

SPARSPAK: Waterloo Sparse Matrix Package
User's Guide for SPARSPAK-B

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SPARSPAK: Waterloo Sparse Matrix Package

User's Guide for SPARSPAK-B

**A collection of modules
to be used with SPARSPAK-A for solving
sparse constrained linear least squares problems**

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SPARSPAK-B User's Guide

This document describes the use of a system called SPARSPAK-B, which is an enhancement to the SPARSPAK-A package to allow for the solution of large sparse constrained (and unconstrained) linear least squares problems. SPARSPAK-B consists of new interface subroutines and some additional underlying subroutines, but makes extensive use of subroutines in the SPARSPAK-A package. SPARSPAK-B cannot run without SPARSPAK-A.

Although SPARSPAK-B depends upon SPARSPAK-A, it is in an important sense independent; a user can simultaneously solve a least squares problem and a problem from the class treated by the basic SPARSPAK-A package.

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IMPORTANT NOTE

The numerical algorithm used in *LSQSLV* (see Section 2.5) is a prototype implementation of an algorithm that is due to Bjorck [1]. The behaviour of the numerical algorithm, in the presence of roundoff errors in finite precision computer arithmetic, is not well-understood. In the course of solving a constrained linear least squares problem, some small dense subproblems may have to be solved. Some of these resulting subproblems may be sensitive to roundoff errors and numerical solutions to these subproblems may be inaccurate when a small tolerance is supplied to *LSQSLV*.

We would appreciate receiving any comments and feedback the user may have in using the package to solve practical problems. Such comments and feedback are important and useful since they may allow us to refine the numerical algorithm in the future.

When the package fails to produce an accurate solution, we would be grateful if the user could send us a copy of the data (if possible) so that we may locate where problems occur.

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1. Introduction and basic structure of SPARSPAK-B

SPARSPAK-B is designed to solve the problem

$$\min_{\beta \in \Omega} \| W_X(X\beta - y) \|_2 ,$$

where

$$\Omega = \{ \beta \mid \beta \text{ minimizes } \| W_Y(Y\beta - z) \|_2 \} .$$

Here X and Y are respectively $m \times n$ and $p \times n$ sparse matrices, y and z are vectors of length m and p respectively, and β is a vector of length n . The matrices W_X and W_Y are respectively $m \times m$ and $p \times p$ diagonal weight matrices. The package is capable of handling the very general problem in which X and Y may be either of full rank or rank-deficient, and there is no restriction on the dimensions of X and Y . Moreover, the constraints need not be consistent. When the constrained linear least squares problem does not have a unique solution, the package computes the solution which has minimal Euclidean norm.

Even though SPARSPAK-B is designed to solve a very general constrained linear least squares problem, it can also handle problems that may be much simpler than this general case. For example, the package is capable of solving an unconstrained linear least squares problem; that is, $p=0$. In particular, SPARSPAK-B can be used to solve a sparse general square system of linear equations ($p=0$ and $m=n$).

As we have noted above, the package does not impose any restrictions on the dimensions of X and Y . That is, the package also handles the case in which $m=0$ but $p \neq 0$ (even though such a problem may not have any physical meaning). In this situation, SPARSPAK-B simply treats the nonempty constraints as a linear least squares problem and computes the minimal norm least squares solution.

The basic computational technique used in SPARSPAK-B is due to George and Heath [3].

Let M denote the $(m+p) \times n$ matrix $\begin{bmatrix} Y \\ X \end{bmatrix}$. It is assumed that the Cholesky factor of $M^T M$ is sparse. Then M is reduced to upper trapezoidal form $\begin{bmatrix} R \\ O \end{bmatrix}$ by applying Givens transformations and Gaussian eliminations to the rows of M . Here R is an $n \times n$ upper triangular matrix. Finally the upper triangular matrix R is used to compute the solution. It can be shown that the structure of R is contained in the structure of the Cholesky factor of the symmetric positive definite matrix $M^T M$. Thus, using techniques developed for solving sparse symmetric positive definite systems, one can predict the structure of R by analyzing the structure of $M^T M$ [7]. This allows a storage scheme for R to be set up before numerical factorization begins and hence the numerical computation of R can be carried out using a static data structure. Experience has shown that this approach is efficient (both in terms of storage and execution time) compared to schemes that employ dynamic storage allocation [4].

In most cases, the matrix $M^T M$ is sparse when both the "least squares matrix" X and the "constraint matrix" Y are sparse. However, there are instances in which $M^T M$ is dense even though X and Y are sparse. Fortunately this usually occurs when there are only a few "dense rows" in X and Y . Such problems can be handled in a special way by the package. More precisely, the least squares problem and the constraints may be regarded as being partitioned as follows:

$$X\beta - y = \begin{bmatrix} A \\ B \end{bmatrix} \beta - \begin{bmatrix} y_A \\ y_B \end{bmatrix}$$

$$Y\beta - z = \begin{bmatrix} E \\ F \end{bmatrix} \beta - \begin{bmatrix} z_E \\ z_F \end{bmatrix}$$

where A and E contain respectively the sparse equations and constraints, and B and F contain respectively the dense equations and constraints. It is now assumed that M denotes the matrix $\begin{bmatrix} E \\ A \end{bmatrix}$. Furthermore, it is assumed that the Cholesky factor of $M^T M$ is sparse. The package reduces M to upper trapezoidal form using the approach described above. Then the upper trapezoidal form, together with B and F , are used to derive the solution to the original problem. The algorithm is due to Bjorck [1]. Detailed description of the implementation can be found in [11].

In general the algorithms, the data structures and the storage management for solving sparse matrix problems are quite complicated. Thus, in order to insulate the user from these considerations, a set of simple user interface subroutines is used in the package. These interface subroutines will be described in detail in the following sections.

The user and the package interact to solve the problem through the following basic steps.

- Step 1. The user supplies the rows of $[X \mid y]$ and $[Y \mid z]$ to the package, in any order, along with the corresponding diagonal element of W_X and W_Y .
- Step 2. The user calls a subroutine which initiates a reordering of the columns of $\begin{bmatrix} E \\ A \end{bmatrix}$, in order to preserve sparsity in subsequent calculations. (See Section 2.3.)
- Step 3. The user calls a subroutine which initiates a reordering of the rows of X and Y according to one of several criteria. (See Section 2.4.)
- Step 4. The user calls a subroutine which computes the solution β .

The package has facilities to allow the user to compute conveniently the norm of the residual vectors

$$\|y - X\beta\|_2 \quad \text{and} \quad \|z - Y\beta\|_2 ,$$

where β is the computed solution.

Important notes:

1. Note that SPARSPAK-B is designed to handle problems in which X and Y may have any dimensions. However, the package will perform more efficiently (in terms of storage and execution time) when $m + p \geq n$ (that is, overdetermined problems). When $m + p \ll n$ (that is, underdetermined problems), the package will still be able to solve the problems, but both the storage and time requirements may be high. See [5] for some examples and algorithms for handling sparse unconstrained underdetermined problems.
2. The discussions above indicate that the package employs heavily techniques for handling sparse symmetric positive definite systems of linear equations. Indeed, SPARSPAK-B makes extensive use of the subroutines in SPARSPAK-A, which is a package designed for solving efficiently sparse symmetric positive definite linear systems [2]. SPARSPAK-B cannot run

without SPARSPAK-A. Although SPARSPAK-B depends upon SPARSPAK-A, it is in an important sense independent. A user can simultaneously solve a sparse constrained linear least squares problem and a sparse symmetric positive definite linear system in the same program.

An early version of SPARSPAK-B was designed and implemented by Dr. M.T. Heath at the Oak Ridge National Laboratory. This early version includes algorithms for solving the basic sparse unconstrained linear least squares problems, and for handling constraints, dense rows and rank deficiency [12]. Those algorithms are special cases of a more general algorithm due to Bjorck for handling more general sparse constrained linear least squares problems [1]. This general algorithm is used in the current version of SPARSPAK-B. The design of SPARSPAK-B is similar to that of SPARSPAK-A [2]. The reader is referred to [6] for a discussion of the design and implementation issues.

2. Modules of SPARSPAK-B and how to use them

2.1. User mainline program and an example

SPARSPAK-B allocates all of its storage from a single one-dimensional floating-point array⁽¹⁾ which for purposes of discussion we will denote by T . In addition, the user must provide its size $MAXSB$, which is transmitted to the package via a common block $SPBUSR$, (SPARSPAK-B USER), which has eight variables.

```
COMMON /SPBUSR/ MSGLVB, IERRB, MAXSB, NCOLS,
              NSEQNS, NDEQNS, NSCONS, NDCONS
```

Here $MSGLVB$ is the message level indicator which is used to control the amount of information printed by the package. The second variable $IERRB$ is an error code, which the user can examine in his mainline program for possible errors detected by the package. Detailed discussion of the roles of $MSGLVB$ and $IERRB$ is provided in Section 6. The variable $NCOLS$ is the number of columns in X and Y , and $NSEQNS$, $NDEQNS$, $NSCONS$, $NDCONS$ are respectively the number of rows in A , B , E and F . Thus, $NSEQNS + NDEQNS = m$ and $NSCONS + NDCONS = p$.

The following program illustrates how one might use SPARSPAK-B. The various subroutines referenced are described in the subsequent parts of this section. The problem solved is assumed to be stored on an external file (FORTRAN unit 1) in a binary format.

```

      INTEGER SUBS(10)
      INTEGER FILE, IERRB, INPUT, K, MAXSB, MSGLVB,
1          NCOLS, NDCONS, NDEQNS, NSCONS, NSEQNS,
1          NSUBS, OPTION, ROWNUM, TYPE, TYPTOL
      REAL T(5000), VALUES(10)
      REAL RESCON, RESEQN, RHS, TOL, WEIGHT
      COMMON /SPBUSR/ MSGLVB, IERRB, MAXSB, NCOLS,
1          NSEQNS, NDEQNS, NSCONS, NDCONS
C
C      -----
C      INITIALIZATION.
C      -----
      INPUT = 1
      FILE = 2
      OPTION = 0
      TOL = 1.0E-6
      TYPTOL = 0
C
      CALL SPRSPK
      MSGLVB = 2
      MAXSB = 5000
C
      CALL FILEB ( FILE )
C      -----
C      INPUT ROWS FROM EXTERNAL FILE.
C      -----
      REWIND INPUT
100  CONTINUE
      READ ( INPUT ) ROWNUM, TYPE, NSUBS,
1          ( SUBS(K), VALUES(K), K=1, NSUBS ),
```

(1) Declared either REAL or DOUBLE PRECISION, depending on the version of SPARSPAK-A and SPARSPAK-B that is available. The examples in this manual assume a single precision version is being used.


```

      1          RHS, WEIGHT
      IF ( NSUBS .EQ. 0 ) GO TO 200
      CALL INXYWB ( ROWNUM, TYPE, NSUBS, SUBS, VALUES,
      1          RHS, WEIGHT, T )
      GO TO 100
200    CONTINUE
C      -----
C      ORDER COLUMNS AND ROWS.
C      -----
      CALL ORCOLB ( T )
      CALL ORROWB ( OPTION, T )
C      -----
C      COMPUTE LEAST SQUARES SOLUTION AND RESIDUALS.
C      -----
      CALL LSQSLV ( TOL, TYPTOL, T )
      CALL RESIDB ( RESEQN, RESCON, T )
C      -----
C      PRINT THE SOLUTION, FOUND IN THE FIRST NCOLS
C      LOCATIONS IN THE WORKING STORAGE ARRAY T, AND
C      PRINT THE RESIDUALS.
C      -----
      WRITE ( 6,11 ) ( T(K),K=1,NCOLS)
11     FORMAT ( / 10H SOLUTION / (5F12.5) )
      WRITE ( 6,22 ) RESEQN, RESCON
22     FORMAT ( / 22H EQUATION RESIDUAL   =, F12.5
      1          / 22H CONSTRAINT RESIDUAL =, F12.5 )
C      -----
C      PRINT STATISTICS GATHERED BY SPARSPAK-B.
C      -----
      CALL STATSB
C
      STOP
      END

```

Note: If the SPARSPAK-B package available to you is a double precision version, the REAL declarations in this example should be changed to DOUBLE PRECISION.

