7861420

Lecture Notes in Computer Science

Edited by G. Goos and J. Hartmanis

51

B. S. Garbow J. M. Boyle
J. J. Dongarra C. B. Moler

Matrix Eigensystem Routines – EISPACK Guide Extension

Springer-Verlag
Berlin · Heidelberg · New York

TP31
G3
7861420

Lecture Notes in Computer Science

Edited by G. Goos and J. Hartmanis

51

B. S. Garbow J. M. Boyle
J. J. Dongarra C. B. Moler

华南工学院
图书馆藏书

Matrix Eigensystem Routines – EISPACK Guide Extension

E7861420

Springer-Verlag
Berlin · Heidelberg · New York 1977

Editorial Board
P. Brinch Hansen, D. Gries, C. Mol
N. Wirth

Author
Burton S. Garbow
Applied Mathematics Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439 USA

TP31 7861420
G3

Matrix eigensystem routines
EISPACK guide exide extensio

龙志扬	20122	1985	
龙志扬	20122	1986	
[illegible]	807881	988	5

Library of Congress Cataloging in Publication Data
Main entry under title:

Matrix eigensystem routines.

(Lecture notes in computer science ; 51)
Supplements the 2d. ed of Matrix eigensystem
EISPACK guide.
1. EISPACK (Computer program) I. Garbow,
1930- II. Series.
QA193.M38 001.6'425 77-2802

AMS Subject Classifications (1970): 15A18, 65F15
CR Subject Classifications (1974): 5.14

ISBN 3-540-08254-9 Springer-Verlag Berlin · Heidelberg · New York
ISBN 0-387-08254-9 Springer-Verlag New York · Heidelberg · Berlin

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically those of translation, re-printing, re-use of illustrations, broadcasting, reproduction by photocopying machine or similar means, and storage in data banks.

Under § 54 of the German Copyright Law where copies are made for other than private use, a fee is payable to the publisher, the amount of the fee to be determined by agreement with the publisher.

© by Springer-Verlag Berlin · Heidelberg 1977

Printed in Germany
Printing and binding: Beltz Offsetdruck, Hemsbach/Bergstr.
2145/3140-543210

Lecture Notes in Computer Science

Vol. 1: GI-Gesellschaft für Informatik e.V. 3. Jahrestagung, Hamburg, 8.–10. Oktober 1973. Herausgegeben im Auftrag der Gesellschaft für Informatik von W. Brauer. XI, 508 Seiten. 1973.

Vol. 2: GI-Gesellschaft für Informatik e.V. 1. Fachtagung über Automatentheorie und Formale Sprachen, Bonn, 9.–12. Juli 1973. Herausgegeben im Auftrag der Gesellschaft für Informatik von K.-H. Böhling und K. Indermark. VII, 322 Seiten. 1973.

Vol. 3: 5th Conference on Optimization Techniques, Part I. (Series: I.F.I.P. TC7 Optimization Conferences.) Edited by R. Conti and A. Ruberti. XIII, 565 pages. 1973.

Vol. 4: 5th Conference on Optimization Techniques, Part II. (Series: I.F.I.P. TC7 Optimization Conferences.) Edited by R. Conti and A. Ruberti. XIII, 389 pages. 1973.

Vol. 5: International Symposium on Theoretical Programming. Edited by A. Ershov and V. A. Nepomniaschy. VI, 407 pages. 1974.

Vol. 6: B. T. Smith, J. M. Boyle, J. J. Dongarra, B. S. Garbow, Y. Ikebe, V. C. Klema, and C. B. Moler, Matrix Eigensystem Routines – EISPACK Guide. XI, 551 pages. 2nd Edition 1974. 1976.

Vol. 7: 3. Fachtagung über Programmiersprachen, Kiel, 5.–7. März 1974. Herausgegeben von B. Schlender und W. Frielinghaus. VI, 225 Seiten. 1974.

Vol. 8: GI-NTG Fachtagung über Struktur und Betrieb von Rechensystemen, Braunschweig, 20.–22. März 1974. Herausgegeben im Auftrag der GI und der NTG von H.-O. Leilich. VI, 340 Seiten. 1974.

Vol. 9: GI-BIFOA Internationale Fachtagung: Informationszentren in Wirtschaft und Verwaltung. Köln, 17./18. Sept. 1973. Herausgegeben im Auftrag der GI und dem BIFOA von P. Schmitz. VI, 259 Seiten. 1974.

Vol. 10: Computing Methods in Applied Sciences and Engineering, Part 1. International Symposium, Versailles, December 17–21, 1973. Edited by R. Glowinski and J. L. Lions. X, 497 pages. 1974.

Vol. 11: Computing Methods in Applied Sciences and Engineering, Part 2. International Symposium, Versailles, December 17–21, 1973. Edited by R. Glowinski and J. L. Lions. X, 434 pages. 1974.

