Section 1

INTRODUCTION

The package of Fortran IV programs given the acronym EISPACK is a systematized collection of subroutines which compute the eigenvalues and/or eigenvectors of six classes of matrices; namely, complex general, complex Hermitian, real general, real symmetric, real symmetric tridiagonal, and special real tridiagonal matrices. The subroutines are based mainly upon Algol procedures published in the Handbook series of Springer-Verlag by Wilkinson and Reinsch [1], have been adapted and thoroughly tested on several different machines, and have been certified and are supported by the NATS project [3,4,5]. The machines for which they are certified include IBM 360-370, CDC 6000-7000, Univac 1110, Honeywell 6070, DEC PDP-10, and Burroughs 6700.

This manual is a user guide to EISPACK and to a control program EISPAC available with the IBM version of the package. It contains program segments which illustrate each of the basic computations with EISPACK and discusses variants of these that provide mild tradeoffs of efficiency, storage, and accuracy. Other sections of the guide discuss the validation procedures used for testing EISPACK, report execution times of the EISPACK subroutines on several machines, advertise the certified status and availability of EISPACK, and describe the major differences between the published Algol procedures in [1] and their Fortran counterparts. The final section includes detailed documentation with Fortran listings of each EISPACK subroutine and the document for the control program.

Section 1.1

ORGANIZATION OF THE GUIDE

This guide is organized for the convenience, hopefully, of the user. Material most pertinent to the basic uses of the package and the control program appears in the early sections and references the more detailed and specific information in later sections. Here follows a brief description of the organization of the guide.

The remaining subsection of this introduction is a general statement with regard to the expected accuracy of the results from EISPACK. This statement is based upon the careful and detailed analyses of Wilkinson and others. Only a brief overview is provided in this subsection and the interested reader is directed to [1] and [2] for more detailed statements of accuracy.

Section 2 is divided into a prologue and three major subsections. The prologue introduces the concept of an EISPACK path, discusses the economies that can be realized with the use of the control program if available, and instructs on the selection among the 22 basic paths. The first subsection establishes several conventions that are useful in clarifying the discussions of the paths. It then details the 22 basic paths and associated control program calls in the form of program segments. Each program segment is introduced by a brief description of the problem it solves and any specific considerations needed for the path, and is followed by a summary of array storage requirements for the path and sample execution times on the IBM 370/195 computer. The next subsection describes possible variants of the 22 basic paths, focusing on those conditions for which the variants are to be preferred. The last subsection provides further information about specific details of EISPACK and the control program and suggests several additional applications of the package. Complete sample programs illustrating the use of EISPACK and EISPAC to solve a specified eigenproblem appear at the end of this subsection.

Section 3 outlines the validation procedures for EISPACK that led to the certification of the package. Section 4 reports sample execution times of the individual subroutines and of several of the program segments of Section 2 and also discusses such considerations as the dependence of the execution times upon the matrix and the computer. The statement of certification for EISPACK, the machines and operating systems on which it has been certified, and its availability appear in Section 5. Section 6 itemizes the principal differences between the Fortran subroutines and their Algol antecedents published in [1]. Finally, the documentation and Fortran listing for each subroutine appear in edited form in Section 7.

Section 1.2

ACCURACY OF THE EISPACK SUBROUTINES

The most useful statement that can be made with regard to the accuracy of the EISPACK subroutines is that they are based on algorithms which are numerically stable; that is, for every computed eigenpair (λ,z) associated with a matrix A, there exists a matrix E with norm small compared to that of A for which λ and z are an exact eigenpair of A+E. This backward or inverse approach in describing the accuracy of the subroutines is necessitated by the inherent properties of the problem which, in general, preclude the more familiar forward approach. However, for real symmetric and complex Hermitian matrices the forward approach also applies, and indeed is a consequence of the backward analysis. For these matrices the eigenvalues computed by EISPACK must be close to the exact ones, but a similar claim for the eigenvectors is not possible. What is true in this case is that the computed eigenvectors will be closely orthogonal if the subroutines that accumulate the transformations are used.

The size of E, of course, is crucial to a meaningful statement of accuracy, and the reader is referred to the detailed error analyses of Wilkinson and others ([1],[2]). In our many tests of EISPACK, we have seldom observed an E with norm larger than a small multiple of the product of the order of the matrix A, its norm, and the precision of the machine.