The module *SPRSPK* must be called before any part of the package is used. Its role is to initialize some system parameters (e.g. the logical unit numbers for output files), to set default values for options (e.g. the message level indicator), and to initialize the timing routine. The routine needs only to be called once in the user program, and the FORTRAN statement is shown below.

CALL SPRSPK

(In fact, *SPRSPK* is the initialization routine for the entire SPARSPAK package, including both SPARSPAK-A and SPARSPAK-B.) Note that the only variable in the common block *SPBUSR* that *must* be explicitly assigned a value by the user is *MAXSB*, although he may wish to set others as well, such as *MSGLVB*.

It is assumed that the subroutines which comprise SPARSPAK-A and SPARSPAK-B have been compiled into a *library*, and that the user can reference them from his FORTRAN program just as he references the standard FORTRAN library subroutines, such as *SIN*, *COS*, etc. Normally, a user will use only a small fraction of the subroutines provided in SPARSPAK-A and SPARSPAK-B.

SPARSPAK-B requires an external sequential file for the storage of intermediate results. Before beginning to solve a problem, the user must call a subroutine *FILEB* to tell SPARSPAK-B which FORTRAN unit it should use. The FORTRAN statement to be used is

CALL FILEB (IONUM)

where *IONUM* is the required FORTRAN logical unit.

Important Notes:

- (1) The module *FILEB* must be called when a new problem is to be solved.
- (2) The user is responsible for defining the external file for the FORTRAN logical unit *IONUM* using the appropriate system control statement or command. (This depends on the environment in which the program is being executed.) Furthermore, the file should be preserved throughout the execution of the program.

Warning:

The modules of SPARSPAK-B communicate with each other through labelled common blocks whose names are *SPKSYS*, *SPBUSR*, *SPBCON*, *SPBMAP*, and *SPBDTA*. (Note that *SPKSYS* is shared by SPARSPAK-A and SPARSPAK-B.) Thus, the user must not use labelled common blocks with these names in his program.

If these common block names cause conflicts in your program or at your computer installation, it is possible to have the package distributed with these common blocks having *specifically requested names*. These names should be specified when the package is acquired.

2.2. Modules for input of the problem

The subroutine *INXYWB* allows the user to provide the structure and the numerical values of *X* and *Y* to the package, along with the numerical values of *y*, *z*, *W_X*, and *W_Y*. They are provided one row at a time, as shown in the example below.

CALL INXYWB (ROWNUM, TYPE, NSUBS, SUBS, VALUES, RHS, WEIGHT, T)

The parameters of the subroutine are as follows.

ROWNUM: An integer variable associated with each row. Usually, $1 \leq \text{ROWNUM} \leq (m+p)$ and the rows of *X* and *Y* are labelled from 1 to $m+p$. The rows of *X* and *Y* can be intermixed in this labelling. It should be emphasized that *ROWNUM* is used only as a label for a row. In some contexts, it may be reasonable for several rows to have the same value for *ROWNUM*. The use of *ROWNUM* along with the use of *ORROWB* with *OPTION* set to 5 (see Section 2.4) allows the user to impose a specific row ordering.

TYPE: An integer variable having value 1, 2, 3 or 4, indicating the following.

- 1 - a row of A (sparse equation in X), with corresponding element of y and W_X .
- 2 - a row of B (dense equation in X), with corresponding element of y and W_X . (See below for an explanation.)
- 3 - a row of E (sparse constraint in Y), with corresponding element of z and W_Y .
- 4 - a row of F (dense constraint in Y), with corresponding element of z and W_Y . (See below for an explanation.)

NSUBS: An integer variable containing the number of nonzeros in the input row.

SUBS: An integer array containing the column indices (subscripts) of the nonzeros in the input row.

VALUES: A floating-point array containing the numerical values of the nonzeros in the input row in positions corresponding to the column indices stored in **SUBS**.

RHS: The right-hand side element of y or z corresponding to the input row.

WEIGHT: The diagonal element of the weight matrix W_X or W_Y corresponding to the input row. It is assumed that **WEIGHT** is positive.

T: The floating-point working storage array from which all storage for the package is allocated. (See Section 2.1 and the example there.)

Dense rows

Some problems may yield a few rows of X and of Y that have relatively many nonzeros. Such rows wreak havoc with the sparsity preservation techniques used in SPARSPAK-B. At the moment the package has no robust scheme for *deciding* which rows will cause unacceptable damage, but it does have a way of circumventing problems caused by such rows. Accordingly, the user can indicate dense rows of X or of Y by setting the corresponding value of the input parameter **TYPE** to 2 or 4 when such a row is input. See Example 2 in Section 8 for an illustration of the use of this feature.

Important Note:

The floating-point values transmitted to SPARSPAK-B by **INXYWB** are either *single or double precision floating-point numbers*, depending on the version of SPARSPAK-B being used. The examples in this manual assume that a single precision version of the package is being used.

2.3. Module for ordering the columns

Recall that the Cholesky factor of the symmetric positive definite matrix $M^T M$ plays an important role in the solution process, where $M = \begin{bmatrix} E \\ A \end{bmatrix}$. It is well known that if $M^T M$ is sparse, the sparsity of its Cholesky factor depends crucially on the symmetric ordering of the rows and columns of $M^T M$ [7]. Note that a symmetric ordering of $M^T M$ is the same as a column ordering of M . Thus, in order to reduce storage and execution time, one should find a "good" column ordering for M before any numerical computation begins so that the Cholesky factor of the reordered matrix is (hopefully) sparse. This can be achieved after the problem has been supplied to

the package using *INXYWB*. The column ordering process is invoked by executing the following FORTRAN statement.

CALL ORCOLB (T)

The algorithm used in SPARSPAK-B is an implementation of the minimum degree algorithm due to Liu [14]. The module *ORCOLB* is also responsible for setting up the appropriate data structures for the matrices involved in subsequent numerical computations.

Common Errors:

The most common cause of premature termination of the *ORCOLB* module is insufficient working storage. As mentioned above, this module performs two functions: *column ordering* and *storage allocation*. The ordering step determines the column permutation, and the allocation step sets up the appropriate data structures.

In general, the ordering and allocation subroutines require different amounts of storage. Furthermore, their storage requirements are often unpredictable, because the number of data structure pointers, and the number of nonzeros to be stored are not known until the subroutines have been executed.

Thus, the interface module *ORCOLB* may terminate in several distinctly different ways.

- (a) There was not enough storage to execute the column ordering subroutine.
- (b) The ordering was successfully obtained, but there was insufficient storage to initiate execution of the data structure set-up (storage allocation) subroutine.
- (c) The data structure set-up subroutine was executed, and the amount of storage required for the data structure pointers etc. was determined, but there was insufficient storage for these pointers.
- (d) The data structure was successfully generated, but there is insufficient storage for the actual numerical values in the upper trapezoidal matrix, so the next step (numerical computation) cannot be executed.
- (e) *ORCOLB* was successfully executed, and there is sufficient storage to proceed to the next step.

If any of the above conditions occurs, the user may execute *SAVEB*, and re-initiate the computation after adjusting the storage declarations (either up or down) and executing *RSTRTB*⁽²⁾. If (a) or (b) occurs, information is supplied indicating the minimum value of *MAXSB* needed so that (c) or (d) will occur upon re-execution. If (c) occurs, the minimum value of *MAXSB* needed for (d) is provided.

When (c) or (d) occurs, after executing *SAVEB*, adjusting the storage declaration, then executing *RSTRTB*, one must again call *ORCOLB*. However, the interface will detect that the ordering and/or storage allocation have already been performed, and will skip that part of the computation.

(2) See Section 4 for details on how to use *SAVEB* and *RSTRTB*, and Examples 3 and 4 in Section 8.

2.4. Module for reordering the rows

The execution time or the numerical stability of the module *LSQSLV* described in Section 2.5 can be affected significantly by the row ordering [3,13]. Accordingly, SPARSPAK-B provides a row-ordering module which may be invoked (optionally) by the following FORTRAN statement.

CALL ORROWB (OPTION, T)

When the weights W_X and W_Y vary widely in magnitude, it is important for numerical accuracy that the rows of A and E be arranged in order of increasing weight. See [13] for details. This can be achieved by setting the integer parameter *OPTION* to 1.

If the rows of $W_X X$ and $W_Y Y$ do not vary greatly, the user may wish to sort the rows in order to reduce execution time, although the user should be aware that this sorting might require *more* storage than would otherwise be required to solve the problem. The following options are provided.

<i>OPTION</i>	Details
0	Rows are processed in the order they were supplied, regardless of the values of <i>ROWNUM</i> (see Section 2.2).
1	Rows are sorted in order of increasing weight (i.e., the parameter <i>WEIGHT</i>).
2	Rows are sorted in order of increasing number of nonzeros (i.e., the parameter <i>NSUBS</i>).
3	Rows are sorted in order of increasing minimum column subscripts (see below).
4	Rows are sorted in order of increasing maximum column subscripts (see below).
5	Rows are sorted in order of the parameter <i>ROWNUM</i> (see Section 2.2).

Here the *maximum* {*minimum*} column subscript of a row is the column subscript (index) of the *last* {*first*} nonzero in that row. Moreover, the column indices referred to those of the (column) *permuted* matrix obtained from *ORCOLB*.

The effectiveness of these strategies is not well understood, and varies with the problem. In the absence of any prior knowledge, setting *OPTION* to 4 is recommended. See [8,9,10] for discussions on the row ordering problem in the solution of sparse linear least squares problems.

Note:

The amount of storage required to perform row ordering may be substantially larger than those required by the other interface subroutines.

2.5. Module for numerical solution

The actual numerical computation which produces the solution β is initiated by executing the FORTRAN statement

CALL LSQSLV (TOL, TYPTOL, T)

where T is the working storage array.

