



Warning: Subroutine MA29 performs functions which are adequately treated by routines in other standard subroutine libraries (for example, LAPACK). The use of this routine is not recommended, and it may be removed from future releases of this library.

1 SUMMARY

These subroutines are for factorizing, or solving systems involving, a non-sparse matrix \mathbf{A} which is symmetric but not necessarily positive definite.

MA29A/AD solves the system of linear equations

$$\mathbf{A}x=b,$$

where the vector b is given, to obtain the solution vector x .

MA29B/BD factorizes the matrix \mathbf{A} (permuted) into the form \mathbf{LDL}^T where \mathbf{L} is a lower triangular matrix, and \mathbf{D} a simple block diagonal matrix.

MA29C/CD, given a factored \mathbf{A} , solves the system $\mathbf{A}x=b$ by a forward and back substitution.

MA29A/AD calls both MA29B/BD and MA29C/CD, but these subroutines can be used independently (see Sections 4 and 5). The matrix \mathbf{A} (or its factorization) is stored in all three routines in a compact form requiring only $n(n+1)/2$ locations, thus allowing full storage advantage to be taken of symmetry.

To solve problems when more than one right-hand side vector b is given, the factors given by MA29B/BD do not have to be recalculated and it is merely necessary to call MA29C/CD again for each additional right-hand side b (see Section 5).

The method is that described by R. Fletcher (Factorizing symmetric indefinite matrices, *Journal of Linear Algebra and its Applications*, 1975-76). Previously, it has been recommended that symmetry should be ignored for this type of problem, and that LU decompositions of \mathbf{A} should be calculated using partial pivoting. The new routine MA29A/AD however is twice as efficient on storage and number of operations, and also usually requires fewer interchanges to be made. Since round-off errors are controlled satisfactorily by this routine, it is now recommended that it be used.

ATTRIBUTES — **Version:** 1.0.0. **Types:** MA29A, MA29AD. **Calls:** MA29A/AD calls MA29B/BD, MA29C/CD (see Sections 5, 6). **Original date:** August 1975. **Origin:** R. Fletcher, University of Dundee.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version

```
CALL MA29A (N,A,LT,B,W)
```

The double precision version

```
CALL MA29AD (N,A,LT,B,W)
```

N is an INTEGER ($N > 1$) in which the number of equations must be set.

A is a REAL (DOUBLE PRECISION in the D version) array of $N(N+1)/2$ elements in which the matrix \mathbf{A} must be given. The order in which the elements of \mathbf{A} are given must be $a_{11}, a_{21}, \dots, a_{N1}, a_{22}, a_{32}, \dots, a_{N2}, \dots, a_{N-1,N-1}, a_{N,N-1},$

a_{NN} ; that is to say, as successive columns of its lower triangle. These elements are overwritten by the factors of **A** as described in Section 4. These factors must be passed on unchanged if further calls of MA29C/CD are intended.

- LT is an INTEGER one dimensional array of N elements used to record row and column interchanges in **A** – see Section 4 for details. No initial setting is required. However LT must be passed on unchanged if further calls of MA29C/CD are intended.
- B is a REAL (DOUBLE PRECISION in the D version) one dimensional array of N elements in which the vector b must be given. B is overwritten by the solution vector x , in its natural ordering.
- W is a REAL (DOUBLE PRECISION in the D version) one dimensional array of N elements, used as working space. No initial setting is required.

3 THE COMMON AREA

MA29D/DD, MA29A/AD and MA29B/BD have a common area which can be referenced by the user. However in straightforward applications this will usually not be necessary.

The single precision version

COMMON/MA29D/GR, IRANK, LP

The double precision version

COMMON/MA29AD/GR, IRANK, LPGR

- A is a REAL (DOUBLE PRECISION in the D version) variable in which the error growth control factor for MA29B/BD is stored. This is automatically set by default to 4.0 and it should not be necessary to change it. However it can be reset, and users wishing to experiment should first read R. Fletcher (*loc.cit.*).