Vol. 12: GFK-GI-GMR Fachtagung Prozessrechner 1974. Karlsruhe, 10.–11. Juni 1974. Herausgegeben von G. Krüger und R. Friehmelt. XI, 620 Seiten. 1974.

Vol. 13: Rechnerstrukturen und Betriebsprogrammierung, Erlangen, 1970. (GI-Gesellschaft für Informatik e.V.) Herausgegeben von W. Händler und P. P. Spies. VII, 333 Seiten. 1974.

Vol. 14: Automata, Languages and Programming – 2nd Colloquium, University of Saarbrücken, July 29–August 2, 1974. Edited by J. Loeckx. VIII, 611 pages. 1974.

Vol. 15: L Systems. Edited by A. Salomaa and G. Rozenberg. VI, 338 pages. 1974.

Vol. 16: Operating Systems, International Symposium, Rocquencourt 1974. Edited by E. Gelenbe and C. Kaiser. VIII, 310 pages. 1974.

Vol. 17: Rechner-Gestützter Unterricht RGU '74, Fachtagung, Hamburg, 12.–14. August 1974, ACU-Arbeitskreis Computer-Unterstützter Unterricht. Herausgegeben im Auftrag der GI von K. Brunnstein, K. Haefner und W. Händler. X, 417 Seiten. 1974.

Vol. 18: K. Jensen and N. E. Wirth, PASCAL – User Manual and Report. VII, 170 pages. Corrected Reprint of the 2nd Edition 1976.

Vol. 19: Programming Symposium. Proceedings 1974. V, 425 pages. 1974.

Vol. 20: J. Engelfriet, Simple Program Schemes and Formal Languages. VII, 254 pages. 1974.

Vol. 21: Compiler Construction, An Advanced Course. Edited by F. L. Bauer and J. Eickel. XIV. 621 pages. 1974.

Vol. 22: Formal Aspects of Cognitive Processes. Proceedings 1972. Edited by T. Storer and D. Winter. V, 214 pages. 1975.

Vol. 23: Programming Methodology. 4th Informatik Symposium, IBM Germany Wildbad, September 25–27, 1974. Edited by C. E. Hackl. VI, 501 pages. 1975.

Vol. 24: Parallel Processing. Proceedings 1974. Edited by T. Feng. VI, 433 pages. 1975.

Vol. 25: Category Theory Applied to Computation and Control. Proceedings 1974. Edited by E. G. Manes. X, 245 pages. 1975.

Vol. 26: GI-4. Jahrestagung, Berlin, 9.–12. Oktober 1974. Herausgegeben im Auftrag der GI von D. Siefkes. IX, 748 Seiten. 1975.

Vol. 27: Optimization Techniques. IFIP Technical Conference. Novosibirsk, July 1–7, 1974. (Series: I.F.I.P. TC7 Optimization Conferences.) Edited by G. I. Marchuk. VIII, 507 pages. 1975.

Vol. 28: Mathematical Foundations of Computer Science. 3rd Symposium at Jadwisin near Warsaw, June 17–22, 1974. Edited by A. Blikle. VII, 484 pages. 1975.

Vol. 29: Interval Mathematics. Procedings 1975. Edited by K. Nickel. VI, 331 pages. 1975.

Vol. 30: Software Engineering. An Advanced Course. Edited by F. L. Bauer. (Formerly published 1973 as Lecture Notes in Economics and Mathematical Systems, Vol. 81) XII, 545 pages. 1975.

Vol. 31: S. H. Fuller, Analysis of Drum and Disk Storage Units. IX, 283 pages. 1975.

Vol. 32: Mathematical Foundations of Computer Science 1975. Proceedings 1975. Edited by J. Bečvář. X, 476 pages. 1975.

Vol. 33: Automata Theory and Formal Languages, Kaiserslautern, May 20–23, 1975. Edited by H. Brakhage on behalf of GI. VIII, 292 Seiten. 1975.

Vol. 34: GI – 5. Jahrestagung, Dortmund 8.–10. Oktober 1975. Herausgegeben im Auftrag der GI von J. Mühlbacher. X, 755 Seiten. 1975.

Vol. 35: W. Everling, Exercises in Computer Systems Analysis. (Formerly published 1972 as Lecture Notes in Economics and Mathematical Systems, Vol. 65) VIII, 184 pages. 1975.

Vol. 36: S. A. Greibach, Theory of Program Structures: Schemes, Semantics, Verification. XV, 364 pages. 1975.

Vol. 37: C. Böhm, λ-Calculus and Computer Science Theory. Proceedings 1975. XII, 370 pages. 1975.