The parameter TOL is a user-specified tolerance which is used to determine when a diagonal element of the upper triangular matrix produced in the numerical computation should be regarded as *numerically* zero. Suppose R denotes the upper triangular matrix. A diagonal element R_{ii} will be regarded as numerically zero if

$$|R_{ii}| \leq TOL \quad \text{when} \quad TYPTOL = 0 \quad ,$$

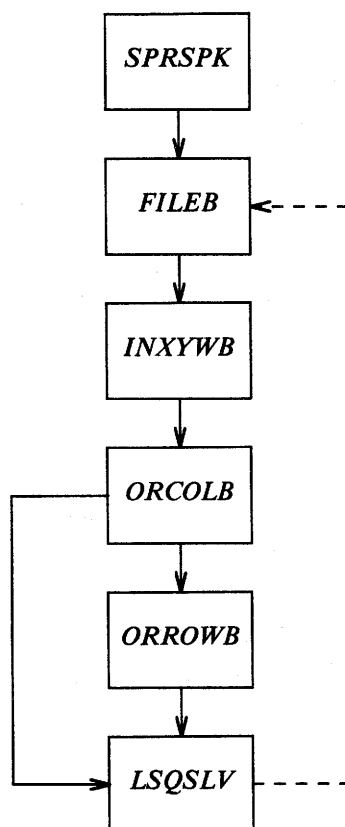
and

$$\frac{|R_{ii}|}{\max_k |R_{kk}|} \leq TOL \quad \text{when} \quad TYPTOL = 1 \quad .$$

The choice of TOL is usually problem-dependent. In general, TOL should be chosen so that it reflects the accuracy of X , Y , y and z . For example, if the input numerical values are known to be accurate to t significant digits, then one should use a relative test ($TYPTOL=1$) and TOL should be set to about 10^{-t} .

3. Summary of the use of the basic interface modules

The following flowchart depicts the sequence of calls to SPARSPAK-B interface subroutines which occur when a constrained linear least squares problem is solved. After *LSQSLV* has been executed, the solution to the problem can be found in the first *NCOLS* locations in the working storage array *T*, where *NCOLS* is the third variable in the labelled common block *SPBUSR*.



A second and subsequent problems can be solved by simply starting at the beginning of the module sequence again, as implied by the broken line.

4. Save and restart facilities

As in SPARSPAK-A, SPARSPAK-B provides two subroutines called *SAVEB* and *RSTRTB* which allow the user to stop the calculation at some point, save the results on an external sequential file, and then restart the calculation at exactly the same point some time later. To save the results of the computation done thus far, the user executes the FORTRAN statement

CALL SAVEB (K, T)

where *K* is the FORTRAN logical unit on which the results are to be written, along with other information needed to restart the computation. If execution is then terminated, the state of the computation can be re-established by executing the FORTRAN statement

CALL RSTRTB (K, T)

Example 3 provided in Section 8 illustrates the use of *SAVEB* and *RSTRTB*.

Note that executing *SAVEB* does not destroy any information; the computation can proceed just as if *SAVEB* were not executed.

When errors occur in a module, the routines *SAVEB* and *RSTRTB* are useful in saving the results of previous modules executed successfully (see Section 6.3 and Example 4 in Section 8).

Another potential use of the *SAVEB* and *RSTRTB* modules is to make the working storage array *T* available to the user in the middle of a sparse matrix computation. After *SAVEB* has been executed, the working storage array *T* can be used by some other computation.

Finally, the *SAVEB* and *RSTRTB* modules allow the user to segment the computation into several distinct phases, and thereby reduce the amount of program that must be resident in storage at any given time.

Important Notes:

- (a) In the subroutines *SAVEB* and *RSTRTB*, information is either written on or read from the FORTRAN logical unit *K* using *binary format*.
- (b) If the subroutines *SAVEB* and *RSTRTB* are used, then before the user executes his program, he must define a file for the FORTRAN logical unit *K* using the appropriate system control statement or command. (This depends on the environment in which the program is being executed.) Furthermore, this file must be preserved by the user for later access by the *RSTRTB* subroutine.
- (c) The external file for the logical unit *K* must be different from the working file specified in the *FILEB* statement.

5. Residual calculation

SPARSPAK-B provides a subroutine for computing the Euclidean norm of the residual vectors. The FORTRAN statement to be used is as follows:

CALL RESIDB (RESEQN, RESCON, T)

where *T* is the working storage array. After the subroutine is called,

$$RESEQN = || y - X\beta ||_2$$

and

$$RESCON = || z - Y\beta ||_2$$

where β is the computed solution.

Important Note:

RESIDB should be called only when the least squares solution has been computed (that is, after *LSQSLV* has been executed successfully).

6. Output from SPARSPAK-B

As noted earlier in Section 2.1, the user supplies a one-dimensional floating-point array T , from which all array storage is allocated. In particular, the interface allocates the first $NCOLS$ storage locations in T for the solution vector of the constrained linear least squares problem. After all the interface modules for a particular problem have been successfully executed, the user can retrieve the solution from these $NCOLS$ locations.

In addition to the least squares solution β , SPARSPAK-B may provide other information about the computation, depending upon the value of $MSGLVB$ (the first variable in the common block $SPBUSR$), whether or not errors occur, and whether or not the module $STATSB$ is called. This section discusses these features of SPARSPAK-B.

Notes:

Two logical output units ($IPRNTS$ and $IPRNTE$) are required by SPARSPAK-B. Any information and/or statistics which the user has requested are recorded on the output unit $IPRNTS$, while any error messages that might be raised by SPARSPAK-B during the execution of the program are recorded on the output unit $IPRNTE$. These two logical output units are set in the initialization module $SPRSPK$, and it is the responsibility of the user and/or the computer installation to ensure that the files associated with these two logical units are defined before attempting to execute the program. The default output units are both 6. (These two output units are also used by SPARSPAK-A.)

6.1. Message level indicator ($MSGLVB$)

The first variable $MSGLVB$ in the common block $SPBUSR$ stands for "message level", and governs the amount of information printed by the interface modules. Its default value is two, and for this value a relatively small amount of summary information is printed, indicating the initiation of each phase. When $MSGLVB$ is set to one by the user, only fatal error messages are printed; this option could be useful if SPARSPAK-B is being used in the "inner loop" of a large computation, where even summary information would generate excessive output. Increasing the value of $MSGLVB$ (up to 4) provides increasingly detailed information about the computation. Note that the module $SPRSPK$ sets $MSGLVB$ to its default value; if the user wishes $MSGLVB$ to be different from two, he must reset it *after* $SPRSPK$ has been called.

In many circumstances, SPARSPAK-B will be embedded in still another "super package" which models phenomena producing sparse constrained linear least squares problems. Messages printed by SPARSPAK-B may be useless or even confusing to the ultimate users of the super package, or the super package may wish to field the error conditions and perhaps take some corrective action which makes the error messages irrelevant. Thus, *all* printing by SPARSPAK-B can be prevented by setting $MSGLVB$ to zero.

We summarize our discussion in this section in the following table.

<i>MSGLVB</i>	amount of output
0	no information is provided.
1	only warnings and errors are printed.
2	warnings, errors and summary are printed.
3	warnings, errors, summary and some statistics are printed.
4	detailed information for debugging purposes.

Warning:

It should be noted that a high volume of output may be generated if *MSGLVB* is set to four, since the input data would also be echoed.

6.2. Statistics gathering (*STATSB*)

SPARSPAK-B gathers a number of statistics which the user will find useful if he is comparing SPARSPAK-B with other packages, or is going to solve numerous similar problems and wants to adjust the working storage to the minimum necessary. The package has a common block called *SPBDTA* containing variables whose values can be printed by executing the following FORTRAN statement.

CALL STATSB

The information printed includes

- the size of the working storage array *T*,
- the number of columns in *X* and *Y*,
- the number of rows in *A*, *B*, *E* and *F*,
- the number of nonzeros in the matrices *X* and *Y*,
- the maximum number of nonzeros in the rows of *X* and *Y*,
- the number of nonzeros in $\begin{pmatrix} E^T & A^T \end{pmatrix} \begin{pmatrix} E \\ A \end{pmatrix}$,
- the number of off-diagonal nonzeros in the upper triangular matrix obtained after the numerical reduction,
- the time used to find the column ordering,
- the storage used by the column ordering subroutine,
- the time used for data structure set-up,
- the storage used by the storage allocation subroutine,
- the time used to find the row ordering,
- the storage used by the row ordering subroutine,
- the time used for computing the solution,
- the number of operations required by the solution subroutine,

the storage used by the solution subroutine,
 the time used for computing the residuals,
 the number of operations required by the residual calculation subroutine,
 the storage used by the residual calculation subroutine,
 the total time used by the solution process,
 the maximum storage required by the solution process,
 the Euclidean norm of the residual vectors.

Since the module *STATSB* can be called at any time, some of the above information may not be available, and will not be printed. Furthermore, the amount of information printed also depends on the message level *MSGLVB*. The word "operations" here means multiplicative operations (multiplications and divisions). Since most of the arithmetic performed in sparse matrix computation occurs in multiply-add pairs, the number of operations (as defined here) is a useful measure of the amount of arithmetic performed.

The reader is referred to the examples in Section 8 for more discussion about the output from *STATSB*.

6.3. Error messages (*IERRB*)

When a fatal error is detected, so that the computation cannot proceed, a positive code is assigned to *IERRB*. The user can simply check the value of *IERRB* to see if the execution of the module has been successful. This error flag can be used in conjunction with the save and restart feature described in Section 4 to retain the results of successfully completed parts of the computation, as shown by the program fragment below.

```

      .
      .
      .
      CALL ORCOLB ( T )
      IF ( IERRB .EQ. 0 ) GO TO 100
      CALL SAVEB ( 3 , T )
      STOP
100 CONTINUE
      .
      .
      .
  
```

The variable *IERRB* is set to the value $10 \times k + l$, where $1 \leq l \leq 9$ distinguishes the error, and k is determined by the type of module that sets *IERRB* positive.

<i>k</i>	interface modules
20	save and restart modules (<i>SAVEB</i> and <i>RSTRTB</i>)
21	problem initialization module (<i>FILEB</i>)
22	row input module (<i>INXYWB</i>)
23	column ordering and data structure set-up module (<i>ORCOLB</i>)
24	row reordering module (<i>ORROWB</i>)
25	solution module (<i>LSQSLV</i>)
26	residual calculation module (<i>RESIDB</i>)

6.3.1. Save and restart subroutines*IERRB**SAVEB* and *RSTRTB*

- | | |
|-----|---|
| 201 | Output unit given to <i>SAVEB</i> is not positive. |
| 202 | Input unit given to <i>RSTRTB</i> is not positive. |
| 203 | Insufficient storage in working storage array to restart the computational process. The minimum value of <i>MAXSB</i> required is printed in the error message. |

6.3.2. Problem initialization subroutine*IERRB**FILEB*

- | | |
|-----|--|
| 211 | Input/output unit given to <i>FILEB</i> is not positive. |
|-----|--|

6.3.3. Row input subroutine*IERRB**INXYWB*

- | | |
|-----|--|
| 221 | Incorrect execution sequence. Probable cause of error: routine <i>FILEB</i> was not executed successfully. |
| 222 | Incorrect execution sequence. Probable cause of error: routine <i>ORCOLB</i> has already been executed. To start a new problem, <i>FILEB</i> must be called first. |
| 223 | Number of nonzeros (<i>NSUBS</i>) is not positive. |
| 224 | Input row type (<i>TYPE</i>) is invalid. |
| 225 | Input index (or subscript) is not positive. |
| 226 | Input weight (<i>WEIGHT</i>) is not positive. |
| 227 | Insufficient storage in working storage array to form matrix structure. The minimum value of <i>MAXSB</i> required is printed in the error message. |

6.3.4. Column ordering subroutine*IERRB**ORCOLB*

- | | |
|-----|--|
| 231 | Incorrect execution sequence. Probable cause of error: routine <i>INXYWB</i> was not executed successfully. |
| 232 | Incorrect execution sequence. Probable cause of error: routine <i>ORCOLB</i> was called after having already been executed successfully. |

*IERRB**ORCOLB*

- 233 Insufficient storage in working storage array to create adjacency structure. The minimum value of *MAXSB* required is printed in the error message. Response: execute *SAVEB*, and restart the computation using *ORCOLB* with *MAXSB* at least as large as that indicated in the error message.
- 234 Number of variables or columns (*NCOLS*) is zero.
- 235 Number of equations and constraints is zero (i.e., $m + p = 0$).
- 236 Insufficient storage in working storage array to execute the column ordering routine. The minimum value of *MAXSB* required is printed in the error message. Response: execute *SAVEB*, and restart the computation using *ORCOLB* with *MAXSB* at least as large as that indicated in the error message.
- 237 Insufficient storage in working storage array to execute the storage allocation routine. The column ordering routine was successfully executed. Response: same as for error 236.
- 238 Insufficient storage in working storage array to hold the data structure pointers. The column ordering and storage allocation routines were successfully executed. Response: same as for error 236.