IRANK is an INTEGER variable in which the rank of the matrix **A** is set by MA29B/BD. Usually IRANK will be equal to N in which case no user intervention is required. If IRANK is not equal to N, then a diagnostic is printed out by MA29A/AD (but see LP below). This usually indicates that the matrix **A** is singular, although it may of course be due to an error in setting up **A**. The diagnostic is

```
A IS SINGULAR WITH RANK EQUAL TO...
A HAS BEEN REPLACED BY ITS FACTORS
IF THE EQUATIONS ARE KNOWN TO BE CONSISTENT, THEN B
CONTAINS A SOLUTION (NOT UNIQUE)
OTHERWISE B SHOULD BE IGNORED
```

- LP is an INTEGER variable which stores the FORTRAN stream number to be used for the above diagnostic printing. It is set automatically by default to 6 (line printer), but the user can change this to any valid stream number. If LP is set less than or equal to zero, then the diagnostic is suppressed, in which case users are recommended to check the value of IRANK by program.

4 GENERAL INFORMATION

Use of common: : There is a COMMON block labelled MA29D/DD – See Section 3.

Workspace: : N elements in the argument W. below) in turn; otherwise no other routines.

Input/output: : MA29A/AD may output a diagnostic – see Section 3.

5 THE SUBROUTINE MA29B

The information in this section need not be read when using MA29A/AD alone or in conjunction with further calls of MA29C/CD. MA29B/BD is called by MA29A/AD to calculate \mathbf{LDL}^T factors of a permutation \mathbf{PAP}^T of **A**. **D** is a simple

block diagonal matrix with either 1×1 or 2×2 symmetric blocks (pivots). **L** is a unit lower triangular matrix with, in addition,

$$l_{i+1,i}=0$$

whenever

$$d_{i,i}d_{i,i+1}d_{i+1,i}d_{i+1,i+1}$$

forms a 2×2 block diagonal element of **D**.

The single precision version

```
CALL MA29B(N,A,LT)
```

The double precision version

```
CALL MA29BD(N,A,LT)
```

N is an INTEGER variable which must be set to the dimension of the matrix **A**.

A is a REAL (DOUBLE PRECISION in the D version) array of $N(N+1)/2$ elements in which **A** must be set, as described for MA29A/AD in Section 2. The factors are set by MA29B/BD and are stored as follows. The elements of **L** (other than the known 0 and 1 elements) overwrite the corresponding elements of **A**. The remaining block diagonal elements of **A** are overwritten by the corresponding lower triangular part of **D**−1. In the case of a zero 1×1 pivot d_{ii} , a zero is stored. The method in use also has the property that any 2×2 blocks of **D** always have one positive and one negative eigenvalue (assuming $GR > 2$ – see below). Hence a positive or negative definite matrix will invariably be factorised using only 1×1 pivots.

LT is an INTEGER one dimensional array of **N** elements which is set by MA29B/BD as follows. If row **I** of **D** is the first row of a 2×2 block, then **LT(I)** has a negative sign; positive otherwise. Also $|\mathbf{LT(I)}|$ is the row and column of the matrix **A** which is stored in row and column **I** of the matrix \mathbf{PAP}^T . This is equivalent to a matrix **P** for which the **I**th row has zero elements except for a 1 in the $|\mathbf{LT(I)}|$ element. MA29B uses the information in **GR** (labelled COMMON MA29D/DD) and sets **IRANK** – See Section 3.

6 THE SUBROUTINE MA29C/CD

The information in this section need not be read when using MA29A/AD alone. MA29C/CD carries out the back substitution operations to solve

$$\mathbf{Ax}=b$$

for x , given b , and using factors of **A** previously calculated by MA29B/BD (or MA29A/AD) .

The single precision version

```
CALL MA29C(N,A,LT,B,W)
```

The double precision version

```
CALL MA29CD(N,A,LT,B,W)
```

N is an INTEGER giving the number of equations, which must also be the dimension of the matrix **A**.

A is a REAL (DOUBLE PRECISION in the D version) one dimensional array of $N(N+1)/2$ elements. On entry this must contain the factors of the matrix **A** (permuted), as calculated by a previous call of MA29A/AD or MA29B/BD. This array is not changed by MA29C/CD.

LT is an INTEGER one dimensional array of **N** elements. On entry, this must contain the permutation vector **LT** which was set at the same time as the factors of **A** were calculated. This array is not changed by MA29C/CD.

B is a REAL (DOUBLE PRECISION in the D version) one dimensional array of **N** elements in which the vector b must be given. **B** is overwritten by the solution vector x in its natural ordering.

W is a REAL (DOUBLE PRECISION in the D version) one dimensional array of N elements used as working space.
No initial setting is required.