NAG Library Chapter Introduction

f01 – Matrix Factorizations

Contents

1 Scope of the Chapter

This chapter together with Chapters f07, f08 and f11 provides facilities for two types of problem:

(i) Matrix Inversion (see Chapter f07)

(ii) Matrix Factorizations (see Chapters f01, f07, f08 and f11)

These problems are discussed separately in Section 2.1 and Section 2.2.

2 Background to the Problems

2.1 Matrix Inversion

(i) Non-singular square matrices of order n.

If A, a square matrix of order n, is nonsingular (has rank n), then its inverse X exists and satisfies the equations $AX = XA = I$ (the identity or unit matrix).

It is worth noting that if $AX - I = R$, so that R is the 'residual' matrix, then a bound on the relative error is given by $\|R\|$, i.e.,

$$\frac{\|X - A^{-1}\|}{\|A^{-1}\|} \leq \|R\|.$$

(ii) General real rectangular matrices.

A real matrix A has no inverse if it is square (n by n) and singular (has rank $< n$), or if it is of shape (m by n) with $m \neq n$, but there is a **Generalized** or **Pseudo Inverse** Z which satisfies the equations

$$AZA = A, \qquad ZAZ = Z, \qquad (AZ)^{\mathrm{T}} = AZ, \qquad (ZA)^{\mathrm{T}} = ZA$$

(which of course are also satisfied by the inverse X of A if A is square and nonsingular).

(a) if $m \geq n$ and $\mathrm{rank}(A) = n$ then A can be factorized using a ***QR*** **factorization**, given by

$$A = Q\begin{pmatrix} R \\ 0 \end{pmatrix},$$

where Q is an m by m orthogonal matrix and R is an n by n, nonsingular, upper triangular matrix. The pseudo-inverse of A is then given by

$$Z = R^{-1}\tilde{Q}^{\mathrm{T}},$$

where $\tilde{Q}$ consists of the first n columns of Q.

(b) if $m \leq n$ and $\mathrm{rank}(A) = m$ then A can be factorized using an ***RQ*** **factorization**, given by

$$A = (R \quad 0)P^{\mathrm{T}}$$

where P is an n by n orthogonal matrix and R is an m by m, nonsingular, upper triangular matrix. The pseudo-inverse of A is then given by

$$Z = \tilde{P}R^{-1},$$

where $\tilde{P}$ consists of the first m columns of P.

(c) if $m \geq n$ and $\mathrm{rank}(A) = r \leq n$ then A can be factorized using a QR factorization, with column interchanges, as

$$A = Q\begin{pmatrix} R \\ 0 \end{pmatrix}P^{\mathrm{T}},$$

where Q is an m by m orthogonal matrix, R is an r by n upper trapezoidal matrix and P is an n by n permutation matrix. The pseudo-inverse of A is then given by

$$Z = PR^{\mathrm{T}}\left(RR^{\mathrm{T}}\right)^{-1}\tilde{Q}^{\mathrm{T}},$$

where $\tilde{Q}$ consists of the first r columns of Q.

(d) if rank$(A) = r \leq k = \min(m, n)$, then A can be factorized as the **singular value decomposition**

$$A = QDP^{\mathrm{T}},$$

where Q is an m by m orthogonal matrix, P is an n by n orthogonal matrix and D is an m by n diagonal matrix with non-negative diagonal elements. The first k columns of Q and P are the **left-** and **right-hand singular vectors** of A respectively and the k diagonal elements of D are the **singular values** of A. D may be chosen so that

$$d_1 \geq d_2 \geq \cdots \geq d_k \geq 0$$

and in this case if rank$(A) = r$ then

$$d_1 \geq d_2 \geq \cdots \geq d_r > 0, \qquad d_{r+1} = \cdots = d_k = 0.$$

If $\tilde{Q}$ and $\tilde{P}$ consist of the first r columns of Q and P respectively and Σ is an r by r diagonal matrix with diagonal elements $d_1, d_2, \ldots, d_r$ then A is given by

$$A = \tilde{Q}\Sigma\tilde{P}^{\mathrm{T}}$$

and the pseudo-inverse of A is given by

$$Z = \tilde{P}\Sigma^{-1}\tilde{Q}^{\mathrm{T}}.$$

Notice that

$$A^{\mathrm{T}}A = P\left(D^{\mathrm{T}}D\right)P^{\mathrm{T}}$$

which is the classical eigenvalue (spectral) factorization of $A^{\mathrm{T}}A$.