6.3.5. Row ordering subroutine*IERRB**ORROWB*

- 241 Incorrect execution sequence. Probable cause of error: routine *ORCOLB* was not executed successfully.
- 242 Incorrect execution sequence. Probable cause of error: routine *ORROWB* was called after having already been executed successfully.
- 243 Input row ordering option (*OPTION*) is invalid.
- 244 Insufficient storage in working storage array to execute the row ordering routine. The minimum value of *MAXSB* required is printed in the error message. Response: execute *SAVEB*, and restart the computation using *ORROWB* with *MAXSB* at least as large as that indicated in the error message.

6.3.6. Solution subroutine

*IERRB**LSQSLV*

- 251 Incorrect execution sequence. Probable cause of error: routine *ORCOLB* or routine *ORROWB* was not executed successfully.
- 252 Incorrect execution sequence. Probable cause of error: routine *LSQSLV* was called after having already been executed successfully.
- 253 Input tolerance (*TOL*) is negative.
- 254 Input tolerance type (*TYPTOL*) is invalid.
- 255 Insufficient storage in working storage array to execute the solution routines. The minimum value of *MAXSB* required is printed in the error message. Response: execute *SAVEB*, and restart the computation using *LSQSLV* with *MAXSB* at least as large as that indicated in the error message.
- 256 routine *LSQSLV* fails to compute a singular value decomposition of intermediate small dense matrices.

6.3.7. Residual calculation subroutine*IERRB**RESIDB*

- 261 Incorrect execution sequence. Probable cause of error: routine *LSQSLV* was not executed successfully.
- 262 Insufficient storage in working storage array to compute residuals. The minimum value of *MAXSB* required is printed in the error message. Response: execute *SAVEB*, and restart the computation using *RESIDB* with *MAXSB* at least as large as that indicated in the error message.

7. Summary listing of SPARSPAK-B interface subroutines

SPARSPAK initialization	<i>SPRSPK</i>
Problem initialization	<i>FILEB (IONUM)</i>
Row input	<i>INABWB (ROWNUM, TYPE, NSUBS, SUBS, VALUES, RHS, WEIGHT, T)</i>
Column ordering	<i>ORCOLB (T)</i>
Row ordering	<i>ORROWB (OPTION, T)</i>
Numerical solution	<i>LSQSLV (TOL, TYPTOL, T)</i>
Residual calculation	<i>RESIDB (RESEQN, RESCON, T)</i>
Print statistics	<i>STATSB</i>
Save Restart	<i>SAVEB (K, T)</i> <i>RSTRTB (K, T)</i>

8. Examples

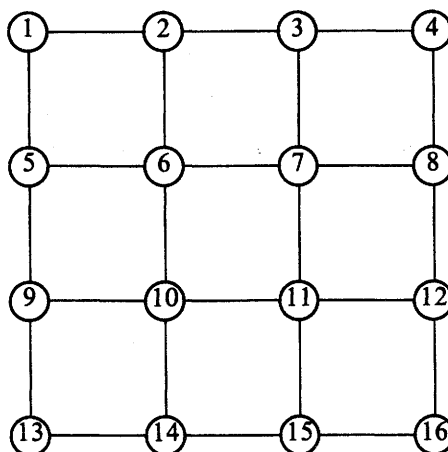
In this section, we provide several examples which illustrate how SPARSPAK-B can be used. The programs were compiled using the Berkeley f77 compiler and run on a DEC VAX 11/780 computer. A single precision version of SPARSPAK-A and SPARSPAK-B was used. All times reported are in seconds. It should be noted that the results may be different if a different version of SPARSPAK-A and SPARSPAK-B are used, or if the programs are compiled and run on a different computer.

The sample problems are variants of the following unconstrained linear least squares problem:

$$\min_{\beta} \|X\beta - y\|_2,$$

where X is defined below.

Consider a $k \times k$ grid (see figure below, where $k=4$). There is a variable associated with each grid point, and for each square in the grid, there is a set of four equations involving the variables at the four grid points in that square. This gives rise to a sparse overdetermined system of linear equations and it will be solved in the least squares sense. The number of variables is $n=k^2$ and the number of equations is $m=4(k-1)^2$. For our purpose, the numerical values of the nonzeros in X and y are generated using a uniform random number generator.



Example 1

In this example, SPARSPAK-B is used to solve a constrained linear least squares problem

$$\min_{\beta \in \Omega} || X\beta - y ||_2 ,$$

where

$$\Omega = \{ \beta \mid \beta \text{ minimizes } || Y\beta - z ||_2 \} .$$

The matrix X is the same as the one defined on a $k \times k$ grid. The constraints are as follows.

$$Y = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \end{bmatrix} , \quad z = \begin{bmatrix} 2 \\ 5 \end{bmatrix}$$

That is, the first and the second variables are assumed to have values 2 and 5 respectively.

The program begins by calling *SPRSPK* to initialize SPARSPAK-B, followed by a call to *FILEB* which tells SPARSPAK-B the unit number to be used to reference the temporary external file required by the package. Then the problem is generated and provided to SPARSPAK-B using the subroutine *INXYWB*. The column ordering is determined and data structure is set up by calling *ORCOLB*. Finally, the solution is obtained by executing *LSQSLV*. The subroutines *RESIDB* and *STATSB* are called to compute the norm of the residual vectors and to print out the statistics gathered by the package.

Note that in this example, the size of the working storage array T was 7500, while the statistic indicates that the maximum amount of storage required by any modules was only 514 which was the storage requirement in *ORCOLB*. Thus if problems with the same structure are to be solved, the user can change the size of T to 514.

Program

```

C --- SPARSPAK-B (ANSI FORTRAN) RELEASE 111 --- NAME = EX1          1SPK
C (C) UNIVERSITY OF WATERLOO JANUARY 1984                          2SPK
C*****                                                              3SPK
C*****                                                              4SPK
C*****      M A I N L I N E      P R O G R A M      *****      5SPK
C*****                                                              6SPK
C*****                                                              7SPK
C*****                                                              8SPK
C      EXAMPLE 1 (SEE USER'S GUIDE).                                9SPK
C                                                                    10SPK
C      REQUIREMENTS :                                              11SPK
C      -- AN EXTERNAL FILE FOR UNIT 1.                             12SPK
C      -- A RANDOM NUMBER GENERATOR (RANDOM).                      13SPK
C                                                                    14SPK
C*****                                                              15SPK
C                                                                    16SPK
C      INTEGER      SUBS(100)                                       17SPK
C      INTEGER      FILE , I , ICASE , IERRB , IPRNTE , IPRNTE , 18SPK
C      1            ISEED , J , K , KGRID , KMI , MAXINT ,         19SPK
C      1            MAXSB , MSGLVB , NCOLS , NDCONS , NDEQNS , NSCONS, 20SPK
C      1            NSEQNS , NSUBS , OUTPUT , ROWNUM , TYPE , TYPTOL 21SPK
C      REAL          MCHEPS , RATIOI , RATIOS , TIME               22SPK
C      REAL          T(7500) , VALUES(100)                      23SPK
C      REAL          RESCON , RESEQN , RHS , TOL , WEIGHT          24SPK
C                                                                    25SPK
C*****                                                              26SPK

```

```

C
COMMON /SPKSYS/ IPRNTE, IPRNTS, MAXINT, RATIOS, RATIOL,
1      MCHEPS, TIME
COMMON /SPBUSR/ MSGGLVB, IERRB, MAXSB, NCOLS, NSEQNS,
1      NDEQNS, NSCONS, NDCONS
C*****
C
C      -----
C      INITIALIZATION.
C      -----
C      CALL SPRSPK
C
C      FILE = 1
C      OUTPUT = IPRNTS
C      TOL = MCHEPS
C      TOL = 100.0E0*TOL
C      TYPTOL = 1
C      ISEED = 1234567
C
C      MSGGLVB = 2
C      MAXSB = 7500
C
C      CALL FILEB ( FILE )
C
C      -----
C      GENERATE PROBLEM FROM THE GRID.
C      -----
C      NSUBS = 4
C      WEIGHT = 1.0E0
C      TYPE = 1
C
C      ROWNUM = 0
C
C      KGRID = 5
C      KMI = KGRID - 1
C      DO 400 I = 1, KMI
C          DO 300 J = 1, KMI
C              -----
C              GENERATE STRUCTURE.
C              -----
C              SUBS(1) = (I - 1)*KGRID + J
C              SUBS(2) = (I - 1)*KGRID + J + 1
C              SUBS(3) = I*KGRID + J
C              SUBS(4) = I*KGRID + J + 1
C              -----
C              GENERATE NUMERICAL VALUES USING
C              A RANDOM NUMBERGENERATOR.
C              -----
C              DO 200 ICASE = 1, 4
C                  DO 100 K = 1, NSUBS
C                      VALUES(K) = RANDOM( ISEED )
100          CONTINUE
C              ROWNUM = ROWNUM + 1
C              RHS = RANDOM( ISEED )
C              CALL INXYWB ( ROWNUM, TYPE, NSUBS, SUBS,
C                          VALUES, RHS, WEIGHT, T )
C
C          200 CONTINUE
C          300 CONTINUE
C          400 CONTINUE
C
C      -----
C      GENERATE CONSTRAINTS.
C      -----
C      ROWNUM = ROWNUM + 1
C      TYPE = 3

```

27SPK
28SPK
29SPK
30SPK
31SPK
32SPK
33SPK
34SPK
35SPK
36SPK
37SPK
38SPK
39SPK
40SPK
41SPK
42SPK
43SPK
44SPK
45SPK
46SPK
47SPK
48SPK
49SPK
50SPK
51SPK
52SPK
53SPK
54SPK
55SPK
56SPK
57SPK
58SPK
59SPK
60SPK
61SPK
62SPK
63SPK
64SPK
65SPK
66SPK
67SPK
68SPK
69SPK
70SPK
71SPK
72SPK
73SPK
74SPK
75SPK
76SPK
77SPK
78SPK
79SPK
80SPK
81SPK
82SPK
83SPK
84SPK
85SPK
86SPK
87SPK
88SPK
89SPK
90SPK
91SPK
92SPK

