1 SUMMARY

To solve an **equality-constrained linear least squares problem.** Given an over-determined system of m linear equations in n unknowns,

$$\sum_{j=1}^{n} a_{ij} x_j = b_i, \quad i=1,2,...m, \qquad m \geq n \geq 1,$$

it calculates the solution vector $\mathbf{x}$ which satisfies the first m_1 equations ($0 \leq m_1 \leq n$) and minimizes the sum of squares of residuals

$$S(\mathbf{x}) = \sum_{i=1}^{m} r_i^2,$$

where

$$r_i = \sum_{j=1}^{n} a_{ij} x_j - b_i, \quad i=1,2,...,m.$$

The matrix $\mathbf{A} = \{a_{ij}\}$ must have rank n, that is its columns must be linearly independent. Also the first m_1 rows of $\mathbf{A}$ must be linearly independent.

There is a re-entry facility which allows further systems having the same left-hand sides to be solved economically.

On the assumption that the first m_1 equations are exact and that the remaining equations have errors which are independent random variables with the same variance, there is an entry to obtain solution standard deviations and the variance-covariance matrix.

The automatic printing of results and the calculation of equation residuals are options.

The subroutine can be used to solve the general linear least squares data fitting problem with or without equality side conditions.

ATTRIBUTES — **Version:** 1.0.0. (12th July 2004) **Types:** Real (single, double). **Original date:** January 1985. **Origin:** J.K.Reid, Harwell. **Remark:** This is a rewritten version of MA14 and supersedes it.

2 HOW TO USE THE PACKAGE

2.1 Argument lists

To calculate the least squares solution of a new system of equations:

The single precision version

```
CALL MA44A(M,N,M1,A,IA,B,RES,X,IW,W,VAR,LP,MP)
```

The double precision version

```
CALL MA44AD(M,N,M1,A,IA,B,RES,X,IW,W,VAR,LP,MP)
```

To solve a new system with the same matrix, taking advantage of the work already done:

The single precision version

```
CALL MA44B(M,N,M1,A,IA,B,RES,X,IW,W,VAR,LP,MP)
```

The double precision version

```
CALL MA44BD(M,N,M1,A,IA,B,RES,X,IW,W,VAR,LP,MP)
```

To calculate estimates of the variances, covariances and standard deviations of the solution:

The single precision version

```
CALL MA44C(M,N,M1,A,IA,IW,W,VAR,LP,MP,V,IV,STD)
```

The double precision version

```
CALL MA44CD(M,N,M1,A,IA,IW,W,VAR,LP,MP,V,IV,STD)
```

`M` is an `INTEGER` variable which must be set by the user to m, the number of equations. It is not altered. **Restriction:** $m \geq n$.

`N` is an `INTEGER` variable which must be set by the user to n, the number of variables. It is not altered. **Restriction:** $n \geq 1$.

`M1` is an `INTEGER` variable which must be set by the user to m_1, the number of constraints. It is not altered. **Restriction:** $0 \leq m_1 \leq n$.

`A` is a `REAL` (`DOUBLE PRECISION` in the D version) two-dimensional array which the user must set prior to calling `MA44A/AD` to hold the coefficients a_{ij}, i=1,2,...m, j=1,2,...,n. `MA44A/AD` overwrites it by its factorized form. It must be passed unchanged to `MA44B/BD` and `MA44C/CD` and is not altered by these subroutines.

`IA` is an `INTEGER` variable which must be set by the user to the first dimension of the array `A`. It is not altered. **Restriction:** `IA`$\geq m$.

`B` is a `REAL` (`DOUBLE PRECISION` in the D version) array of length m which the user must set prior to calling `MA44A/AD` or `MA44B/BD` to hold the coefficients b_i, i=1,2,...m. It is used as workspace. If `RES` is set to `.TRUE.`, `B` is overwritten by the equation residuals r_i, i=1,2,...m.

`RES` is a `LOGICAL` variable which the user must set prior to calling `MA44A/AD` or `MA44B/BD` to `.TRUE.` if residuals are wanted and `.FALSE.` otherwise. It is not altered.