(e) if A is complex then the above relationships are still true if we use 'unitary' in place of 'orthogonal' and conjugate transpose in place of transpose. For example, the singular value decomposition of A is

$$A = QDP^{\mathrm{H}},$$

where Q and P are unitary, P^{H} the conjugate transpose of P and D is as in (d) above.

2.2 Matrix Factorizations

The functions in this section perform matrix factorizations which are required for the solution of systems of linear equations with various special structures. A few functions which perform associated computations are also included.

Other functions for matrix factorizations are to be found in Chapters f03, f07, f08 and f11.

3 Recommendations on Choice and Use of Available Functions

3.1 Matrix Inversion

Note: before using any function for matrix inversion, consider carefully whether it is really needed.

Although the solution of a set of linear equations $Ax = b$ can be written as $x = A^{-1}b$, the solution should **never** be computed by first inverting A and then computing $A^{-1}b$; the functions in Chapters f04 or f07 should **always** be used to solve such sets of equations directly; they are faster in execution, and numerically more stable and accurate. Similar remarks apply to the solution of least-squares problems which again should be solved by using the functions in Chapters f02 or f08 rather than by computing a pseudo-inverse.

(a) Non-singular square matrices of order n

This chapter describes techniques for inverting a general real matrix A and matrices which are positive-definite (have all eigenvalues positive) and are either real and symmetric or complex and Hermitian. It is wasteful and uneconomical not to use the appropriate function when a matrix is known to have one of these special forms. A general function must be used when the matrix is not known to be positive-definite. In most functions the inverse is computed by solving the linear equations $Ax_i = e_i$, for $i = 1, 2, \ldots, n$, where e_i is the ith column of the identity matrix.

The residual matrix $R = AX - I$, where X is a computed inverse of A, conveys useful information in that $\|R\|$ is a bound on the relative error in X.

The decision trees for inversion show which functions in Chapter f07 should be used for the inversion of other special types of matrices not treated in the chapter.

(b) General real rectangular matrices

For real matrices nag_dgeqrf (f08aec) returns a QR factorization of A and nag_dgeqpf (f08bec) returns the QR factorization with column interchanges. The corresponding complex functions are nag_zgeqrf (f08asc) and nag_zgeqpf (f08bsc) respectively. Functions are also provided to form the orthogonal matrices and transform by the orthogonal matrices following the use of the above functions.

Combinations of functions in Chapter f08 (e.g., nag_dgebrd (f08kec), nag_dorgbr (f08kfc) and nag_dbdsqr (f08mec)) compute the singular value decomposition as described in Section 2 for real and complex matrices respectively. If A has rank $r \leq k = \min(m, n)$ then the $k - r$ smallest singular values will be negligible and the pseudo-inverse of A can be obtained as $Z = P\Sigma^{-1}Q^{\mathrm{T}}$ as described in Section 2. If the rank of A is not known in advance it can be estimated from the singular values (see Section 2.4 in the f04 Chapter Introduction). For large sparse matrices, leading terms in the singular value decomposition can be computed using functions from Chapter f12.

3.2 Matrix Factorizations

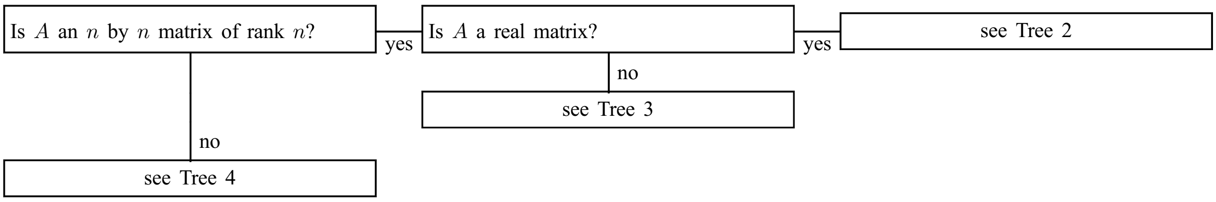
Each of these functions serves a special purpose required for the solution of sets of simultaneous linear equations or the eigenvalue problem. For further details you should consult Sections 3 or 4 in the f02 Chapter Introduction or Sections 3 or 4 in the f04 Chapter Introduction.