Vol. 38: P. Branquart, J.-P. Cardinael, J. Lewi, J.-P. Delescaille, M. Vanbegin. An Optimized Translation Process and Its Application to ALGOL 68. IX, 334 pages. 1976.

Vol. 39: Data Base Systems. Proceedings 1975. Edited by H. Hasselmeier and W. Spruth. VI, 386 pages. 1976.

Vol. 40: Optimization Techniques. Modeling and Optimization in the Service of Man. Part 1. Proceedings 1975. Edited by J. Cea. XIV, 854 pages. 1976.

Vol. 41: Optimization Techniques. Modeling and Optimization in the Service of Man. Part 2. Proceedings 1975. Edited by J. Cea. XIII, 852 pages. 1976.

Vol. 42: James E. Donahue, Complementary Definitions of Programming Language Semantics. VII, 172 pages. 1976.

Vol. 43: E. Specker und V. Strassen, Komplexität von Entscheidungsproblemen. Ein Seminar. V, 217 Seiten. 1976.

Vol. 44: ECI Conference 1976. Proceedings 1976. Edited by K. Samelson. VIII, 322 pages. 1976.

Vol. 45: Mathematical Foundations of Computer Science 1976. Proceedings 1976. Edited by A. Mazurkiewicz. XI, 601 pages. 1976.

Vol. 46: Language Hierarchies and Interfaces. Edited by F. L. Bauer and K. Samelson. X, 428 pages. 1976.

Vol. 47: Methods of Algorithmic Language Implementation. Edited by A. Ershov and C. H. A. Koster. VIII, 351 pages. 1977.

Vol. 48: Theoretical Computer Science, Darmstadt, March 1977. Edited by H. Tzschach, H. Waldschmidt and H. K.-G. Walter on behalf of GI. VIII, 418 pages. 1977.

8. Moler, C. B. and Stewart, G. W., An Algorithm for Generalized Matrix Eigenvalue Problems, SIAM Journal of Numerical Analysis, Vol. 10, 1973, pp. 241-256.

9. Ward, R. C., An Extension of the QZ Algorithm for Solving the Generalized Matrix Eigenvalue Problem, Technical Note NASA TN D-7305, National Aeronautics and Space Administration, Washington, 1973.

10. Smith, B. T., Boyle, J. M., Dongarra, J. J., Garbow, B. S., Ikebe, Y., Klema, V. C., and Moler, C. B., Matrix Eigensystem Routines - EISPACK Guide, Lecture Notes in Computer Science, Vol. 6, Second Edition, Springer-Verlag, New York, Heidelberg, Berlin, 1976.

此为试读，需要完整PDF请访问：www.ertongbook.com

PREFACE

This volume supplements the earlier Volume 6 in this series [10]; together they provide guidance for the complete second release of the EISPACK Eigensystem Package. The stress in this book is on four additional problem classes: the symmetric band eigenproblem, the generalized symmetric eigenproblem, the generalized real eigenproblem, and the singular value decomposition of a rectangular matrix and solution of an associated linear least squares problem.

The organization of material in this volume follows closely that of [10]. Several of the newer problems transform to problems covered earlier in [10]; reference should be made there for details that apply after the problem has been transformed. Towards achieving a certain degree of self-sufficiency, however, the documentation for seven earlier subroutines that recur here in the various recommended paths of Section 2 has been recopied in Section 7.1 of this volume.

The EISPAC control program, available with the IBM version of EISPACK, extends to each of the newer problem classes except Singular Value Decomposition; the discussion of its usage, where applicable, is integrated into the various sections of this volume. Its documentation, earlier provided in [10], has been recopied in Section 7.2 of this volume.

EISPACK is a product of the NATS (National Activity to Test Software) Project ([3],[4],[5]) which has been guided by the principle that the effort to produce high quality mathematical software is justified by the wide use of that software in the scientific community. EISPACK has been distributed to several hundred computer centers throughout the world since the package was first released in May, 1972, and now the second release is available as described in Section 5.

Building a systematized collection of mathematical software is necessarily a collaborative undertaking demanding the interplay of a variety of skills; we wish to acknowledge a few whose roles were especially crucial during the preparation of the second release. J. Wilkinson persisted in his encouragement of the project and his counsel was often sought during his frequent visits to North America. Organization and direction came from W. Cowell and J. Pool. B. Smith and V. Klema provided highly valued consultation. The field testing was carried out at the installations listed in Section 5 through the sustained efforts of M. Berg, A. Cline, D. Dodson, B. Einarsson, S. Eisenstat, I. Farkas, P. Fox, F. Fritsch, C. Frymann, G. Haigler, H. Happ, L. Harding, M. Havens, H. Hull, D. Kincaid, P. Messina, M. Overton, R. Raffenetti, J. Stein, J. Walsh, and J. Wang. Additional assistance in providing the timing information for the tables of Section 4 was given by T. Pinter. Appreciation is also expressed for the very important feedback received from users not formally associated with the testing effort. Finally, we acknowledge the skill and cooperation of our typist, J. Beumer.