`X` is a `REAL` (`DOUBLE PRECISION` in the D version) array of length n which need not be set by the user. `MA44A/AD` and `MA44B/BD` overwrite it by the solution x_j, j=1,2,...n.

`IW` is an `INTEGER` array of length n which is used by `MA44A/AD` as workspace and must be passed unchanged to `MA44B/BD` and `MA44C/CD`. `IW`(j) holds the column interchanged with column j at step j of the decomposition.

`W` is a one-dimensional `REAL` (`DOUBLE PRECISION` in the D version) array of length $2n$ which is used as workspace by `MA44A/AD`. It must be passed unchanged to `MA44B/BD` and `MA44C/CD` and is not altered by them.

`VAR` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which is set by `MA44A/AD` and `MA44B/BD` to an estimate of the residual variance, or to an error flag. Possible error flags are:

–1 One of the simple argument restrictions has been violated.

–2 The first m_1 rows of **A** are linearly dependent.

–3 The columns of **A** are linearly dependent.

It must be passed unchanged to `MA44C/CD` and is not altered by it unless a simple argument restriction is violated, in which case it is reset to –1. Note that roundoff errors may mean that an error return does not occur even though the columns of **A** are linearly dependent or the first m_1 rows of **A** are linearly dependent; however in this case `VAR` will be returned with a very large value.

LP is an INTEGER variable which must be set by the user to a unit number for the printing of diagnostic messages or to a non-positive number if messages are to be suppressed.

MP is an INTEGER variable which must be set by the user to a unit number for the printing of monitor output or to a non-positive number if monitor output is to be suppressed. The following information is output by MA44A/AD and MA44B/BD: the values of m_1, $m-m_1$ and n; the solution; the residual variance estimate; and (if requested) the residuals. The following information is output by MA44C/CD: the residual variance estimate; the solution standard deviations; and the variance-covariance matrix.

V is a two-dimensional REAL (DOUBLE PRECISION in the D version) array in which MA44C/CD returns an estimate of the variance-covariance matrix. The diagonal element v_{ii} estimates the variance of x_i, i=1,2,...,n and the off-diagonal element v_{ij} estimates the covariance of x_i with x_j, i=1,2,...,n, j=1,2,...,n.

IV is an INTEGER variable which must be set by the user to the first dimension of the array V. It is not altered. **Restriction:** IV$\geq n$.

STD is a one-dimensional REAL (DOUBLE PRECISION in the D version) array of length n in which MA44C/CD returns estimates of the standard deviations of the solution components.

3 GENERAL INFORMATION

Workspace: Provided in the arguments A, B, IW and W.

Use of common: None.

Other routines called directly: none.

Input/output: Diagnostic and monitor output are under the control of arguments LP and MP.

Restrictions: $m\geq n$, $n\geq 1$, $0\leq m_1\leq n$, IA$\geq m$, IV$\geq n$.

4 METHOD

The algorithm is based on the work of Bjorck and Golub (1967), BIT **7**, 322-337 and includes the column scaling suggested by Powell and Reid (1968), Harwell Report TP 322.

MA44A/AD processes the matrix and calls MA44B/BD to process the right-hand side. First orthogonal reductions are applied to the leading m_1 rows of **A**, together with column interchanges, to produce the matrix

$$\mathbf{Q}_1\mathbf{A}\mathbf{P}_1 = \begin{pmatrix} \mathbf{U}_{11} & \mathbf{A}_{12}^{(1)} \\ \mathbf{A}_{21}^{(1)} & \mathbf{A}_{22}^{(1)} \end{pmatrix} \tag{1}$$

where $\mathbf{Q}_1$ is orthogonal, $\mathbf{P}_1$ is a permutation matrix and $\mathbf{U}_{11}$ is an upper-triangular matrix of order $m_1\times m_1$. The column interchanges are chosen with the aim of ensuring that $\mathbf{U}_{11}$ is non-singular and well-conditioned.

