NAG Library Chapter Introduction

F03 – Determinants

Contents

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 $U = L^{\mathrm{T}}$, 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

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

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

It is extremely wasteful of computer time and storage to use an inappropriate routine, for example to use a routine requiring 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**

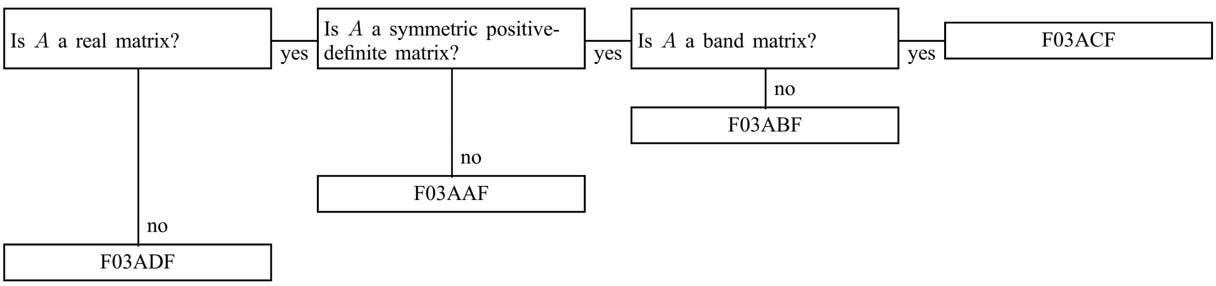
These should be used if only the determinant is required. The scaled representation $d1 \times 2^{d2}$ is evaluated as a floating-point number and a failure is indicated if the floating-point number is outside the range of the machine.

(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 Trees

Tree 1



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6 Routines Withdrawn or Scheduled for Withdrawal

Withdrawn Routine	Mark of Withdrawal	Replacement Routine(s)
F03AGF	17	F07HDF (DPBTRF)
F03AHF	17	F07ARF (ZGETRF)
F03AMF	17	No replacement; 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