

NAG Fortran Library Chapter Introduction

F03 – Determinants

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1 Scope of the Chapter

This chapter is concerned with the calculation of determinants of square matrices.

2 Background to the Problems

The routines in this chapter compute the determinant of a square matrix A . The matrix is first decomposed into triangular factors

$$A = LU.$$

If A is positive-definite, then $U = L^T$, and the determinant is the product of the squares of the diagonal elements of L . Otherwise, the routines in this chapter use the Crout form of the LU decomposition, where U has unit elements on its diagonal. The determinant is then the product of the diagonal elements of L , taking account of possible sign changes due to row interchanges.

To avoid overflow or underflow in the computation of the determinant, some scaling is associated with each multiplication in the product of the relevant diagonal elements. The final value is represented by

$$\det A = d1 \times 2^{d2}$$

where $d2$ is an integer and

$$\frac{1}{16} \leq |d1| < 1.$$

Most of the routines of the chapter are based on those published in the book edited by Wilkinson and Reinsch (1971). We are very grateful to the late Dr J H Wilkinson FRS for his help and interest during the implementation of this chapter of the Library.

3 Recommendations on Choice and Use of Available Routines

Note: refer to the Users' Note for your implementation to check that a routine is available.

3.1 General Discussion

It is extremely wasteful of computer time and storage to use an inappropriate routine, for example one for a complex matrix when A is real. Most programmers will know whether their matrix is real or complex, but may be less certain whether or not a real symmetric matrix A is positive-definite, i.e., all eigenvalues of $A > 0$. A real symmetric matrix A not known to be positive-definite must be treated as a general real matrix. In all other cases either the band routine or the general routines must be used.

The routines in this chapter fall into two easily defined categories.

(i) Black Box Routines

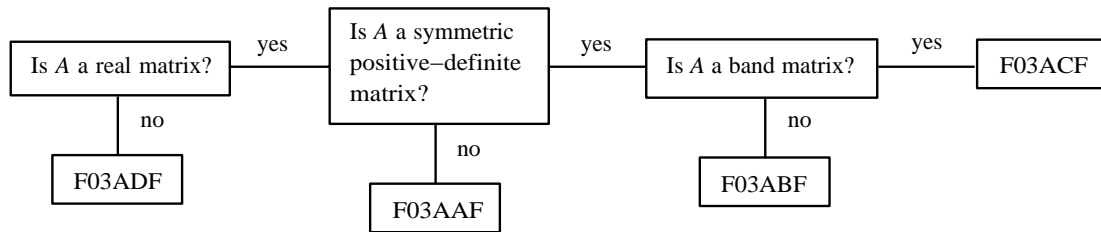
These should be used if only the determinant is required. The scaled representation $d1 \times 2^{d2}$ is evaluated as a floating-point number and a failure is indicated if the floating-point number is outside the range of the machine.

(ii) General Purpose Routines

These give the value of the determinant in its scaled form, $d1$ and $d2$, and also give the triangular decomposition of the matrix A in a form suitable for input to either the inversion routines of Chapter F01 or the solution of linear equation routines in Chapter F04.

4 Decision Tree

If at any stage the answer to a question is ‘Don’t know’ this should be read as ‘No’.



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Black Box Routines

Complex matrix	F03ADF
Real matrix	F03AAF
Real symmetric positive-definite matrix	F03ABF
Real symmetric positive-definite band matrix	F03ACF

General Purpose Routines

Including the decomposition into triangular factors:

Real matrix	F03AFF
Real symmetric positive-definite matrix	F03AEF

6 Routines Withdrawn or Scheduled for Withdrawal

The following routines have been withdrawn. Advice on replacing calls to those withdrawn since Mark 13 is given in the document ‘Advice on Replacement Calls for Withdrawn/Superseded Routines’.

Withdrawn Routine	Mark of Withdrawal	Replacement Routine(s)
F03AGF	17	F07HDF (SPBTRF/DPBTRF)
F03AHF	17	F07ARF (CGETRF/ZGETRF)
F03AJF	8	F01BRF
F03AKF	8	F01BSF
F03ALF	9	F07BDF (SGBTRF/DGBTRF)
F03AMF	17	none; see Chapter F03

7 References

Fox L (1964) *An Introduction to Numerical Linear Algebra* Oxford University Press

Wilkinson J H and Reinsch C (1971) *Handbook for Automatic Computation II, Linear Algebra* Springer-Verlag