Next Gaussian elimination steps are applied to reduce the (2,1) block (that is rows m_1 to m and columns 1 to m_1) to zero. Now the matrix has the form

$$\mathbf{G}_1\mathbf{Q}_1\mathbf{A}\mathbf{P}_1 = \begin{pmatrix} \mathbf{U}_{11} & \mathbf{A}_{12}^{(1)} \\ 0 & \mathbf{A}_{22}^{(2)} \end{pmatrix}. \tag{2}$$

The reduction is completed by orthogonal reductions in the last $m-m_1$ rows, together with column interchanges, to produce the matrix

$$\mathbf{Q}_2\mathbf{G}_1\mathbf{Q}_1\mathbf{A}\mathbf{P}_1\mathbf{P}_2 = \begin{pmatrix} \mathbf{U}_{11} & \mathbf{A}_{12}^{(2)} \\ 0 & \mathbf{U}_{22} \end{pmatrix}. \tag{3}$$

where $\mathbf{U}_{22}$ is an upper-triangular matrix of order $m-m_1$ by $n-m_1$. Details of this reduction are stored by MA44A/AD.

MA44B/BD processes the right-hand side vector and calculates the solution and, optionally, the corresponding residuals. It begins by premultiplying $\mathbf{b}$ in turn by $\mathbf{Q}_1$, $\mathbf{G}_1$ and $\mathbf{Q}_2$. The permuted solution is then found by back-substitution through the upper-triangular matrix formed by the first n rows of (3). It is then permuted to the original order.

The residuals of the transformed system have their first n components zero and their remaining components in the last $m-n$ components of the right-hand side vector. The residual vector for the original system is available by premultiplying this vector by $\mathbf{Q}_2^T$ (note that $\mathbf{G}^{-1}$ and $\mathbf{Q}_1^T$ do not affect this vector since its first m_1 components are zero). This computation is performed only if requested. The variance σ^2 of the residuals is estimated by the residual sum of squares divided by the number of degrees of freedom, $m-n$.

`MA44C/CD` estimates the variances and covariances of the solution components. The variance-covariance matrix for the reduced system is

$$\sigma^2 \begin{pmatrix} \mathbf{BVB}^T & -\mathbf{BV} \\ -\mathbf{VB}^T & \mathbf{V} \end{pmatrix},$$

where $\mathbf{V}=\mathbf{U}_{22}^{-1}\mathbf{U}_{22}^{-T}$ and $\mathbf{B}=\mathbf{U}_{11}^{-1}\mathbf{A}_{12}^{(2)}$. This can be calculated from the inverse of (2)

$$\mathbf{U}^{-1}=\begin{pmatrix} \mathbf{U}_{11} & \mathbf{A}_{12}^{(1)} \\ & \mathbf{A}_{22}^{(2)} \end{pmatrix}^{-1}=\begin{pmatrix} \mathbf{U}_{11}^{-1} & -\mathbf{BU}_{22}^{-1} \\ & \mathbf{U}_{22}^{-1} \end{pmatrix}$$

and the product

$$\mathbf{U}^{-1}\begin{pmatrix} \mathbf{0} & \\ & \mathbf{I} \end{pmatrix}\mathbf{U}^{-T}=\begin{pmatrix} \mathbf{U}_{11}^{-1} & -\mathbf{BU}_{22}^{-1} \\ & \mathbf{U}_{22}^{-1} \end{pmatrix}\begin{pmatrix} \mathbf{0} & \mathbf{0} \\ -\mathbf{U}_{22}^{-T}\mathbf{B}^T & \mathbf{U}_{22}^{-T} \end{pmatrix}=\begin{pmatrix} \mathbf{BVB}^T & -\mathbf{BV} \\ -\mathbf{V}^T\mathbf{B}^T & \mathbf{V} \end{pmatrix}.$$

Finally row and column permutations that account for $\mathbf{P}_1\mathbf{P}_2$ are applied.