Work performed under the auspices of the United States Energy Research and Development Administration and the National Science Foundation.

TABLE OF CONTENTS

SECTION 1

SECTION 2

SECTION 3

SECTION 4

SECTION 5

SECTION 6

SECTION 7

LIST OF TABLES

此为试读，需要完整PDF请访问： www.ertongbook.com

Section 1

INTRODUCTION

The subset of the EISPACK package of Fortran IV programs included within this volume is a systematized collection of subroutines which compute the eigenvalues and/or eigenvectors for three special classes of matrix problems and the singular value decomposition of an arbitrary matrix. The three problem classes are real symmetric band, generalized real symmetric, and generalized real. The singular value decomposition, in turn, enables the solution of certain linear least squares problems. The subroutines are based mainly upon Algol procedures published in the Handbook series of Springer-Verlag by Wilkinson and Reinsch [1] and the QZ algorithm of Moler and Stewart [8] as extended by Ward [9]. They 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 these newer capabilities of EISPACK (complementing [10]) 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 referenced herein 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 four 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 10 basic paths of this volume. The first subsection establishes several conventions that are useful in clarifying the discussions of the paths. It then details the 10 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 10 basic paths, focusing on those conditions for which the variants are to be preferred. The third 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. The last subsection describes the EISPACK capabilities to compute the singular value decomposition of a matrix and to solve an associated linear least squares problem.

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 referenced 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. For generalized problems, the corresponding claim can be made after associating also with B a matrix of small relative norm. 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 band matrices the forward approach also applies, and indeed is a consequence of the backward analysis. For these problems 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 or system, an appropriate norm, and the precision of the machine.

Section 2

HOW TO USE EISPACK

This section is designed to provide, in readily accessible form, the basic information you need to correctly use subroutines from EISPACK to solve an eigenproblem. The way in which this information is presented is influenced by the design of the eigensystem package; hence we will first consider briefly the global structure of EISPACK.

EISPACK is capable of performing 32 different basic computations (22 of them described in [10]), plus several variations of them. If each of these computations (and variations) were performed completely within a single EISPACK subroutine, the package would be unwieldy indeed. It also would be highly redundant, since the same steps appear in many of the computations. To avoid these problems, the subroutines in EISPACK are designed so that each performs a basic step which appears in one or more of the computations. (See [7] for an introduction to the modularization of EISPACK.) Consequently, the redundancy (hence the size) of the package is minimized.

Another consequence is that, in general, more than one subroutine from EISPACK is required to perform a given computation. These subroutines must of course be called in the correct order and with the proper parameters; in addition, some computations also require certain auxiliary actions, e.g., initializing parameters and testing for errors. Throughout the remainder of this book such an ordered set of subroutine calls and associated auxiliary actions will be called an EISPACK *path*.

As a result of this structure the documentation for the use of EISPACK comprises two main parts: a description of the basic paths and their variations, and a description of the individual subroutines in EISPACK. The information about the paths constitutes the remainder of this section while the subroutine documentation is collected in Section 7.

The path descriptions are divided into three parts. Section 2.1 describes the 10 basic paths and includes a table to facilitate reference to them. Section 2.2 describes some of the variations of these paths and suggests when such variations might be useful. Section 2.3 contains certain additional information about and examples of the use of EISPACK. To keep the descriptions of the basic paths and their variants simple, we have omitted much of the detailed information (e.g., the meanings of non-zero error indicators and the descriptions of certain parameters) and collected it in Section 2.3. Detailed information about each subroutine may be obtained from the documentation for the individual subroutines in Section 7. We hope, however, that the information given in this section will be sufficient to permit you to correctly solve most eigenproblems.

The detail of path information that you must know to solve certain basic eigenproblems can be reduced by using an appropriate driver subroutine to build the desired path from other EISPACK members. Applicability of the driver subroutines is limited to those problems where all eigenvalues and eigenvectors or all eigenvalues only are desired. There is a driver subroutine for each class of problems handled by the package; driver subroutine calls corresponding to six of the 10 basic paths are given as part of the discussion of the paths in this section.

Substantial further reduction in the detail of path information that you must know to solve an eigenproblem, with wider applicability, can be achieved by use of a control program, called EISPAC, which is available with the IBM version of the eigensystem package [6]. (It is only practical to implement this control program on those computing systems which adequately support execution-time loading of subroutines.) EISPAC accepts a relatively straightforward problem description stated in terms of the

此为试读，需要完整PDF请访问：www.ertongbook.com