NSUBS = 1	93SPK
SUBS(1) = 1	94SPK
VALUES(1) = 1.0E0	95SPK
RHS = 2.0E0	96SPK
WEIGHT = 1.0E0	97SPK
CALL INXYWB (ROWNUM, TYPE, NSUBS, SUBS, VALUES,	98SPK
1 RHS, WEIGHT, T)	99SPK
C	100SPK
ROWNUM = ROWNUM + 1	101SPK
TYPE = 3	102SPK
NSUBS = 1	103SPK
SUBS(1) = 2	104SPK
VALUES(1) = 1.0E0	105SPK
RHS = 5.0E0	106SPK
WEIGHT = 1.0E0	107SPK
CALL INXYWB (ROWNUM, TYPE, NSUBS, SUBS, VALUES,	108SPK
1 RHS, WEIGHT, T)	109SPK
C	110SPK
C	111SPK
C ORDER COLUMNS.	112SPK
C	113SPK
CALL ORCOLB (T)	114SPK
C	115SPK
C	116SPK
C COMPUTE LEAST SQUARES SOLUTION AND RESIDUALS.	117SPK
C	118SPK
CALL LSQSLV (TOL, TYPTOL, T)	119SPK
CALL RESIDB (RESEQN, RESCON, T)	120SPK
C	121SPK
C	122SPK
C PRINT THE SOLUTION, FOUND IN THE FIRST NCOLS	123SPK
C LOCATIONS IN THE WORKING STORAGE ARRAY T.	124SPK
C	125SPK
WRITE (OUTPUT,11) (T(K),K=1,NCOLS)	126SPK
11 FORMAT (/ 10H SOLUTION / (1P5E15.5))	127SPK
C	128SPK
C PRINT STATISTICS GATHERED BY SPARSPAK-B.	129SPK
C	130SPK
CALL STATSB	131SPK
C	132SPK
STOP	133SPK
END	134SPK

Output

```

***** UNIVERSITY OF WATERLOO
***** SPARSE MATRIX PACKAGE
***** ( S P A R S P A K )
***** RELEASE 3
***** (C) JANUARY 1984
***** ANSI FORTRAN
***** SINGLE PRECISION
***** LAST UPDATE JANUARY 1984

```

```

OUTPUT UNIT FOR ERROR MESSAGES 6
OUTPUT UNIT FOR STATISTICS      6

```

```

FILEB - FILE INITIALIZATION ...

```

INXYWB - INPUT ROWS ...

ORCOLB - FIND COLUMN ORDERING ...

LSQSLV - LEAST SQUARES SOLVE ...

RESIDB - COMPUTE RESIDUAL ...

SOLUTION

2.00000e+00	5.00000e+00	-2.64674e+00	2.11532e+00	-3.95429e-01
-3.00018e+00	-1.18907e+00	2.28644e-01	4.77276e-01	-6.61121e-03
3.82073e-01	1.95622e+00	3.16640e-02	1.93660e-01	3.61554e-01
5.77518e-01	-3.68422e-01	9.56243e-02	2.84502e-01	1.24321e+00
6.70207e-01	5.10281e-01	3.93671e-01	1.24445e-02	-1.10439e+00

STATSB - SYSTEM-B STATISTICS ...

SIZE OF STORAGE ARRAY (MAXSB)	=	7500
NUMBER OF COLUMNS (UNKNOWN)	=	25
NUMBER OF SPARSE EQUATIONS	=	64
NUMBER OF DENSE EQUATIONS	=	0
NUMBER OF SPARSE CONSTRAINTS	=	2
NUMBER OF DENSE CONSTRAINTS	=	0
TIME FOR COLUMN ORDERING	=	0.017
STORAGE FOR COLUMN ORDERING	=	514.
TIME FOR ALLOCATION	=	0.033
STORAGE FOR ALLOCATION	=	425.
TIME FOR ROW ORDERING	=	0.
STORAGE FOR ROW ORDERING	=	0.
TIME FOR SOLUTION	=	0.650
OPERATION COUNT FOR SOLUTION	=	21758.
STORAGE FOR SOLUTION	=	451.
TIME FOR COMPUTING RESIDUAL	=	0.133
OPN COUNT FOR COMPUTING RESIDUAL	=	390.000
STORE FOR COMPUTING RESIDUAL	=	376.
TOTAL TIME REQUIRED	=	0.833
MAXIMUM STORAGE REQUIRED	=	514.
RESIDUAL IN EQUATIONS	=	7.900e+00
RESIDUAL IN CONSTRAINTS	=	0.000e-01

Example 2

The purpose of this example is to illustrate the effect of dense rows. The problem being solved is the unconstrained linear least squares problem

$$\min_{\beta} || X\beta - y ||_2 ,$$

where X is partitioned into two portions

$$X = \begin{bmatrix} A \\ B \end{bmatrix} .$$

Here A is the matrix defined on a $k \times k$ grid, and B and y_B are given below.

$$B = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 & 1 \end{bmatrix} , \quad y_B = \begin{bmatrix} 7 \end{bmatrix} .$$

In the first run, all rows of X are treated as sparse ($TYPE=1$). In the second run, the rows of A are regarded as sparse ($TYPE=1$) whereas the row of B is treated as dense ($TYPE=2$). Note the difference in storage requirements and execution times in the output.

Program 1

```

C--- SPARSPAK-B (ANSI FORTRAN) RELEASE III --- NAME = EX2A
C (C) UNIVERSITY OF WATERLOO JANUARY 1984
C*****
C*****
C***** M A I N L I N E P R O G R A M *****
C*****
C*****
C
C   EXAMPLE 2 (SEE USER'S GUIDE).
C
C   REQUIREMENTS :
C       -- AN EXTERNAL FILE FOR UNIT 1.
C       -- A RANDOM NUMBER GENERATOR (RANDOM).
C*****
C
C   INTEGER      SUBS(100)
C   INTEGER      FILE , I , ICASE , IERRB , IPRNTE , IPRNTS ,
1   ISEED , J , K , KGRID , KMI , MAXINT ,
1   MAXSB , MSGLVB , NCOLS , NDCONS , NDEQNS , NSCONS ,
1   NSEQNS , NSUBS , OUTPUT , ROWNUM , TYPE , TYPTOL
C   REAL         MCHEPS , RATIOI , RATIOS , TIME
C   REAL         T(7500) , VALUES(100)
C   REAL         RESCON , RESEQN , RHS , TOL , WEIGHT
C
C*****
C
C   COMMON /SPKSYS/ IPRNTE , IPRNTS , MAXINT , RATIOS , RATIOI ,
1   MCHEPS , TIME
C   COMMON /SPBUSR/ MSGLVB , IERRB , MAXSB , NCOLS , NSEQNS ,
1   NDEQNS , NSCONS , NDCONS
C
C*****
C
C   -----
C   INITIALIZATION.
C   -----

```

1SPK
2SPK
3SPK
4SPK
5SPK
6SPK
7SPK
8SPK
9SPK
10SPK
11SPK
12SPK
13SPK
14SPK
15SPK
16SPK
17SPK
18SPK
19SPK
20SPK
21SPK
22SPK
23SPK
24SPK
25SPK
26SPK
27SPK
28SPK
29SPK
30SPK
31SPK
32SPK
33SPK
34SPK
35SPK
36SPK
37SPK

```

C      CALL  SPRSPK
C      FILE = 1
C      OUTPUT = IPRNTS
C      TOL = MCHEPS
C      TOL = 100.0E0*TOL
C      TYPTOL = 1
C      ISEED = 1234567
C      MSGLVB = 2
C      MAXSB = 7500
C      CALL  FILEB ( FILE )
C      -----
C      GENERATE PROBLEM FROM THE GRID.
C      -----
C      NSUBS = 4
C      WEIGHT = 1.0E0
C      TYPE = 1
C      ROWNUM = 0
C      KGRID = 7
C      KMI = KGRID - 1
C      DO 400 I = 1, KMI
C          DO 300 J = 1, KMI
C              -----
C              GENERATE STRUCTURE.
C              -----
C              SUBS(1) = (I - 1)*KGRID + J
C              SUBS(2) = (I - 1)*KGRID + J + 1
C              SUBS(3) = I*KGRID + J
C              SUBS(4) = I*KGRID + J + 1
C              -----
C              GENERATE NUMERICAL VALUES USING
C              A RANDOM NUMBER GENERATOR.
C              -----
C              DO 200 ICASE = 1, 4
C                  DO 100 K = 1, NSUBS
C                      VALUES(K) = RANDOM(ISEED)
100          CONTINUE
C              ROWNUM = ROWNUM + 1
C              RHS = RANDOM(ISEED)
C              CALL INXYWB ( ROWNUM, TYPE, NSUBS, SUBS,
C                          VALUES, RHS, WEIGHT, T )
C              CONTINUE
200          CONTINUE
300          CONTINUE
400          CONTINUE
C      -----
C      GENERATE LAST EQUATION.
C      -----
C      ROWNUM = ROWNUM + 1
C      TYPE = 1
C      NSUBS = KGRID*KGRID
C      DO 500 I = 1, NSUBS
C          SUBS(I) = I
C          VALUES(I) = 1.0E0
500          CONTINUE
C      RHS = 7.0E0
C      WEIGHT = 1.0E0
C      CALL INXYWB ( ROWNUM, TYPE, NSUBS, SUBS, VALUES,
C                  1    RHS, WEIGHT, T )
C      -----

```

38SPK
39SPK
40SPK
41SPK
42SPK
43SPK
44SPK
45SPK
46SPK
47SPK
48SPK
49SPK
50SPK
51SPK
52SPK
53SPK
54SPK
55SPK
56SPK
57SPK
58SPK
59SPK
60SPK
61SPK
62SPK
63SPK
64SPK
65SPK
66SPK
67SPK
68SPK
69SPK
70SPK
71SPK
72SPK
73SPK
74SPK
75SPK
76SPK
77SPK
78SPK
79SPK
80SPK
81SPK
82SPK
83SPK
84SPK
85SPK
86SPK
87SPK
88SPK
89SPK
90SPK
91SPK
92SPK
93SPK
94SPK
95SPK
96SPK
97SPK
98SPK
99SPK
100SPK
101SPK
102SPK
103SPK

```

C      ORDER COLUMNS.                                104SPK
C      -----                                105SPK
C      CALL ORCOLB ( T )                                106SPK
C      -----                                107SPK
C      -----                                108SPK
C      COMPUTE LEAST SQUARES SOLUTION AND RESIDUALS.    109SPK
C      -----                                110SPK
C      CALL LSQSLV ( TOL, TYPTOL, T )                    111SPK
C      CALL RESIDB ( RESEQN, RESCON, T )                  112SPK
C      -----                                113SPK
C      -----                                114SPK
C      PRINT THE SOLUTION, FOUND IN THE FIRST NCOLS      115SPK
C      LOCATIONS IN THE WORKING STORAGE ARRAY T.         116SPK
C      -----                                117SPK
C      WRITE (OUTPUT,11) (T(K),K=1,NCOLS)                118SPK
11 11 FORMAT ( / 10H SOLUTION / (1P5E15.5) )            119SPK
C      -----                                120SPK
C      PRINT STATISTICS GATHERED BY SPARSPAK-B.          121SPK
C      -----                                122SPK
C      CALL STATS                                         123SPK
C      -----                                124SPK
C      STOP                                              125SPK
C      END                                              126SPK

```

Output

```

***** UNIVERSITY OF WATERLOO
***** SPARSE MATRIX PACKAGE
***** ( S P A R S P A K )
***** RELEASE 3
***** (C) JANUARY 1984
***** ANSI FORTRAN
***** SINGLE PRECISION
***** LAST UPDATE JANUARY 1984

```

```

OUTPUT UNIT FOR ERROR MESSAGES      6
OUTPUT UNIT FOR STATISTICS          6

```

FILEB - FILE INITIALIZATION ...

INXYWB - INPUT ROWS ...

