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 assumued to have first been decomposed into triangular factors

$$A = LU,$$

using routines from Chapter F07.

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 Dolittle form of the LU decomposition, where L has unit elements on its diagonal. The determinant is then the product of the diagonal elements of U, 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

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

For complex valued determinants the real and imaginary parts are scaled separately.

Most of the original routines of the chapter were 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 are general purpose routines. These give the value of the determinant in its scaled form, $d1$ and $d2$, given the triangular decomposition of the matrix from a suitable routine from Chapter F07.

4   Decision Trees

Tree 1
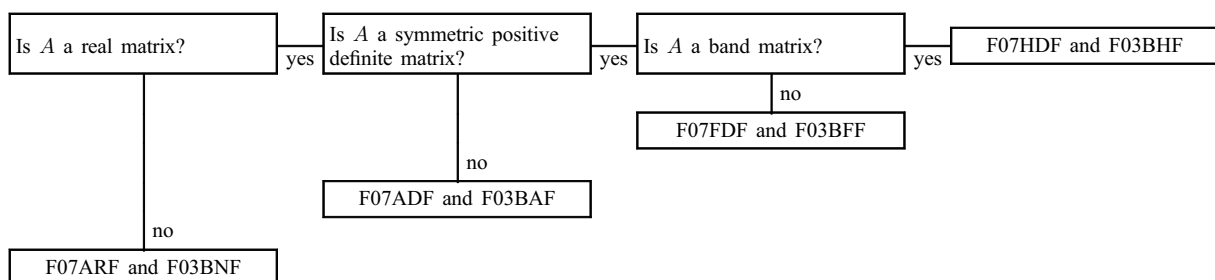
5   Functionality Index

Determinants of factorized matrices,

6   Auxiliary Routines Associated with Library Routine Parameters

None.

7   Routines Withdrawn or Scheduled for Withdrawal

The following lists all those routines that have been withdrawn since Mark 17 of the Library or are scheduled for withdrawal at one of the next two marks.

Withdrawn Routine	Mark of Withdrawal	Replacement Routine(s)
F03AAF	25	F07ADF (DGETRF) and F03BAF
F03ABF	25	F07FDF (DPOTRF) and F03BFF
F03ACF	25	F07HDF (DPBTRF) and F03BHF
F03ADF	25	F07ARF (ZGETRF) and F03BNF
F03AEF	25	F07FDF (DPOTRF) and F03BFF
F03AFF	25	F07ADF (DGETRF) and F03BAF
F03AGF	17	F07HDF (DPBTRF)
F03AHF	17	F07ARF (ZGETRF)
F03AMF	17	No replacement required; see Chapter F03

8   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

_____