function

$$X = ELEM (IROW, ICOLUM, FLAG)$$

where

IROW = row number.

ICOLUM = column number.

FLAG, a logical variable, = TRUE if the element requested
is within the column profile.

= FALSE if the requested location
is above the column profile.

EXAMPLE OF APPLICATION

The example of the subroutine ADJUST shown in the appendix was coded for
T. Vincenty of NGS to use in a three-dimensional geodetic adjustment program
(Vincenty 1979). Vincenty has written the observation equations C and the
associated subscripts of the unknowns IU to a disk file during the processing
of the data. This subroutine then reads that file and does the adjustment.
The subroutine is set up like the outline for implementation with the addi-
tion of two sections of code. One adds special connections into the reorder
phase. Connections which are not specified in the observation equations are
added to the neighbor list. These special connections are those needed for
error analysis after the adjustment. This process ensures that the inverse
terms needed for error analysis are available and that no special programs
are needed for this purpose. Another section of code replaces the right-hand
side of the equations and resolves without rebuilding and rereducing the nor-
mal equations.

This package was originally prepared with the assumption that a subroutine
similar to ADJUST would be coded for each different application, or that the
code would be included in the main program. In fact, the majority of the
code in subroutine ADJUST could be used in many different applications.

ACKNOWLEDGMENTS

The subroutines in this package were written by various members of the
National Geodetic Survey. Robert Hanson wrote HERESI, and the later sub-
routines HEIR and HERES, which were created to compute the inverse more
efficiently. The other subroutines in this publication were developed to
support HERESI. John Isner wrote the subroutines for designing and setting

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up the random file of HERESI records and subsequently filling the normal equation matrix. He also coded the subroutines for building the neighbor list records prior to reordering. The subroutine for reording using the banker's algorithm was coded by Richard Snay. Charles Schwarz coded the subroutines to emulate READMS and WRITMS on the IBM 360 and the UNIVAC 1140. Edward Herbrechtsmeier coded the subroutine BLOKNL, which buffers neighbor list records.

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```
      SUBROUTINE ADJUST( NOBS,NUNK,IT,IREO,IFORM,MSG, IUNIT,IUR,IUS
     .              , KTO,KFR, NERLIN, ISPACE
     .              , IW,W, IU, C
     .              , SIGMA, ANS, DI )
C
C.
C.
C.    THE FOLLOWING INPUT PARAMETERS ARE REQUIRED BY THIS SUBROUTINE
C.
C.    NOBS =   NUMBER OF OBSERVATION EQUATIONS TO PROCESS
C.    NUNK =   NUMBER OF UNKNOWNS IN THE PROBLEM
C.    IT   =   ITERATION COUNTER , THE FIRST TIME THROUGH IN THE
C.             CALL TO BIBB   IT MUST = 0 , THEREAFTER  IT   MUST BE
C.             GREATER THAN  0
C.    IREO =   PARAMETER TO SPECIFY WHICH REORDER ALGORITHM TO USE
C.    IFORM =  INTEGER SWITCH
C.             IFORM = 1  MEANS TO FORM AND REDUCE THE COMPLETE
C.                         NORMAL EQUATIONS
C.             IFORM = 0  MEANS TO REPLACE AND REREDUCE THE RIGHT HAND
C.                          SIDE OF THE EQUATIONS, WITHOUT REFORMING OR
C.                          REREDUCING THE LEFT HAND SIDE OF THE EQUATIONS
C.    MSG  =  PRINT SWITCH
C.             0 =  NO PRINT BY ADJUSTMENT PACKAGE
C.             1 =  MINIMUN PRINT, INCLUDING SINGULAR UNKNOWNS AND
C.                   WHICH REORDER ALGORITHM WAS USED
C.             2 =  IN ADDITION TO THE ABOVE PRINT INFORMATION ABOUT
C.                   COMPONENTS OF THE CONNECTIVITY GRAPH IF THEY ARE
C.                   DISCOVERED
C.             3 =  IN ADDITION TO THE ABOVE PRINT THE  NEW  ORDER ARRAY
C.    IUNIT = FORTRAN UNIT HOLDING OBSERVATION EQUATIONS
C.    IUR  =  RANDOM ACCESS SCRATCH UNIT NUMBER FOR THE NORMAL EQUATIONS
C.    IUS  =  SEQUENTIAL SCRATCH UNIT NUMBER,  NO LONGER NEEDED AFTER
C.             THE CALL TO  NEWORD
C.    KTO, KFR  =   ARRAYS CONTAINING A LIST OF UNKNOWN NUMBERS NOT
C.             CONNECTED BY THE OBSERVATION EQUATIONS BUT WHICH
C.             MUST HAVE CONNECTING INVERSE TERMS AVAILABLE FOR A
C.             NEEDED ERROR ANALYSIS   KTO(I)  WILL BE CONNECTED
C.             TO  KFR(I)
C.    NERLIN = NUMBER OF CONNECTIONS CONTAINED IN THE ARRAYS  KTO,KFR
C.    ISPACE = LENGTH IN SINGLE PRECISION WORDS OF THE SPACE
C.             AVAILABLE IN THE ARRAY  IW
C.
C.      THE FOLLOWING ARRAYS ARE NEEDED AS SCRATCH SPACE
C.
C.    IW  =   LARGE SCRATCH ARRAY TO BE USED FOR THE SOLUTION PROCESS
C.    W   =   A DOUBLE PRECISION ARRAY EQUIVALENCED TO THE ARRAY IW
C.             THROUGH THE CALLING SEQUENCE
```

