Chapter F02

Eigenvalues and Eigenvectors

Contents

1 Scope of the Chapter

This chapter provides two routines for the solution of eigenvalue problems. One routine solves the Symmetric Eigenvalue Problem, for real symmetric matrices, the other routine solves the Hermitian Eigenvalue Problem, for complex Hermitian matrices.

The computation of the Singular Value Decomposition (SVD) is also supported by a further two routines, for real and complex rectangular matrices, respectively. Chapter F08 contains further routines for symmetric and Hermitian eigenvalue problems.

2 Background to the Problems

In this section we describe the symmetric and Hermitian eigenvalue problems and the SVD for real and complex rectangular matrices. For more details, consult a standard textbook on matrix computations, such as Parlett [3] for the symmetric and Hermitian eigenvalue problems, Golub and Van Loan [1] for symmetric and Hermitian eigenvalue problems and the SVD.

The phrase 'eigenvalue problem' is sometimes abbreviated to **eigenproblem**.

2.1 Symmetric Eigenvalue Problem

Let A be a real square symmetric matrix of order n. The symmetric eigenproblem is to find the eigenvalues, λ, and the corresponding eigenvectors, $z \neq 0$, such that

$$Az = \lambda z. \tag{1}$$

The eigenvalues λ are all real, and the eigenvectors can be chosen to be mutually orthogonal. That is, we can write

$$Az_i = \lambda_i z_i \;\text{ for }\; i = 1, \ldots, n$$

or equivalently:

$$AZ = Z\Lambda \tag{2}$$

where Λ is a real diagonal matrix whose diagonal elements λ_i are the eigenvalues, and Z is a real orthogonal matrix whose columns z_i are the eigenvectors. This implies that $z_i^T z_j = 0$ if $i \neq j$, and $\|z_i\|_2 = 1$ where z_i^T denotes the transpose of the vector z_i.

Equation (2) can be rewritten

$$A = Z\Lambda Z^T. \tag{3}$$

This is known as the **eigendecomposition** or **spectral factorization** of A.

Eigenvalues of a real symmetric matrix are well conditioned, that is, they are not unduly sensitive to perturbations in the original matrix A. The sensitivity of an eigenvector depends on how small the gap is between its eigenvalue and any other eigenvalue; the smaller the gap, the more sensitive the eigenvector.

The parallel algorithm for computing the spectral decomposition is based on an extension to the one-sided Jacobi method due to Hestenes, see [2]. This is an implicit Jacobi method and uses odd-even permutations to shuffle the columns of the matrix across the logical processors in the Library Grid.

2.2 Hermitian Eigenvalue Problem

The Hermitian eigenproblem is the complex equivalent of the symmetric eigenproblem. In the Hermitian eigenproblem, the matrix A is complex Hermitian but all its eigenvalues are real. However, the eigenvectors z_i, $i = 1, \ldots, n$ are, in general, complex. The eigendecomposition of A is given by

$$A = Z\Lambda Z^H \tag{4}$$

where the matrix Z is now unitary. That is, $z_i^H z_j = 0$ if $i \neq j$, and $\|z_i\|_2 = 1$ where z_i^H represents the complex conjugate transpose of the vector z_i.

The same method of solution as used for the symmetric eigenproblem (see Section 2.1) is used to solve the Hermitian eigenproblem.

2.3 Singular Value Decomposition of Matrices (SVD)

The SVD of a real m by n matrix A is given by

$$A = U\Sigma V^T,$$

where U and V are orthogonal and Σ is an m by n diagonal matrix with real diagonal elements, σ_i, such that

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min(m,n)} \geq 0.$$

The σ_i are the **singular values** of A and the first $\min(m,n)$ columns of U and V are, respectively, the **left** and **right singular vectors** of A. The singular values and singular vectors satisfy

$$Av_i = \sigma_i u_i \text{ and } A^T u_i = \sigma_i v_i, \quad i = 1, \ldots, \min(m,n),$$

where u_i and v_i are the ith columns of U and V, respectively.

The SVD of A is closely related to the eigendecompositions of the symmetric matrices A^TA and AA^T, because:

$$A^TAv_i = \sigma_i^2 v_i \text{ and } AA^T u_i = \sigma_i^2 u_i.$$

However, these relationships are not recommended as a means of computing singular values or vectors.

Singular values are well conditioned, that is, they are not unduly sensitive to perturbations in A. The sensitivity of a singular vector depends on how small the gap is between its singular value and any other singular value; the smaller the gap, the more sensitive the singular vector.

The singular value decomposition is useful for the numerical determination of the rank of a matrix, and for solving linear least-squares problems, especially when they are rank deficient, or nearly so.

The SVD of complex matrices has many similarities with the real matrix problem and it is given by

$$A = U\Sigma V^H.$$

In the complex case, the singular vector matrices U and V are complex unitary but the singular value matrix Σ is still real. Note that the transpose operation ^{T} in the real case is replaced by the complex conjugate operation ^{H}.

The parallel algorithm for computing the SVD is similar to the parallel algorithm for the symmetric eigenproblem and the Hermitian eigenproblem. It is based on an extension to the one-sided Jacobi method due to Hestenes (see [2]). This is an implicit Jacobi method and uses odd-even permutations to shuffle the columns of the matrix across the logical processors.

2.4 References

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

[2] Hestenes M R (1958) Inversion of matrices by biorthogonalization and related results *J. SIAM* **6** 51–90

[3] Parlett B N (1980) *The Symmetric Eigenvalue Problem* Prentice–Hall

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

3.1 Symmetric Eigenvalue Problem

F02FQFP computes the eigenvalues and eigenvectors of a real symmetric matrix.

3.2 Hermitian Eigenvalue Problem

F02FRFP Eigenvalues and eigenvectors of complex Hermitian matrix, one-sided Jacobi method.

3.3 Singular Value Decomposition of Real Matrices

F02WQFP Singular Value Decomposition (SVD) of real matrix, one-sided Jacobi method.

3.4 Singular Value Decomposition of Complex Matrices

F02WRFP Singular Value Decomposition (SVD) of complex matrix, one-sided Jacobi method.