

NAG Library Chapter Introduction

f – Linear Algebra

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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 you decide which particular f Chapter is relevant to your problem. The following Chapters are currently available:

- Chapter f01 – Matrix Operations, Including Inversion
- Chapter f02 – Eigenvalues and Eigenvectors
- Chapter f03 – Determinants
- Chapter f04 – Simultaneous Linear Equations
- Chapter f06 – Linear Algebra Support Functions
- Chapter f07 – Linear Equations (LAPACK)
- Chapter f08 – Least Squares and Eigenvalue Problems (LAPACK)
- Chapter f11 – Large Scale Linear Systems
- Chapter f12 – Large Scale Eigenproblems
- Chapter 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 Chapter f16. You will not normally need to be concerned with these support functions.

NAG has been involved in a project, called LAPACK (see 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 emphasized that, while the LAPACK project has been concerned with high-performance computers, the functions do not compromise efficiency on conventional machines.

Chapters f11 and f12 contain functions for solving large scale problems, but a few earlier functions are still located in Chapters f01, f02 and f04.

For background information on numerical algorithms for the solution of linear algebra problems see Golub and Van Loan (1996). In some problem areas you have 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 nonsingular matrix, are to be found in Chapters f04 and f07. 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 large 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 Chapters f02, f04 and 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, you are recommended to consult the f04 Chapter Introduction in the first instance, although the decision trees will often in fact point to a function in Chapters f07 or f11.

3 Linear Least Squares

Functions for solving linear least squares problems of the form

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

and A is an m by n , possibly rank deficient, matrix, can be solved by selecting one or more general purpose factorization functions from Chapters f02 or 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, you are recommended to consult the f04 Chapter Introduction in the first instance, but if you have additional statistical requirements you may prefer to consult Section 2.2 in the g02 Chapter Introduction.

Chapter f08 also contains functions for solving linear equality constrained least squares problems, and the general Gauss–Markov linear model problem. Chapter e04 contains a function to solve general linearly constrained linear least squares problems.

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

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

where B is also an n by n matrix, are to be found in Chapters f02, f08 and f12. 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 Chapters f02 and f08, and such problems may also be solved by functions from Chapter f12, and by combining functions from Chapter f08.

In order to select the appropriate function, you 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 you 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. You are recommended to consult Chapter f03 in the first instance.

6 Support Functions

Chapter f16 contains 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. Chapter f16 contains functions that meet the specification of the BLAS (Basic Linear Algebra Subprograms) (see Lawson *et al.* (1979), Dodson *et al.* (1991), Dongarra *et al.* (1988), Dongarra *et al.* (1990) and Blackford *et al.* (2002)). 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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