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Band 186

Handbook for Automatic Computation

Volume II

J. H. Wilkinson · C. Reinsch

Linear Algebra

Handbook for Automatic Computation

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Linear Algebra

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in Einzeldarstellungen
mit besonderer Berücksichtigung
der Anwendungsgebiete

Band 186

Preface

The development of the internationally standardized language ALGOL has made it possible to prepare procedures which can be used without modification whenever a computer with an ALGOL translator is available. Volume Ia in this series gave details of the restricted version of ALGOL which is to be employed throughout the Handbook, and volume Ib described its implementation on a computer. Each of the subsequent volumes will be devoted to a presentation of the basic algorithms in some specific areas of numerical analysis.

This is the first such volume and it was felt that the topic Linear Algebra was a natural choice, since the relevant algorithms are perhaps the most widely used in numerical analysis and have the advantage of forming a well defined class. The algorithms described here fall into two main categories, associated with the solution of linear systems and the algebraic eigenvalue problem respectively and each set is preceded by an introductory chapter giving a comparative assessment.

In spite of the self-contained nature of the linear algebra field, experience has shown that even here the preparation of a fully tested set of algorithms is a far greater task than had been anticipated. Almost all the algorithms presented here have received pre-publication in Numerische Mathematik and the need to check very carefully whenever an algorithm is modified, even in a minor detail, has meant that the preparation of a paper in the Handbook series has usually taken longer than would be required for a normal research paper. Failure to check may result in the introduction of an error into an algorithm which previously had enjoyed a long period of successful use.

It soon became obvious that it would be impractical, even if desirable, to aim at completeness in this volume. In general we have aimed to include only algorithms which at least in some limited area provide something approaching an optimum solution, this may be from the point of view of generality, elegance, speed or economy of storage. The omission of an algorithm should not be taken as indicating that it has been found wanting; in some cases it merely means that we were not fully satisfied with current implementations.

From its very nature a volume of this kind is essentially a joint effort. In many instances the basic mathematical concept of an algorithm has had a long period of evolution and many people have played a part in the progressive refinement of the original concept. Thanks are due to all who have thereby contributed indirectly to this volume but I would like to pay a special tribute to those who have submitted the ALGOL procedures published here and have assisted in testing them.

Professor F. L. Bauer and the late Professor H. Rutishauser, who are authors of the Handbook series, have been invaluable sources of information and have supervised much of the work in this volume. Three colleagues at the National

Physical Laboratory, Miss. H. Bowdler, Mr. R. S. Martin and Mrs. G. Peters have between them been responsible for the preparation of some half of the published algorithms, have made substantial contributions to them and have played a major part in their testing at all stages in their development. Special thanks are due to Mrs. E. Mann of the Technische Universität München, who tested a number of the earlier variants and virtually all of the final versions of the algorithms and gave valuable assistance in the proof reading.

The publication of a volume of this kind has special problems since a good deal of the typeset material has had to be retained in almost finished form over a long period. We are particularly grateful to the publishers for their patient courteous assistance in what must have been an unusually exacting task.

We are very much aware that the production of reliable algorithms is a continuing process and we shall appreciate it if users will inform us of failures or shortcomings in the performance of our procedures.

Teddington and München
October 1970

J. H. Wilkinson
C. H. Reinsch

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Part I Linear Systems, Least Squares and Linear Programming

Part II The Algebraic Eigenvalue Problem

General guide to the use of the volume

Most of the contributions have been subdivided into the following seven sections.

1. Theoretical Background
   briefly collecting the relevant formulae.
2. Applicability
   which sketches the scope of the algorithms.
3. Formal Parameter List
   with a specification of all input, output and exit parameters.
4. ALGOL Programs
   presenting the algorithms in the ALGOL 60 reference language.
5. Organisational and Notational Details
   explaining and commenting on special features, and showing why particular realizations of the formulae have been preferred to others.
6. Discussion of Numerical Properties
   usually referring to a published error analysis of the underlying algorithms.
7. Test Results and Examples of the Use of the Procedures
   giving the solutions obtained on a digital computer to a number of sample problems in order to facilitate the correct use of the procedures.