ORCOLB - FIND COLUMN ORDERING ...

LSQSLV - LEAST SQUARES SOLVE ...

RESIDB - COMPUTE RESIDUAL ...

SOLUTION

4.27624e-01	3.45387e-02	1.26388e-01	3.57653e-01	3.13657e-01
1.31271e-01	-6.67795e-01	3.41637e-02	4.47426e-01	4.08073e-01
3.17152e-03	1.02795e-01	3.66493e-01	7.21198e-01	-3.65426e-01
3.04172e-01	-9.93216e-02	5.65310e-01	4.02508e-01	5.26987e-02
-6.21576e-02	2.51969e-01	5.16541e-01	1.59729e-01	6.74453e-02
-3.53609e-02	4.96227e-01	-3.99947e-01	-3.46666e-01	3.04208e-01
2.86251e-01	3.20507e-01	5.32274e-01	2.22485e-01	4.58984e-01
6.90003e-01	4.31956e-01	-1.54123e-01	9.86527e-02	3.88556e-03
1.82578e-01	-4.59611e-01	-1.64609e+00	7.08693e-01	-6.20304e-02
5.53662e-01	1.02702e-03	7.23422e-01	-1.13267e-01	

STATSB - SYSTEM-B STATISTICS ...

SIZE OF STORAGE ARRAY (MAXSB)	=	7500
NUMBER OF COLUMNS (UNKNOWN)	=	49
NUMBER OF SPARSE EQUATIONS	=	145
NUMBER OF DENSE EQUATIONS	=	0
NUMBER OF SPARSE CONSTRAINTS	=	0
NUMBER OF DENSE CONSTRAINTS	=	0
TIME FOR COLUMN ORDERING	=	0.050
STORAGE FOR COLUMN ORDERING	=	5146.
TIME FOR ALLOCATION	=	0.200
STORAGE FOR ALLOCATION	=	2795.
TIME FOR ROW ORDERING	=	0.
STORAGE FOR ROW ORDERING	=	0.
TIME FOR SOLUTION	=	2.550
OPERATION COUNT FOR SOLUTION	=	248739.
STORAGE FOR SOLUTION	=	1814.
TIME FOR COMPUTING RESIDUAL	=	0.367
OPN COUNT FOR COMPUTING RESIDUAL	=	915.000
STORE FOR COMPUTING RESIDUAL	=	1667.
TOTAL TIME REQUIRED	=	3.167
MAXIMUM STORAGE REQUIRED	=	5146.
RESIDUAL IN EQUATIONS	=	3.663e+00
RESIDUAL IN CONSTRAINTS	=	0.000e-01

Program 2

```

C--- SPARSPAK-B (ANSI FORTRAN) RELEASE III --- NAME = EX2B          1SPK
C (C) UNIVERSITY OF WATERLOO JANUARY 1984                          2SPK
C*****                                                              3SPK
C*****                                                              4SPK
C*****      M A I N L I N E      P R O G R A M      *****      5SPK
C*****                                                              6SPK
C*****                                                              7SPK
C                                                              8SPK
C      EXAMPLE 2 (SEE USER'S GUIDE).                                9SPK
C                                                              10SPK
C      REQUIREMENTS :                                              11SPK
C      -- AN EXTERNAL FILE FOR UNIT 1.                             12SPK
C      -- A RANDOM NUMBER GENERATOR (RANDOM).                      13SPK
C                                                              14SPK
C*****                                                              15SPK
C                                                              16SPK
C      INTEGER      SUBS(100)                                       17SPK
C      INTEGER      FILE , I , ICASE , IERRB , IPRNTE , IPRNTE , 18SPK
1      ISEED , J , K , KGRID , KM1 , MAXINT.                      19SPK
1      MAXSB , MSGVLB , NCOLS , NDCONS , NDEQNS , NSCONS ,        20SPK
1      NSEQNS , NSUBS , OUTPUT , ROWNUM , TYPE , TYPTOL          21SPK
      REAL          MCHEPS , RATIO , RATIOS , TIME                22SPK
      REAL          T(7500) , VALUES(100)                      23SPK
      REAL          RESCON , RESEQN , RHS , TOL , WEIGHT          24SPK
C                                                              25SPK
C*****                                                              26SPK
C                                                              27SPK
C      COMMON /SPKSYS/ IPRNTE , IPRNTE , MAXINT , RATIOS , RATIO , 28SPK
1      MCHEPS , TIME                                              29SPK
      COMMON /SPBUSR/ MSGVLB , IERRB , MAXSB , NCOLS , NSEQNS , 30SPK
1      NDEQNS , NSCONS , NDCONS                                  31SPK
C                                                              32SPK
C*****                                                              33SPK

```

C		34SPK
C	-----	35SPK
C	INITIALIZATION.	36SPK
C	-----	37SPK
	CALL SPRSPK	38SPK
C		39SPK
	FILE = 1	40SPK
	OUTPUT = IPRNTS	41SPK
	TOL = MCHEPS	42SPK
	TOL = 100.0E0*TOL	43SPK
	TYPTOL = 1	44SPK
	ISEED = 1234567	45SPK
C		46SPK
	MSGVLB = 2	47SPK
	MAXSB = 7500	48SPK
C		49SPK
	CALL FILEB (FILE)	50SPK
C		51SPK
C	-----	52SPK
C	GENERATE PROBLEM FROM THE GRID.	53SPK
C	-----	54SPK
	NSUBS = 4	55SPK
	WEIGHT = 1.0E0	56SPK
	TYPE = 1	57SPK
C		58SPK
	ROWNUM = 0	59SPK
C		60SPK
	KGRID = 7	61SPK
	KM1 = KGRID - 1	62SPK
	DO 400 I = 1, KM1	63SPK
	DO 300 J = 1, KM1	64SPK
C	-----	65SPK
C	GENERATE STRUCTURE.	66SPK
C	-----	67SPK
	SUBS(1) = (I - 1)*KGRID + J	68SPK
	SUBS(2) = (I - 1)*KGRID + J + 1	69SPK
	SUBS(3) = I*KGRID + J	70SPK
	SUBS(4) = I*KGRID + J + 1	71SPK
C	-----	72SPK
C	GENERATE NUMERICAL VALUES USING	73SPK
C	A RANDOM NUMBER GENERATOR.	74SPK
C	-----	75SPK
	DO 200 ICASE = 1, 4	76SPK
	DO 100 K = 1, NSUBS	77SPK
	VALUES(K) = RANDOM(ISEED)	78SPK
100	CONTINUE	79SPK
	ROWNUM = ROWNUM + 1	80SPK
	RHS = RANDOM(ISEED)	81SPK
	CALL INXYWB (ROWNUM, TYPE, NSUBS, SUBS,	82SPK
	VALUES, RHS, WEIGHT, T)	83SPK
200	CONTINUE	84SPK
300	CONTINUE	85SPK
400	CONTINUE	86SPK
C		87SPK
C	-----	88SPK
C	GENERATE LAST EQUATION AND TREAT IT AS DENSE.	89SPK
C	-----	90SPK
	ROWNUM = ROWNUM + 1	91SPK
	TYPE = 2	92SPK
	NSUBS = KGRID*KGRID	93SPK
	DO 500 I = 1, NSUBS	94SPK
	SUBS(I) = I	95SPK
	VALUES(I) = 1.0E0	96SPK
500	CONTINUE	97SPK
	RHS = 7.0E0	98SPK
	WEIGHT = 1.0E0	99SPK

```

      CALL INXYWB ( ROWNUM, TYPE, NSUBS, SUBS, VALUES,
1      RHS, WEIGHT, T )
C
C      -----
C      ORDER COLUMNS.
C      -----
C      CALL ORCOLB ( T )
C
C      -----
C      COMPUTE LEAST SQUARES SOLUTION AND RESIDUALS.
C      -----
C      CALL LSQSLV ( TOL, TYPTOL, T )
C      CALL RESIDB ( RESEQN, RESCON, T )
C
C      -----
C      PRINT THE SOLUTION, FOUND IN THE FIRST NCOLS
C      LOCATIONS IN THE WORKING STORAGE ARRAY T.
C      -----
C      WRITE (OUTPUT,11) (T(K),K=1,NCOLS)
11  FORMAT ( / 10H SOLUTION / (1P5E15.5) )
C
C      PRINT STATISTICS GATHERED BY SPARSPAK-B.
C      -----
C      CALL STATS
C
C      STOP
C      END

```

100SPK
101SPK
102SPK
103SPK
104SPK
105SPK
106SPK
107SPK
108SPK
109SPK
110SPK
111SPK
112SPK
113SPK
114SPK
115SPK
116SPK
117SPK
118SPK
119SPK
120SPK
121SPK
122SPK
123SPK
124SPK
125SPK
126SPK

Output

```

***** UNIVERSITY OF WATERLOO
***** SPARSE MATRIX PACKAGE
***** ( S P A R S P A K )
***** RELEASE 3
***** (C) JANUARY 1984
***** ANSI FORTRAN
***** SINGLE PRECISION
***** LAST UPDATE JANUARY 1984

```

```

      OUTPUT UNIT FOR ERROR MESSAGES      6
      OUTPUT UNIT FOR STATISTICS          6

```

FILEB - FILE INITIALIZATION ...

INXYWB - INPUT ROWS ...

ORCOLB - FIND COLUMN ORDERING ...

LSQSLV - LEAST SQUARES SOLVE ...

RESIDB - COMPUTE RESIDUAL ...

SOLUTION

4.27621e-01	3.45408e-02	1.26385e-01	3.57654e-01	3.13655e-01
1.31271e-01	-6.67797e-01	3.41631e-02	4.47427e-01	4.08074e-01
3.17158e-03	1.02797e-01	3.66493e-01	7.21199e-01	-3.65426e-01
3.04172e-01	-9.93229e-02	5.65309e-01	4.02507e-01	5.26985e-02
-6.21579e-02	2.51969e-01	5.16541e-01	1.59730e-01	6.74474e-02
-3.53588e-02	4.96227e-01	-3.99947e-01	-3.46664e-01	3.04207e-01

2.86252e-01	3.20503e-01	5.32275e-01	2.22484e-01	4.58985e-01
6.90001e-01	4.31955e-01	-1.54122e-01	9.86543e-02	3.88643e-03
1.82577e-01	-4.59609e-01	-1.64609e+00	7.08693e-01	-6.20310e-02
5.53660e-01	1.02709e-03	7.23423e-01	-1.13268e-01	

STATSB - SYSTEM-B STATISTICS ...

SIZE OF STORAGE ARRAY (MAXSB)	=	7500
NUMBER OF COLUMNS (UNKNOWN)	=	49
NUMBER OF SPARSE EQUATIONS	=	144
NUMBER OF DENSE EQUATIONS	=	1
NUMBER OF SPARSE CONSTRAINTS	=	0
NUMBER OF DENSE CONSTRAINTS	=	0
TIME FOR COLUMN ORDERING	=	0.117
STORAGE FOR COLUMN ORDERING	=	1066.
TIME FOR ALLOCATION	=	0.017
STORAGE FOR ALLOCATION	=	902.
TIME FOR ROW ORDERING	=	0.
STORAGE FOR ROW ORDERING	=	0.
TIME FOR SOLUTION	=	1.400
OPERATION COUNT FOR SOLUTION	=	128442.
STORAGE FOR SOLUTION	=	1132.
TIME FOR COMPUTING RESIDUAL	=	0.317
OPN COUNT FOR COMPUTING RESIDUAL	=	915.000
STORE FOR COMPUTING RESIDUAL	=	985.
TOTAL TIME REQUIRED	=	1.850
MAXIMUM STORAGE REQUIRED	=	1132.
RESIDUAL IN EQUATIONS	=	3.663e+00
RESIDUAL IN CONSTRAINTS	=	0.000e-01

Example 3

The effect of row ordering on execution time is illustrated. The problem being considered is the unconstrained problem defined on a $k \times k$ grid.

