Chapter F

Linear Algebra

Contents

1 Introduction

The F Chapters of the Library are concerned with linear algebra and cover a large area. This general introduction is intended to help users decide which particular F Chapter is relevant to their problem. There are currently nine F Chapters with the following titles:

Chapter F01 – Matrix Operations, including Inversion

Chapter F02 – Eigenvalues and Eigenvectors

Chapter F03 – Determinants

Chapter F04 – Simultaneous Linear Equations

Chapter F05 – Orthogonalisation

Chapter F06 – Linear Algebra Support Routines

Chapter F07 – Linear Equations (LAPACK)

Chapter F08 – Least-squares and Eigenvalue Problems (LAPACK)

Chapter F11 – Sparse Linear Algebra

The principal problem areas addressed by the above Chapters are:

Systems of linear equations

Linear least-squares problems

Eigenvalue and singular value problems

The solution of these problems usually involves several matrix operations, such as a matrix factorization followed by the solution of the factorized form, and the routines for these operations themselves utilize lower level support routines, typically routines from Chapter F06. Most users will not normally need to be concerned with these support routines.

NAG has been involved in a project, called LAPACK [1], to develop a linear algebra package for modern high-performance computers, and the routines developed within that project are being incorporated into the Library as two new Chapters, Chapter F07 and Chapter F08. It should be emphasised that, while the LAPACK project has been concerned with high-performance computers, the routines do not compromise efficiency on conventional machines.

Chapter F11 is a new chapter, introduced at Mark 17, and currently containing a new suite of routines for sparse symmetric systems of linear equations. Earlier routines for sparse linear algebra are still located in Chapter F01, Chapter F02 and Chapter F04. For a wider selection of routines for sparse linear algebra, users are referred to the Harwell Sparse Matrix Library (available from NAG).

For background information on numerical algorithms for the solution of linear algebra problems see Golub and Van Loan [5]. For the three main problem areas listed above the user generally has the choice of selecting a single routine to solve the problem, a so-called *Black Box* routine, or selecting more than one routine to solve the problem, such as a factorization routine followed by a solve routine, so-called *General Purpose* routines. The following sections indicate which chapters are relevant to particular problem areas.

2 Linear Equations

The Black Box routines for solving linear equations of the form

$$Ax = b \text{ and } AX = B,$$

where A is an n by n real or complex, non-singular matrix, are to be found in Chapter F04. Such equations can also be solved by selecting a General Purpose factorization routine from Chapter F01 or Chapter F03 and combining them with a solve routine in Chapter F04, or by selecting a factorization and a solve routine from Chapter F07. For sparse symmetric problems routines from Chapter F11 should be used. In addition there are routines to estimate condition numbers in Chapter F04 and Chapter F07, and routines to give error estimates in Chapter F07.

There are routines to cater for a variety of types of matrix, including general, symmetric or Hermitian, symmetric or Hermitian positive definite, banded, skyline and sparse matrices.

In order to select the appropriate routine, users are recommended to consult the F04 Chapter Introduction in the first instance, although the decision trees for the General Purpose routines will usually in fact point to an F07 or F11 routine.

3 Linear Least-squares

The Black Box routines for solving linear least-squares problems of the form

$$\underset{x}{\text{minimize}}\ r^T r,\ \text{where } r = b - Ax,$$

where A is an m by n, possibly rank deficient, matrix are to be found in Chapter F04. Such problems can also be solved by selecting a General Purpose factorization routine from Chapter F02 or Chapter F08 and combining them with a solve routine in Chapter F04, which also contains a routine to compute covariance matrices. Linear least-squares problems can also be solved by routines in the statistical Chapter G02.

In order to select the appropriate routine, users are recommended to consult the F04 Chapter Introduction in the first instance, but users with additional statistical requirements may prefer to consult Section 2.2 of the G02 Chapter Introduction.

4 Eigenvalue Problems and Singular Value Problems

The Black Box routines for solving standard matrix eigenvalue problems of the form

$$Ax = \lambda x,$$

where A is an n by n real or complex matrix, and generalized matrix eigenvalue problems of the form

$$Ax = \lambda Bx \text{ and } ABx = \lambda x,$$

where B is also an n by n matrix, are to be found in Chapter F02. These eigenvalue problems can also be solved by a combination of General Purpose routines (which are mostly in Chapter F08, but a few in Chapter F01 or Chapter F02).

There are routines to cater for various types of matrices, including general, symmetric or Hermitian, banded and sparse matrices.

Similarly, the Black Box routines for finding singular values and/or singular vectors of an m by n real or complex matrix A are to be found in Chapter F02, and such problems may also be solved by combining routines from Chapter F08.

In order to select the appropriate routine, users are recommended to consult the F02 Chapter Introduction in the first instance.

5 Inversion and Determinants

Routines for matrix inversion are to be found in Chapter F01 and Chapter F07. Users are recommended to consult the F01 Chapter Introduction in the first instance, although the decision tree will often in fact point to an F07 routine. It should be noted that users are strongly encouraged not to use matrix inversion routines for the solution of linear equations, since these can be solved more efficiently and accurately using routines directed specifically at such problems. Indeed many problems, which superficially appear to be matrix inversion, can be posed as the solution of a system of linear equations and this is almost invariably preferable.

Routines to compute determinants of matrices are to be found in Chapter F03. Users are recommended to consult the F03 Chapter Introduction in the first instance.

6 Matrix Operations

Routines for various sorts of matrix operation are to be found in Chapter F01, including matrix transposition, addition and multiplication, and conversion between different matrix representation storage formats. Facilities for matrix manipulation can also be found in Chapter F06 (see next section).

7 Support Routines

Chapter F06 contains a variety of routines to perform elementary algebraic operations involving scalars, vectors and matrices, such as setting up a plane rotation, performing a dot product and computing a matrix norm. Chapter F06 contains routines that meet the specification of the BLAS (Basic Linear Algebra Subprograms) [6], [2], [4] and [3]. The routines in this chapter will not normally be required by the general user, but are intended for use by those who require to build specialist linear algebra modules. These routines, especially the BLAS, are extensively used by other NAG Fortran Library routines.

8 References

[1] Anderson E, Bai Z, Bischof C, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A, Ostrouchov S and Sorensen D (1995) *LAPACK Users' Guide* (2nd Edition) SIAM, Philadelphia

[2] Dodson D S, Grimes R G and Lewis J G (1991) Sparse extensions to the Fortran basic linear algebra subprograms *ACM Trans. Math. Software* **17** 253–263

[3] Dongarra J J, Du Croz J J, Duff I S and Hammarling S (1990) A set of Level 3 basic linear algebra subprograms *ACM Trans. Math. Software* **16** 1–28

[4] Dongarra J J, Du Croz J J, Hammarling S and Hanson R J (1988) An extended set of FORTRAN basic linear algebra subprograms *ACM Trans. Math. Software* **14** 1–32

[5] Golub G H and van Loan C F (1996) *Matrix Computations* Johns Hopkins University Press (3rd Edition), Baltimore

[6] Lawson C L, Hanson R J, Kincaid D R and Krogh F T (1979) Basic linear algebra subprograms for Fortran usage *ACM Trans. Math. Software* **5** 308–325