In some earlier contributions section 7 above was subdivided into two sections:

7. Examples of the Use of the Procedures.
8. Test Results.

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Introduction to Part I

Linear Systems, Least Squares and Linear Programming

by J. H. WILKINSON

1. Introduction

Algorithms associated with linear systems may be roughly classified under three headings:

i) Solution of non-singular systems of linear equations, matrix inversion and determinant evaluation.

ii) Linear least squares problems and calculation of generalized inverses.

iii) Linear programming

though the last two overlap to some extent with the first.

Nearly all the methods we describe for solving $n \times n$ systems of equations start by performing some factorization of the matrix A of coefficients and as a by-product the determinant of A is readily available. By taking the n columns of the unit matrix as right-hand sides, the inverse of A can be computed, though the volume of work can be reduced somewhat by taking account of the special nature of these n columns.

It was decided that iterative techniques for the solution of linear algebraic equations should be excluded from this volume since they have mainly been developed in connexion with the solution of partial differential equations.

It will be appreciated that the selection of the most efficient algorithms may be to some extent machine dependent. This is usually true, for example, when storage considerations become relevant. In the algorithms presented in this book no reference is made to the use of a backing store such as a magnetic tape or disc. For this reason the storage requirements in practice may be different from what they appear to be. For example, if iterative refinement of the solution of a system of linear equations is required, a copy of the original system must be retained. In practice this could be held in the backing store.

While it is hoped that many users will wish to take advantage of the tested algorithms in exactly the form in which they are published, others will probably wish to adapt them to suit their own special requirements. The descriptions accompanying the algorithms should make this easier to do.

2. List of Procedures

To facilitate reference to the procedures they are listed below in alphabetical order, together with the chapters in which they are described. Sets of related procedures are grouped together. We also include a number of basic procedures associated with complex arithmetic, etc. in this list.

acc inverse, acc solve, I/2
bandet1, bansol1, I/6
bandet2, bansol2, I/6
cabs, cdiv, csqrt, II/13
cg, I/5
chobanddet, chobandsol, I/4
choldet1, cholsol1, cholinversion1, I/1 and I/2
choldet2, cholsol2, cholinversion2, I/1
compdet, compsol, cx acc solve, I/7
gjdef1, gjdef2, I/3
innerprod, cx innerprod, I/2 and I/7
least squares solution, I/8
lp, I/11
minfit, svd, I/10
ortho1, ortho2, ortholin1, ortholin2, I/9
svd, minfit, I/10
symdet, symsol, syminversion, I/1
unsym acc solve, unsymdet, unsymsol, I/7

3. Positive Definite Symmetric Matrices

The solution of an $n \times n$ system of linear equations with a positive definite symmetric matrix of coefficients is a simpler problem than that of a system with a matrix of general form or even with a non-positive definite symmetric matrix. Most of the algorithms we give for positive definite symmetric matrices are based on the Cholesky factorization $A = LL^T$, where L is a lower triangular matrix, or on the related factorization $A = LDL^T$ where L is unit lower triangular and D is a positive diagonal matrix. Such algorithms are numerically stable and very economical as regards the number of arithmetic operations. There is no significant difference between the effectiveness of the LL^T and LDL^T factorizations, but the former uses square roots and the latter does not. For some purposes the Cholesky factor L is specifically required.

3.1. Dense Positive Definite Matrices

a) Cholesky Factorizations

There are two main sets associated with the Cholesky factorization of a dense $n \times n$ positive definite matrix. They are *choldet1, cholsol1* and *cholinversion1*; and *choldet2, cholsol2* and *cholinversion2*. The second of these sets achieves economy of storage by working only with a linear array of $\frac{1}{2}n(n+1)$ elements consisting initially of the lower triangle of A which is later overwritten with L. This second set is marginally slower than the first, but should be used when storage considerations are paramount.

In each case *choldet* gives the LL^T factorization of A and computes the determinant as a by-product. After using *choldet*, systems of equations having A as the matrix of coefficients may be solved by using the corresponding *cholsol* and the inverse of A may be found by using the corresponding *cholinversion*.

Although the algorithms based on the Cholesky factorization are very accurate, indeed of optimal accuracy having regard to the precision of computation, the computed solutions or the computed inverse may not be of sufficient accuracy if the matrix A is ill-conditioned. The accuracy of the solutions or of the inverse can be improved while still using the original factorization of A. This is achieved in the algorithms *acc solve* and *acc inverse*. These algorithms enable us to determine by means of an iterative refinement process solutions or inverses which are "correct to working accuracy" provided A is not "singular to working accuracy". Iterative refinement ultimately gives a computed solution $\bar{x}$ such that

$$\|x - \bar{x}\|_\infty / \|x\|_\infty \leqq k \times macheps,$$

where *macheps* is the machine precision and k is a constant of the order of unity.