Note that when row ordering option (*OPTION*) is set to four, there is a reduction in execution time for *LSQSLV*. However, one should also note that the amount of storage required to perform row ordering is larger than that required by the other modules.

This example also illustrates the use of the save and restart facilities. After *ORCOLB* is called, *SAVEB* is executed to save the current state of the computation. After the problem is solved with no row ordering, the state after the execution of *ORCOLB* is restored by executing *RSTRTB* so that the problem can now be solved without invoking *FILEB*, *INXYWB*, and *ORCOLB* again.

Program

```

C--- SPARSPAK-B (ANSI FORTRAN) RELEASE III --- NAME = EX3
C (C) UNIVERSITY OF WATERLOO JANUARY 1984
C*****
C*****
C*****      M A I N L I N E      P R O G R A M      *****
C*****
C*****
C
C      EXAMPLE 3 (SEE USER'S GUIDE).
C
C      REQUIREMENTS :
C      -- AN EXTERNAL FILE FOR UNIT 1.
C      -- AN EXTERNAL FILE FOR UNIT 2.
C      -- A RANDOM NUMBER GENERATOR (RANDOM).
C
C*****
C
C      INTEGER      SUBS(100)
C      INTEGER      FILE , I , ICASE , IERRB , IPRNTE , IPRNTS ,
1      ISEED , J , K , KGRID , KMI , MAXINT ,
1      MAXSB , MSGLYB , NCOLS , NDCONS , NDEQNS , NSCONS ,
1      NSEQNS , NSUBS , OPTION , ROWNUM , SAVE , TYPE ,
1      TYPTOL
C      REAL      MCHEPS , RATIOI , RATIOS , TIME
C      REAL      T(7000) , VALUES(100)
C      REAL      RESCON , RESEQN , RHS , TOL , WEIGHT
C
C*****
C
C      COMMON /SPKSYS/ IPRNTE , IPRNTS , MAXINT , RATIOS , RATIOI ,
1      MCHEPS , TIME
C      COMMON /SPBUSR/ MSGLYB , IERRB , MAXSB , NCOLS , NSEQNS ,
1      NDEQNS , NSCONS , NDCONS
C
C*****
C
C      -----
C      INITIALIZATION.
C      -----
C      CALL SPRSPK
C
C      FILE = 1
C      SAVE = 2

```

```

TOL = MCHEPS
TOL = 100.0E0*TOL
TYPTOL = 1
ISEED = 1234567
C
MSGVLVB = 2
MAXSB = 7000
C
CALL FILEB ( FILE )
C
-----
C GENERATE PROBLEM FROM THE GRID.
C -----
NSUBS = 4
WEIGHT = 1.0E0
TYPE = 1
C
ROWNUM = 0
C
KGRID = 10
KMI = KGRID - 1
DO 400 I = 1, KMI
  DO 300 J = 1, KMI
C
-----
C GENERATE STRUCTURE.
C -----
SUBS(1) = (I - 1)*KGRID + J
SUBS(2) = (I - 1)*KGRID + J + 1
SUBS(3) = I*KGRID + J
SUBS(4) = I*KGRID + J + 1
C
-----
C GENERATE NUMERICAL VALUES USING
C A RANDOM NUMBER GENERATOR.
C -----
DO 200 ICASE = 1, 4
  DO 100 K = 1, NSUBS
    VALUES(K) = RANDOM(ISEED)
100 CONTINUE
    ROWNUM = ROWNUM + 1
    RHS = RANDOM(ISEED)
    CALL INXYWB ( ROWNUM, TYPE, NSUBS, SUBS,
1          VALUES, RHS, WEIGHT, T )
200 CONTINUE
300 CONTINUE
400 CONTINUE
C
-----
C ORDER COLUMNS.
C -----
CALL ORCOLB ( T )
C
-----
C SAVE STATE OF COMPUTATION.
C -----
CALL SAVEB ( SAVE, T )
C
OPTION = 0
500 CONTINUE
    CALL ORROWB ( OPTION, T )
C
-----
C COMPUTE LEAST SQUARES SOLUTION AND RESIDUALS.
C -----
CALL LSQSLV ( TOL, TYPTOL, T )
CALL RESIDB ( RESEQN, RESCON, T )
C
-----

```

44SPK
45SPK
46SPK
47SPK
48SPK
49SPK
50SPK
51SPK
52SPK
53SPK
54SPK
55SPK
56SPK
57SPK
58SPK
59SPK
60SPK
61SPK
62SPK
63SPK
64SPK
65SPK
66SPK
67SPK
68SPK
69SPK
70SPK
71SPK
72SPK
73SPK
74SPK
75SPK
76SPK
77SPK
78SPK
79SPK
80SPK
81SPK
82SPK
83SPK
84SPK
85SPK
86SPK
87SPK
88SPK
89SPK
90SPK
91SPK
92SPK
93SPK
94SPK
95SPK
96SPK
97SPK
98SPK
99SPK
100SPK
101SPK
102SPK
103SPK
104SPK
105SPK
106SPK
107SPK
108SPK
109SPK

C	PRINT STATISTICS GATHERED BY SPARSPAK-B.	110SPK
C	-----	111SPK
	CALL STATSB	112SPK
	IF (OPTION .EQ. 4) STOP	113SPK
C		114SPK
C	-----	115SPK
C	RESTORE STATE OF COMPUTATION.	116SPK
C	-----	117SPK
	CALL RSTRTB (SAVE, T)	118SPK
	OPTION = 4	119SPK
	GO TO 500	120SPK
C		121SPK
	END	122SPK

Output

```

***** UNIVERSITY OF WATERLOO
***** SPARSE MATRIX PACKAGE
***** ( S P A R S P A K )
***** RELEASE 3
***** (C) JANUARY 1984
***** ANSI FORTRAN
***** SINGLE PRECISION
***** LAST UPDATE JANUARY 1984

```

```

OUTPUT UNIT FOR ERROR MESSAGES      6
OUTPUT UNIT FOR STATISTICS          6

```

FILEB - FILE INITIALIZATION ...

INXYWB - INPUT ROWS ...

ORCOLB - FIND COLUMN ORDERING ...

SAVEB - SAVE STORAGE VECTOR ...

ORROWB - FIND ROW ORDERING ...

LSQSLV - LEAST SQUARES SOLVE ...

RESIDB - COMPUTE RESIDUAL ...

STATSB - SYSTEM-B STATISTICS ...

SIZE OF STORAGE ARRAY (MAXSB)	=	7000
NUMBER OF COLUMNS (UNKNOWN)	=	100
NUMBER OF SPARSE EQUATIONS	=	324
NUMBER OF DENSE EQUATIONS	=	0
NUMBER OF SPARSE CONSTRAINTS	=	0
NUMBER OF DENSE CONSTRAINTS	=	0
TIME FOR COLUMN ORDERING	=	0.217
STORAGE FOR COLUMN ORDERING	=	2269.
TIME FOR ALLOCATION	=	0.050
STORAGE FOR ALLOCATION	=	1966.
TIME FOR ROW ORDERING	=	0.
STORAGE FOR ROW ORDERING	=	0.
TIME FOR SOLUTION	=	4.683
OPERATION COUNT FOR SOLUTION	=	379405.
STORAGE FOR SOLUTION	=	2306.

TIME FOR COMPUTING RESIDUAL	=	0.717
OPN COUNT FOR COMPUTING RESIDUAL	=	1944.000
STORE FOR COMPUTING RESIDUAL	=	2006.
TOTAL TIME REQUIRED	=	5.667
MAXIMUM STORAGE REQUIRED	=	2306.
RESIDUAL IN EQUATIONS	=	4.823e+00
RESIDUAL IN CONSTRAINTS	=	0.000e-01

RSTRTB - RESTART SYSTEM-B ...

ORROWB - FIND ROW ORDERING ...

LSQSLV - LEAST SQUARES SOLVE ...

RESIDB - COMPUTE RESIDUAL ...

STATSB - SYSTEM-B STATISTICS ...

SIZE OF STORAGE ARRAY (MAXSB)	=	7000
NUMBER OF COLUMNS (UNKNOWN)	=	100
NUMBER OF SPARSE EQUATIONS	=	324
NUMBER OF DENSE EQUATIONS	=	0
NUMBER OF SPARSE CONSTRAINTS	=	0
NUMBER OF DENSE CONSTRAINTS	=	0
TIME FOR COLUMN ORDERING	=	0.217
STORAGE FOR COLUMN ORDERING	=	2269.
TIME FOR ALLOCATION	=	0.050
STORAGE FOR ALLOCATION	=	1966.
TIME FOR ROW ORDERING	=	0.083
STORAGE FOR ROW ORDERING	=	5850.
TIME FOR SOLUTION	=	3.983
OPERATION COUNT FOR SOLUTION	=	325856.
STORAGE FOR SOLUTION	=	2306.
TIME FOR COMPUTING RESIDUAL	=	0.717
OPN COUNT FOR COMPUTING RESIDUAL	=	1944.000
STORE FOR COMPUTING RESIDUAL	=	2006.
TOTAL TIME REQUIRED	=	5.050
MAXIMUM STORAGE REQUIRED	=	5850.
RESIDUAL IN EQUATIONS	=	4.823e+00
RESIDUAL IN CONSTRAINTS	=	0.000e-01

Example 4

This example illustrates the use of the save and restart facilities to handle errors detected by SPARSPAK-B. The problem being solved is the same as the one in Example 3 and row ordering option is set to four. The size of the working storage array is initially set to 3000 which will be insufficient for *ORROWB* (as illustrated by Example 3). The state of the computation is saved by calling *SAVEB* when the error is detected after *ORROWB* is called. After adjusting the size of the working storage array, we then execute the second program. The routine *RSTRTB* is called to restore the state of the computation before *ORROWB* is called.