5 EXAMPLE OF USE

As a very simple example, suppose the data

```
t       0       1       2       3       4
b   -0.009   1.009   1.991   0.999   0.006
```

arise from experimental measurements of a continuous function that is linear over (0,2) and (2,4). Let the linear parts be x_1+tx_2 and x_3+tx_4. The continuity at t=2 gives the condition

$$x_1+2x_2-x_3-2x_4=0$$

and a typical data equation is

$$x_1+x_2=1.009$$

A suitable program is as follows

```
C EXAMPLE OF THE USE OF MA44
      DOUBLE PRECISION A(10,4),B(10),X(4),W(20),V(5,5),VAR,STD(4)
      INTEGER IW(4),IA,IV,M,N,M1,LP,MP
      LOGICAL RES
      DATA A(1,1),A(1,2),A(1,3),A(1,4)/1.0D0, 2.0D0,-1.0D0,-2.0D0/
      DATA A(2,1),A(2,2),A(2,3),A(2,4)/1.0D0, 0.0D0, 0.0D0, 0.0D0/
      DATA A(3,1),A(3,2),A(3,3),A(3,4)/1.0D0, 1.0D0, 0.0D0, 0.0D0/
      DATA A(4,1),A(4,2),A(4,3),A(4,4)/1.0D0, 2.0D0, 0.0D0, 0.0D0/
      DATA A(5,1),A(5,2),A(5,3),A(5,4)/0.0D0, 0.0D0, 1.0D0, 3.0D0/
      DATA A(6,1),A(6,2),A(6,3),A(6,4)/0.0D0, 0.0D0, 1.0D0, 4.0D0/
      DATA B(1),B(2),B(3),B(4),B(5),B(6)/0.0D0,
     *         -0.009D0,1.009D0,1.991D0,0.999D0,0.006D0/
      IA = 10
      IV = 5
      M = 6
      N = 4
      M1 = 1
```

```
      LP = 6
      MP = 6
      RES = .TRUE.
C
C SOLVE THE PROBLEM, WITH MONITOR PRINTING
      CALL MA44AD(M, N, M1, A, IA, B, RES, X, IW, W, VAR, LP, MP)
      WRITE (6,10) VAR
   10 FORMAT (' ON RETURN FROM MA44AD, VAR = ', 1PE12.4)
C
C FIND VARIANCE-COVARIANCE MATRIX, WITH MONITOR PRINTING
      CALL MA44CD(M, N, M1, A, IA, IW, W, VAR, LP, MP, V, IV, STD)
      WRITE (6,20) VAR
   20 FORMAT (' ON RETURN FROM MA44CD, VAR = ', 1PE12.4)
      END
```

This produces the following output

```
 MA44AD: CONSTRAINT EQUATIONS    =   1
         LEAST SQUARES EQUATIONS =   5
         NUMBER OF PARAMETERS    =   4

 MA44BD: CONSTRAINT EQUATIONS    =   1
         LEAST SQUARES EQUATIONS =   5
         NUMBER OF PARAMETERS    =   4

 MA44BD: SOLUTION
 1 -2.85714285714299D-03  2 9.99571428571428D-01 3 3.98742857142857D 00
 4 -9.95571428571428D-01


 MA44BD: RESIDUAL VARIANCE ESTIMATE  1.101429D-04

 MA44BD: RESIDUALS
 1 0.00000000000000D-01  2  6.14285714285732D-03 3 -1.22857142857146D-02
 4 5.28571428571454D-03  5  1.71428571428554D-03 6 -8.57142857142771D-04
 ON RETURN FROM MA44AD, VAR =   1.1014D-04


 MA44CD: RESIDUAL VARIANCE ESTIMATE  1.101429D-04

 MA44CD: SOLUTION STANDARD DEVIATIONS
   1  9.553074D-03   2  9.553074D-03   3  2.165396D-02   4  2.165396D-02

 MA44CD: VARIANCE-COVARIANCE MATRIX
 1 1  9.1261D-05   1 2 -5.3498D-05  1 3 -3.4616D-05  1 4  9.4408D-06
 2 1 -5.3498D-05   2 2  5.0351D-05  2 3  1.0385D-04  2 4 -2.8322D-05
 3 1 -3.4616D-05   3 2  1.0385D-04  3 3  4.6889D-04  3 4 -1.4791D-04
 4 1  9.4408D-06   4 2 -2.8322D-05  4 3 -1.4791D-04  4 4  5.0351D-05
 ON RETURN FROM MA44CD, VAR =   1.1014D-04
```