# NAG C Library Chapter Introduction

# 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:

f01 – Matrix Factorizations

f02 – Eigenvalues and Eigenvectors

f03 – Determinants

f04 – Simultaneous Linear Equations

f06 – Linear Algebra Support Functions

f07 – Linear Equations (LAPACK)

f08 – Least-squares and Eigenvalue Problems (LAPACK)

f11 – Sparse Linear Algebra

f16 – NAG Interface to BLAS

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 functions for these operations themselves utilize lower level support functions, typically from Chapters f06 and f16. Most users will not normally need to be concerned with these support functions.

NAG has been involved in a project, called LAPACK (Anderson *et al.* (1999)), to develop a linear algebra package for modern high-performance computers, and the functions developed within that project are being incorporated into the Library as Chapters f07 and f08. It should be emphasised that, while the LAPACK project has been concerned with high-performance computers, the functions do not compromise efficiency on conventional machines.

Chapter f11 contains a suite of functions for solving sparse systems of linear equations.

For background information on numerical algorithms for the solution of linear algebra problems see Golub and Van Loan (1996). In some problem areas the user has the choice of selecting a single function to solve the problem, a so-called *Black Box* function, or selecting more than one function to solve the problem, such as a factorization function followed by a solve function, so-called *General Purpose* functions. The following sections indicate which chapters are relevant to particular problem areas.

# 2 Linear Equations

The Black Box functions for solving linear equations of the form

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

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 function from Chapter f01 and combining them with a solve function in Chapter f04, or by selecting a factorization and a solve function from Chapter f07. For sparse problems, functions from Chapter f11 should be used. In addition there are functions to estimate condition numbers and functions to give error estimates in Chapter f07.

There are functions 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 function, users are recommended to consult the f04 Chapter Introduction in the first instance, although the decision trees for the General Purpose functions will usually in fact point to a function in Chapter f07 or Chapter f11.

## 3 Linear Least-squares

Functions for solving linear least-squares problems of the form

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

where $A$ is an $m$ by $n$, possibly rank deficient, matrix, can be solved by selecting a general purpose factorization function from Chapter f02 or Chapter f08 and combining them with a solve function in Chapter f04. Linear least-squares problems can also be solved by functions in the statistical Chapter g02.

In order to select the appropriate function, 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 functions 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 Chapters f02 and f08. These eigenvalue problems can also be solved by a combination of General Purpose functions in Chapter f08.

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

Similarly, the Black Box functions 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 functions from Chapter f08.

In order to select the appropriate function, users are recommended to consult Chapters f02 and f08 in the first instance.

## 5 Inversion and Determinants

Functions for matrix inversion are to be found in Chapter f07. It should be noted that users are strongly encouraged not to use matrix inversion functions for the solution of linear equations, since these can be solved more efficiently and accurately using functions 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.

Functions to compute determinants of matrices are to be found in Chapter f03. Users are recommended to consult Chapter f03 in the first instance.

## 6 Support Functions

Chapters f06 and f16 contain a variety of functions 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. Chapters f06 and f16 contain functions that meet the specification of the BLAS (Basic Linear Algebra Subprograms) (Lawson *et al.* (1979), Dodson *et al.* (1991), Dongarra *et al.* (1988), Dongarra *et al.* (1990) and The BLAS Technical Forum Standard (2001)). The functions 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 functions, especially the BLAS, are extensively used by other NAG C Library functions.

# 7 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia

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