Program 1

```

C --- SPARSPAK-B (ANSI FORTRAN) RELEASE III --- NAME = EX4A          1SPK
C (C) UNIVERSITY OF WATERLOO JANUARY 1984                          2SPK
C*****                                                              3SPK
C*****                                                              4SPK
C*****      M A I N L I N E      P R O G R A M      *****      5SPK
C*****                                                              6SPK
C*****                                                              7SPK
C*****                                                              8SPK
C      EXAMPLE 4 (SEE USER'S GUIDE).                                9SPK
C                                                                    10SPK
C      REQUIREMENTS :                                              11SPK
C      -- AN EXTERNAL FILE FOR UNIT 1.                             12SPK
C      -- AN EXTERNAL FILE FOR UNIT 2.                             13SPK
C      -- A RANDOM NUMBER GENERATOR (RANDOM).                       14SPK
C                                                                    15SPK
C*****                                                              16SPK
C                                                                    17SPK
C      INTEGER      SUBS(100)                                       18SPK
C      INTEGER      FILE , I      , ICASE , IERRB , IPRNTE , IPRNTE , 19SPK
1      ISEED , J      , K      , KGRID , KMI      , MAXINT ,      20SPK
1      MAXSB , MSGLVB , NCOLS , NDCONS , NDEQNS , NSCONS ,      21SPK
1      NSEQNS , NSUBS , OPTION , ROWNUM , SAVE , TYPE ,      22SPK
1      TYPTOL                                             23SPK
C      REAL      MCHEPS , RATIOI , RATIOS , TIME          24SPK
C      REAL      T(3000) , VALUES(100)                 25SPK
C      REAL      RESCON , RESEQN , RHS      , TOL      , WEIGHT 26SPK
C                                                                    27SPK
C*****                                                              28SPK
C                                                                    29SPK
C      COMMON /SPKSYS/ IPRNTE , IPRNTE , MAXINT , RATIOS , RATIOI , 30SPK
1      MCHEPS , TIME                                         31SPK
C      COMMON /SPBUSR/ MSGLVB , IERRB , MAXSB , NCOLS , NSEQNS , 32SPK
1      NDEQNS , NSCONS , NDCONS                             33SPK
C                                                                    34SPK
C*****                                                              35SPK
C                                                                    36SPK
C      -----                                                  37SPK
C      INITIALIZATION.                                           38SPK
C      -----                                                  39SPK
C      CALL SPRSPK                                              40SPK
C                                                                    41SPK
C      FILE = 1                                                42SPK
C      SAVE = 2                                                43SPK
C      OPTION = 4                                              44SPK
C      TOL = MCHEPS                                           45SPK
C      TOL = 100.0E0*TOL                                       46SPK
C      TYPTOL = 1                                              47SPK
C      ISEED = 1234567                                         48SPK

```

```

C          MSGLVB = 2
C          MAXSB = 3000
C          CALL FILEB ( FILE )
C          -----
C          GENERATE PROBLEM FROM THE GRID.
C          -----
C          NSUBS = 4
C          WEIGHT = 1.0E0
C          TYPE = 1
C          ROWNUM = 0
C          KGRID = 10
C          KMI = KGRID - 1
C          DO 400 I = 1, KMI
C             DO 300 J = 1, KMI
C                -----
C                GENERATE STRUCTURE.
C                -----
C                SUBS(1) = (I - 1)*KGRID + J
C                SUBS(2) = (I - 1)*KGRID + J + 1
C                SUBS(3) = I*KGRID + J
C                SUBS(4) = I*KGRID + J + 1
C                -----
C                GENERATE NUMERICAL VALUES USING
C                A RANDOM NUMBER GENERATOR.
C                -----
C                DO 200 ICASE = 1, 4
C                   DO 100 K = 1, NSUBS
C                      VALUES(K) = RANDOM( ISEED )
100          CONTINUE
C                ROWNUM = ROWNUM + 1
C                RHS = RANDOM( ISEED )
C                CALL INXYWB ( ROWNUM, TYPE, NSUBS, SUBS,
C                               VALUES, RHS, WEIGHT, T )
200          CONTINUE
300          CONTINUE
400          CONTINUE
C          IF ( IERRB .NE. 0 ) GO TO 500
C          -----
C          ORDER COLUMNS AND ROWS.
C          -----
C          CALL ORCOLB ( T )
C          IF ( IERRB .NE. 0 ) GO TO 500
C          CALL ORROWB ( OPTION, T )
C          IF ( IERRB .NE. 0 ) GO TO 500
C          -----
C          COMPUTE LEAST SQUARES SOLUTION AND RESIDUALS.
C          -----
C          CALL LSQSLV ( TOL, TYPTOL, T )
C          IF ( IERRB .NE. 0 ) GO TO 500
C          CALL RESIDB ( RESEQN, RESCON, T )
C          IF ( IERRB .NE. 0 ) GO TO 500
C          -----
C          PRINT STATISTICS GATHERED BY SPARSPAK-B.
C          -----
C          CALL STATS
C          STOP
C          500 CONTINUE

```

49SPK
 50SPK
 51SPK
 52SPK
 53SPK
 54SPK
 55SPK
 56SPK
 57SPK
 58SPK
 59SPK
 60SPK
 61SPK
 62SPK
 63SPK
 64SPK
 65SPK
 66SPK
 67SPK
 68SPK
 69SPK
 70SPK
 71SPK
 72SPK
 73SPK
 74SPK
 75SPK
 76SPK
 77SPK
 78SPK
 79SPK
 80SPK
 81SPK
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 83SPK
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 91SPK
 92SPK
 93SPK
 94SPK
 95SPK
 96SPK
 97SPK
 98SPK
 99SPK
 100SPK
 101SPK
 102SPK
 103SPK
 104SPK
 105SPK
 106SPK
 107SPK
 108SPK
 109SPK
 110SPK
 111SPK
 112SPK
 113SPK
 114SPK

```

CALL  SAVEB ( SAVE, T )
CALL  STATS
STOP
C
END

```

```

115SPK
116SPK
117SPK
118SPK
119SPK

```

Output

```

***** UNIVERSITY OF WATERLOO
***** SPARSE MATRIX PACKAGE
***** ( S P A R S P A K )
***** RELEASE 3
***** (C) JANUARY 1984
***** ANSI FORTRAN
***** SINGLE PRECISION
***** LAST UPDATE JANUARY 1984

```

```

      OUTPUT UNIT FOR ERROR MESSAGES      6
      OUTPUT UNIT FOR STATISTICS          6

```

FILEB - FILE INITIALIZATION ...

INXYWB - INPUT ROWS ...

ORCOLB - FIND COLUMN ORDERING ...

ORROWB - FIND ROW ORDERING ...

EMSGB - SYSTEM-B ERROR ...

ORROWB - ERROR NUMBER 244

INSUFF. SPACE FOR ROW ORDERING,
MAXSB MUST AT LEAST BE 5850

SAVEB - SAVE STORAGE VECTOR ...

STATSB - SYSTEM-B STATISTICS ...

```

      SIZE OF STORAGE ARRAY (MAXSB)      =      3000
      NUMBER OF COLUMNS (UNKNOWN)       =      100
      NUMBER OF SPARSE EQUATIONS          =      324
      NUMBER OF DENSE EQUATIONS           =      0
      NUMBER OF SPARSE CONSTRAINTS        =      0
      NUMBER OF DENSE CONSTRAINTS         =      0
      TIME FOR COLUMN ORDERING             =      0.217
      STORAGE FOR COLUMN ORDERING         =     2269.
      TIME FOR ALLOCATION                   =      0.050
      STORAGE FOR ALLOCATION                =     1966.
      TOTAL TIME REQUIRED                   =      0.267
      MAXIMUM STORAGE REQUIRED              =     2269.

```

Program 2

```

C--- SPARSPAK-B (ANSI FORTRAN) RELEASE III --- NAME = EX4B
C (C) UNIVERSITY OF WATERLOO JANUARY 1984
C*****
C*****
C*****      M A I N L I N E      P R O G R A M      *****
C*****
C*****
C
C      EXAMPLE 4 (SEE USER'S GUIDE).
C
C      REQUIREMENTS :
C      -- AN EXTERNAL FILE FOR UNIT 1.
C      -- AN EXTERNAL FILE FOR UNIT 2.
C      -- A RANDOM NUMBER GENERATOR (RANDOM).
C*****
C
C      INTEGER      FILE , IERRB , IPRNTE , IPRNTS , MAXINT , MAXSB ,
1      MSGGLVB , NCOLS , NDCONS , NDEQNS , NSCONS , NSEQNS ,
1      OPTION , SAVE , TYPTOL
C      REAL      MCHEPS , RATIOI , RATIOS , TIME
C      REAL      T(10000)
C      REAL      RESCON , RESEQN , TOL
C
C*****
C
C      COMMON /SPKSYS/ IPRNTE , IPRNTS , MAXINT , RATIOS , RATIOI ,
1      MCHEPS , TIME
C      COMMON /SPBUSR/ MSGGLVB , IERRB , MAXSB , NCOLS , NSEQNS ,
1      NDEQNS , NSCONS , NDCONS
C
C*****
C
C      -----
C      INITIALIZATION.
C      -----
C      CALL SPRSPK
C
C      FILE = 1
C      SAVE = 2
C      OPTION = 4
C      TOL = MCHEPS
C      TOL = 100.0E0*TOL
C      TYPTOL = 1
C
C      MSGGLVB = 2
C      MAXSB = 10000
C
C      CALL RSTRTB ( SAVE , T )
C
C      -----
C      ORDER ROWS.
C      -----
C      CALL ORROWB ( OPTION , T )
C
C      -----
C      COMPUTE LEAST SQUARES SOLUTION AND RESIDUALS.
C      -----
C      CALL LSQSLV ( TOL , TYPTOL , T )
C      CALL RESIDB ( RESEQN , RESCON , T )
C

```

1SPK
2SPK
3SPK
4SPK
5SPK
6SPK
7SPK
8SPK
9SPK
10SPK
11SPK
12SPK
13SPK
14SPK
15SPK
16SPK
17SPK
18SPK
19SPK
20SPK
21SPK
22SPK
23SPK
24SPK
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26SPK
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50SPK
51SPK
52SPK
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54SPK
55SPK
56SPK
57SPK
58SPK
59SPK
60SPK
61SPK

C	-----	62SPK
C	PRINT STATISTICS GATHERED BY SPARSPAK-B.	63SPK
C	-----	64SPK
	CALL STATSB	65SPK
	STOP	66SPK
C		67SPK
	END	68SPK

Output

```

***** UNIVERSITY OF WATERLOO
***** SPARSE MATRIX PACKAGE
***** ( S P A R S P A K )
***** RELEASE 3
***** (C) JANUARY 1984
***** ANSI FORTRAN
***** SINGLE PRECISION
***** LAST UPDATE JANUARY 1984

```

```

OUTPUT UNIT FOR ERROR MESSAGES      6
OUTPUT UNIT FOR STATISTICS          6

```

RSTRTB - RESTART SYSTEM-B ...

ORROWB - FIND ROW ORDERING ...

LSQSLV - LEAST SQUARES SOLVE ...

RESIDB - COMPUTE RESIDUAL ...

STATSB - SYSTEM-B STATISTICS ...

```

SIZE OF STORAGE ARRAY (MAXSB)      = 10000
NUMBER OF COLUMNS (UNKNOWN)       = 100
NUMBER OF SPARSE EQUATIONS          = 324
NUMBER OF DENSE EQUATIONS           = 0
NUMBER OF SPARSE CONSTRAINTS        = 0
NUMBER OF DENSE CONSTRAINTS         = 0
TIME FOR COLUMN ORDERING             = 0.217
STORAGE FOR COLUMN ORDERING          = 2269.
TIME FOR ALLOCATION                   = 0.050
STORAGE FOR ALLOCATION                = 1966.
TIME FOR ROW ORDERING                = 0.100
STORAGE FOR ROW ORDERING             = 5850.
TIME FOR SOLUTION                    = 3.933
OPERATION COUNT FOR SOLUTION         = 324939.
STORAGE FOR SOLUTION                 = 2306.
TIME FOR COMPUTING RESIDUAL           = 0.700
OPN COUNT FOR COMPUTING RESIDUAL     = 1944.000
STORE FOR COMPUTING RESIDUAL         = 2006.
TOTAL TIME REQUIRED                   = 5.000
MAXIMUM STORAGE REQUIRED              = 5850.
RESIDUAL IN EQUATIONS                = 4.823e+00
RESIDUAL IN CONSTRAINTS              = 0.000e-01

```

9. References

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