For the factorization of sparse matrices, see nag_sparse_nsym_fac (f11dac), nag_sparse_sym_chol_fac (f11jac) and nag_superlu_lu_factorize (f11mec). These functions should be used only when A is **not** banded and when the total number of nonzero elements is less than 10% of the total number of elements. In all other cases either the band functions or the general functions should be used.

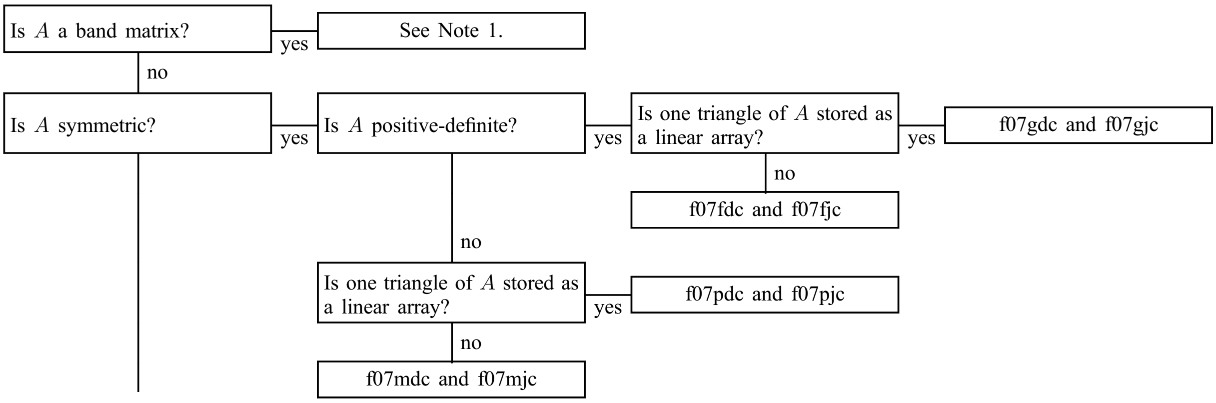
4 Decision Trees

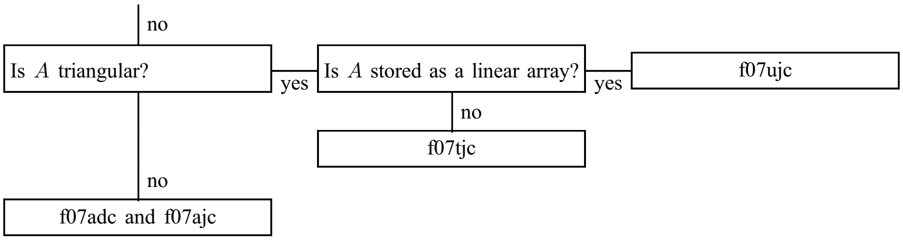
The decision trees show the functions in this chapter and in Chapter f04 that should be used for inverting matrices of various types. Functions marked with an asterisk ($*$) only perform part of the computation – see Section 3.1 for further advice.