```
C.          IU   =   SCRATCH ARRAY USED IN READING OBSERVATION EQUATIONS
C.                    IU  HOLDS THE UNKNOWN SEQUENCE NUMBER
C.          C   =    SCRATCH ARRAY USED IN READING OBSERVATION EQUATIONS
C.                     C  HOLDS THE COEFFICIENTS OF THE OBSERVATION EQUATIONS
C.
C.
C.               THE FOLLOWING VARIABLES ARE DEFINED BY THIS SUBROUTINE
C.
C.          SIGMA =  STANDARD ERROR OF UNIT WEIGHT
C.          ANS   =  ARRAY IN WHICH THE SOLUTION VECTOR IS STORED IN
C.                   ORDER TO ISOLATE THE CALLING PROGRAM FROM THE
C.                   SOLUTION PROCESS
C.          DI   =   ARRAY IN WHICH THE DIAGONAL TERMS OF THE INVERSE
C.                   ARE STORED TO BE PASSED BACK TO THE CALLING PROGRAM
C.
C.
C
      IMPLICIT REAL*8(A-H,O-Z)
      INTEGER   KFR,KTO
      DIMENSION IU(1),C(1),IW(1),ANS(1),DI(1)
       DIMENSION KFR(1) , KTO(1)
      DIMENSION W(1)
      LOGICAL FLAG
C
      REWIND IUNIT
      KS = 1
      IF(IT.GT.0 ) GO TO 8300
C
C.
C.    THE FOLLOWING CODE INITIALIZES THE WORKING ARRAY  IW
C.    FOR SUBROUTINE BIBB  FOR THE CONDITION WHERE THERE IS A FULL
C.    NORMAL EQUATION MATRIX
C.    (( THIS INITIALIZATION DOES NOT HURT,  BUT IS NOT NECESSARY
C.       IF THE MATRIX IS SPARSE AND IS REORDERED IN THE REORDER
C.       SECTION BELOW ))
C.
C
      NUNKA1 = NUNK +1
       DO  8025 I = 1, NUNK
      IW(I) = I
      IW(NUNKA1 +I) = I
 8025 CONTINUE
      IW(NUNKA1) = NUNKA1
      IF(IREO.EQ.0) GO TO 8300
C
```

```
C-----------------------------------------------------------------------
C.     SECTION 1    REORDER A SPARSE NORMAL EQUATION MATRIX
C.
C.     ( SECTION 1 SHOULD BE SKIPPED OVER IF THE NORMAL EQUATION MATRIX
C.      IS FULL  )
C.
C.     TO INITIALIZE THE REORDER SUBROUTINES     CALL NABGEN
C.
C
      CALL PRORD(MSG)
      CALL NABGEN(IW(KS),ISPACE, NUNK, IUS, IUR)
C
C.
C.      THE FOLLOWING  LOOP THROUGH  STMT  8200  READS THROUGH THE
C.      OBSERVATION EQUATIONS AND ADDS CONNECTIONS TO THE NEIGHBOR LIST
C
C
      DO  8200  I = 1, NOBS
      READ(IUNIT) LOBSEQ, (IU(L),C(L),L=1,LOBSEQ), CT,VAR
      DO 8190 K = 1, LOBSEQ
      IF( C(K).EQ. 0 ) IU(K) = 0
 8190 CONTINUE
      CALL ADCON( IU(1), LOBSEQ)
 8200 CONTINUE
C
C.
C.      THE FOLLOWING LOOPS THROUGH  STMT 8255  ADD CONNECTIONS TO THE
C.      NORMAL EQUATION MATRIX TO BE SURE THAT THEIR OFF DIAGONAL TERMS
C.      WILL BE AVAILABLE FOR ERROR STUDIES AFTER THE INVERSE IS DONE
C.      ONLY  CONNECTIONS NOT CONTAINED IN THE DATA NEED TO BE ADDED HERE
C.
C.
C
      IF( NERLIN .EQ. 0 ) GO TO 8255
      DO 8250 I = 1, NERLIN
      IU(1) = KFR(I)
      IU(2) = KTO(I)
      CALL ADCON( IU(1), 2)
 8250 CONTINUE
 8255 CONTINUE
C
C.
C.      THE FOLLOWING CALL WILL GET THE NEW ORDER OF THE UNKNOWNS IN THE
C.      NORMAL EQUATION MATRIX.  THE NEW ORDER AND THE PROFILE ARRAY
C.      ARE STORED AT THE BEGINING OF THE SCRATCH ARRAY  IW  AS NEEDED
C.      BY SUBROUTINE  BIBB
C.
C
      CALL NEWORD(IREO)
      REWIND IUNIT
```

