Chapter 18

Computing Eigenvalues and Eigenvectors

After the problem of solving a linear system, the problem of computing the eigenvalues and the eigenvectors of a real or complex matrix is one of most important problems of numerical linear algebra. Several methods exist, among which we mention Jacobi, Givens–Householder, divide-and-conquer, QR iteration, and Rayleigh–Ritz; see Demmel [48], Trefethen and Bau [176], Meyer [125], Serre [156], Golub and Van Loan [80], and Ciarlet [41]. Typically, better performing methods exist for special kinds of matrices, such as symmetric matrices.

In theory, given an $n \times n$ complex matrix A, if we could compute a Schur form $A = UTU^*$, where T is upper triangular and U is unitary, we would obtain the eigenvalues of A, since they are the diagonal entries in T. However, this would require finding the roots of a polynomial, but methods for doing this are known to be numerically very unstable, so this is not a practical method.

A common paradigm is to construct a sequence (P_k) of matrices such that $A_k = P_k^{-1} A P_k$ converges, in some sense, to a matrix whose eigenvalues are easily determined. For example, $A_k = P_k^{-1} A P_k$ could become upper triangular in the limit. Furthermore, P_k is typically a product of "nice" matrices, for example, orthogonal matrices.

For general matrices, that is, matrices that are not symmetric, the QR iteration algorithm, due to Rutishauser, Francis, and Kublanovskaya in the early 1960s, is one of the most efficient algorithms for computing eigenvalues. A fascinating account of the history of the QR algorithm is given in Golub and Uhlig [79]. The QR algorithm constructs a sequence of matrices (A_k), where A_{k+1} is obtained from A_k by performing a QR-decomposition $A_k = Q_k R_k$ of A_k and then setting $A_{k+1} = R_k Q_k$, the result of swapping Q_k and R_k. It is immediately verified that $A_{k+1} = Q_k^* A_k Q_k$, so A_k and A_{k+1} have *the same eigenvalues*, which are the eigenvalues of A.

The basic version of this algorithm runs into difficulties with matrices that have several eigenvalues with the same modulus (it may loop or not "converge" to an upper triangular matrix). There are ways of dealing with some of these problems, but for ease of exposition,