Tree 1

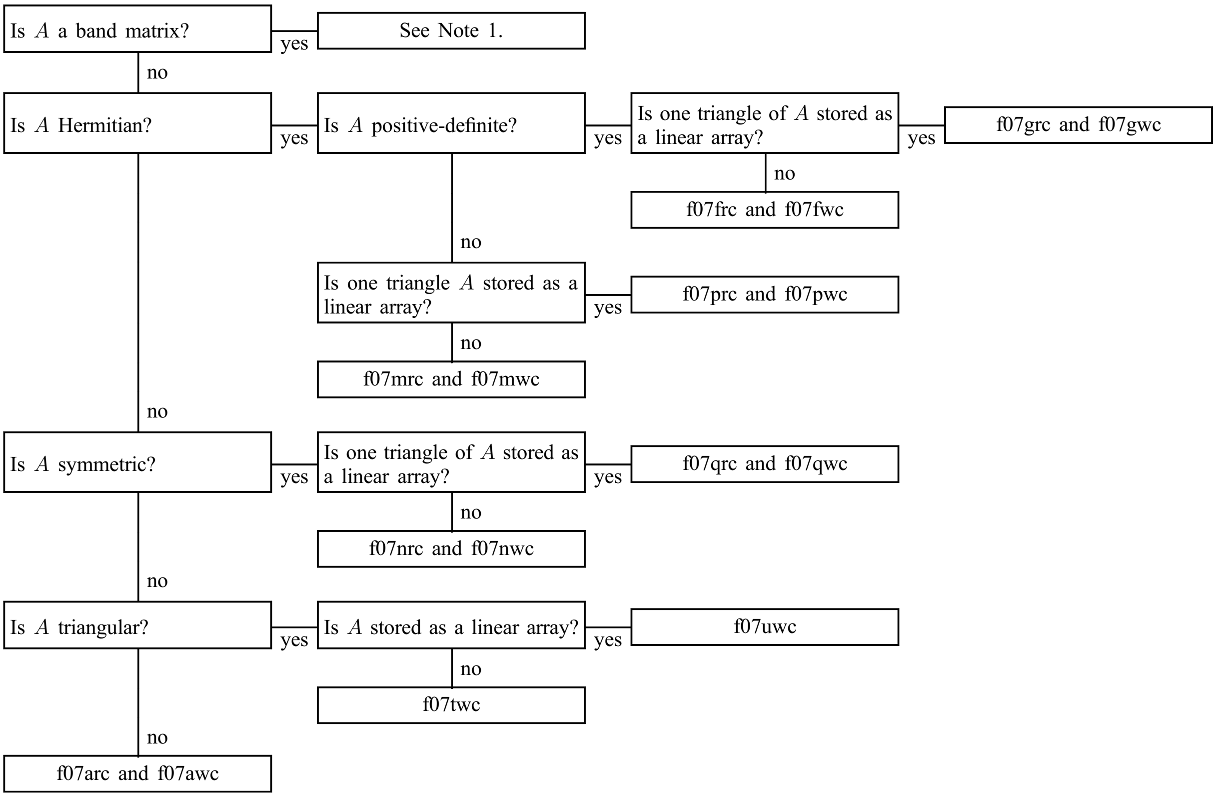


Tree 2: Inverse of a real *n* by *n* matrix of full rank

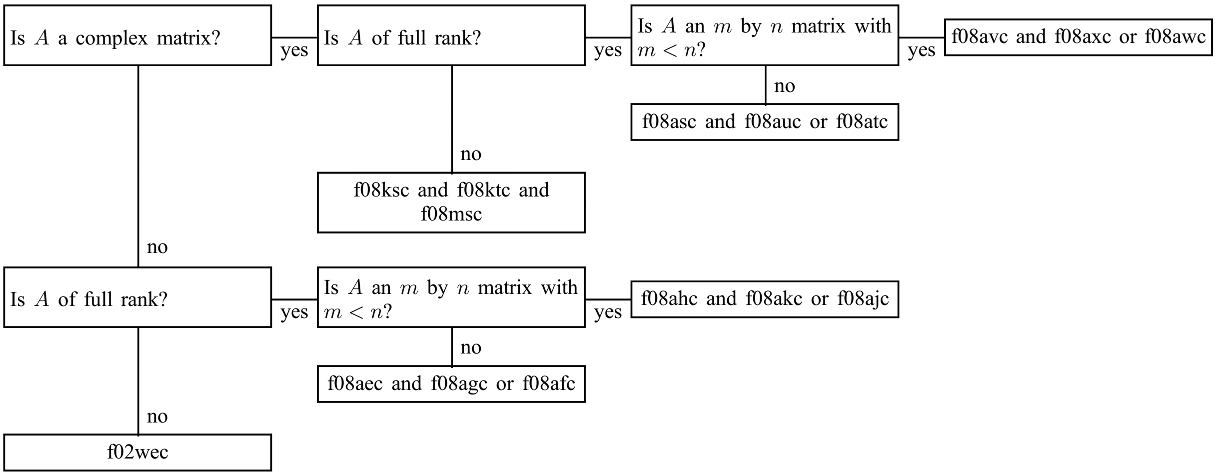




Tree 3: Inverse of a complex *n* by *n* matrix of full rank



Tree 4: Pseudo-inverses



Note 1: the inverse of a band matrix A does not in general have the same shape as A, and no functions are provided specifically for finding such an inverse. The matrix must either be treated as a full matrix, or the equations $AX = B$ must be solved, where B has been initialized to the identity matrix I. In the latter case, see the decision trees in Section 4 in the f04 Chapter Introduction.

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6 Functions Withdrawn or Scheduled for Withdrawal

None.

7 References

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Wilkinson J H and Reinsch C (1971) *Handbook for Automatic Computation II, Linear Algebra* Springer–Verlag

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