```
C
C--------------------------------------------------------------------
C.      SECTION 2
C.                    BUILD  THEN  REDUCE AND SOLVE THE NORMAL EQUATIONS
C.
C.      THE FOLLOWING CALL TO  BIBB  WILL INITIALIZE THE SOLUTION PROGRAM
C.
C
 8300 CONTINUE
      IF(IFORM.EQ.0) GO TO 8500
      CALL BIBB( ISPACE, IW(KS), NUNK, IT)
C
C.
C.      THE FOLLOWING LOOP READS THROUGH THE OBSERVATION EQUATIONS AND
C.      ACCUMULATES THEM IN THE NORMAL EQUATION MATRIX BY ENTRY    ADOBS
C.
C.
C
      DO 8350 I = 1, NOBS
      READ(IUNIT) LOBSEQ, (IU(L),C(L),L=1,LOBSEQ), CT,VAR
      CALL ADOBS( IU, C, LOBSEQ, -CT, 1./VAR)
 8350 CONTINUE
C
C.
C.      REDUCE, SOLVE, AND COMPUTE THE INVERSE OF THE NORMAL EQUATIONS
C.
C
      TOL = 1.D-8
      CALL REDUCE( NE, IERR, TOL)
C
C      TEST FOR ERRORS   THAT IS   UNKNOWNS THAT FAILED TOLERANCE TEST
C
      IF( NE .EQ. 0 ) GO TO 8400
      IERRO = IERR -1
      PRINT 99998, (IW(IERRO+I),I=1,NE)
99998 FORMAT('1',//////,'0THE FOLLOWING UNKNOWNS FAILED THE TOLERANCE TES
     .T ' ,///,(10I10))
C
C      COMPUTE SOLUTION VECTOR
C
 8400 CONTINUE
      CALL SOLVE( NE, IERR; TOL, KEP)
      GO TO 8700
C
```

```
C--------------------------------------------------------------------------------
C.
C.      SECTION  3
C.                    THIS SECTION WILL
C.                    RECOMPUTE THE ABSOLUTE COLUMN OF THE NORMAL EQUATIONS
C.                    THEN RE-REDUCE AND BACK SOLVE THIS COLUMN ONLY WITHOUT
C.                    RECREATING OR REREDUCING THE NORMAL MATRIX ITSELF
C.
C
 8500 CONTINUE
      CALL SETEL( KEEPX )
      KP = (KEP +1)/2
      DO 8515 I=1,NUNK
 8515 W(I+KP)=0.
      PLL=0.
      DO 8550 I=1,NOBS
      READ(IUNIT) LOBSEQ ,(IU(L),C(L),L=1,LOBSEQ),CT,VAR
      DO 8525 K=1,LOBSEQ
      IF(C(K).EQ.0..OR.IU(K).EQ.0) GO TO 8525
      L= IU(K)
      W(KP+L)=W(KP+L)-C(K)*CT/VAR
 8525 CONTINUE
      PLL = PLL + CT*CT/VAR
 8550 CONTINUE
      DO 8600 I=1,NUNK
      WW= W(KP+I)
      CALL REPLA(WW,       I,NUNK+1,FLAG)
 8600 CONTINUE
      CALL REPLA(PLL,NUNK+1,NUNK+1,FLAG)
      CALL RESOLV
C
C.--------------------------------------------------------------------------------
C.      WRAP UP
C.                    RETRIEVE THE VARIANCE, COMPUTE SIGMA AND RETURN
C.
C
 8700 CONTINUE
      SUMPVV=ELEM(NUNK+1,NUNK+1,FLAG)
      DEN=NOBS-NUNK
      IF(DEN.EQ.0.) DEN=1.
      SIGMA =DSQRT(SUMPVV/DEN)
C
C.       RETRIEVE SOLUTION VECTOR
C
      DO 8900 I = 1,NUNK
      ANS(I) = ELEM(I, NUNK+1,FLAG)
 8900 CONTINUE
C
```

```
C.    ( NOTE- THE INVERSE CAN BE COMPUTED AT ANY TIME AFTER THE LAST
C.          CALL TO EITHER  SOLVE  OR  RESOLV BY THE FOLLOWING CALL )
C.
C.      COMPUTE THE INVERSE OF THE NORMAL EQUATIONS
C.      THEN RETRIEVE THE DIAGONAL TERMS OF THE INVERSE
C.          IN A NON-LINEAR LEAST SQUARES PROBLEM THIS STEP
C.          SHOULD BE DONE IN THE CALLING PROGRAM AFTER THE
C.          SOLUTION HAS CONVERGED
C.
C
      CALL INVRSE( NE, IERR, TOL, KEP)
      DO 9100 I =1,NUNK
      DI(I) = ELEM( I,I,FLAG)
 9100 CONTINUE
C
      RETURN
      END
```

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