In order to achieve this high accuracy these algorithms employ a procedure *innerprod* which calculates to double precision the inner-product of two single precision vectors. It is assumed that this is done in machine code. For consistency alternative versions of *choldet1* and *cholsol1* are given in which all inner-products are accumulated in double precision. For computers on which the accumulation of inner-products is inefficient, the standard versions of *choldet1* and *cholsol1* may be used, but the accumulation of inner-products in the computation of the residuals is an *essential* feature of the iterative refinement process.

The procedures *acc solve* and *acc inverse* are of great value even when more accurate solutions are not required. If $\bar{x}^{(1)}$ is the original solution and $\bar{x}^{(2)}$ is the first improved solution, then $\bar{x}^{(2)} - \bar{x}^{(1)}$ usually gives a very good estimate of the effect of end figure changes in the data (i.e. end figure changes from the point of view of *machine* word length) and enables one to assess the significance of the solution when the given matrix A is subject to errors. On a computer which accumulates double precision inner-products efficiently this important information is obtained very economically as regards computing time. However, it is necessary to retain A and the right-hand sides, though this could be done on the backing store.

b) The LDL^T Factorization

The LDL^T factorization is used in the set of procedures *symdet*, *symsol* and *syminversion*. The factorization of A is performed in *symdet* and *det*(A) is produced as a by-product. After using *symdet*, systems of equations having A as the matrix of coefficients may be solved using *symsol* and the inverse of A may be found by using *syminversion*. It may be mentioned that algorithms analogous to *choldet2* etc. could be produced using the LDL^T decomposition and that versions of *acc solve* and *acc inverse* could be based on *symdet* and *symsol*. There is little to choose between corresponding algorithms based on the LL^T and LDL^T decompositions.

c) Gauss-Jordan Inversion

Two algorithms *gjdef1* and *gjdef2* are given for inverting a positive definite matrix *in situ*. The second of these economises in storage in much the same way as *choldet2*. The Gauss-Jordan algorithm should not be used for solving linear equations since it is less efficient than the *choldet-cholsol* combinations. For matrix inversion it provides an elegant algorithm of much the same accuracy as the *cholinversions*.

3.2. Positive Definite Band Matrices

Many physical problems give rise to systems of equations for which the matrix is positive definite and of band form. For such matrices the Cholesky factorization is very effective since it preserves this band form. The procedure *chobanddet* gives the Cholesky factors and the determinant of such a matrix, A, and subsequent use of *chobandsol* provides the solution of systems of equations having A as the matrix of coefficients. It is rare for the inverse of such a matrix to be required (the inverse will be full even when A is of band form) and hence no procedure *choband inverse* is provided. Iterative refinement of the solution could be provided by a procedure analogous to *acc solve*. An alternative method for the solution of banded equations is discussed in the next section.

3.3. Sparse Positive Definite Matrices of Special Form

Many problems in mathematical physics give rise to sparse positive definite matrices in which the non-zero elements a_{ij} are defined in a systematic way as functions of i and j. This is particularly true of systems arising from finite difference approximations to partial differential equations. If the matrix is sufficiently sparse and the functions of i and j are sufficiently simple the procedure *cg* based on the conjugate gradient algorithm may be the most efficient method of solution.

Although the conjugate gradient method is sometimes thought of as an iterative method it would, with exact computation, give the exact solution in a finite number of steps. It has therefore been included, though *true* iterative methods have been excluded.

The *cg* algorithm is optimal in respect of storage since the matrix A is, in general, not stored at all. All that is needed is an auxiliary procedure for determining $A\,x$ from a given vector x. When A is of very high order the use of the conjugate gradient method (or of one of the iterative methods not included in this volume) may be mandatory since it may not be possible to store A even if it is of narrow band form. This is a common situation in connexion with systems arising from partial differential equations. They give rise to narrow banded matrices but in addition most of the elements within the band itself are zero and usually the procedure for computing $A\,x$ is very simple.

It cannot be too strongly emphasized that the procedure *cg* is seldom, if ever, to be preferred to Cholesky type algorithms on the grounds of accuracy. The *cg* method is less competitive in terms of speed if a number of different right-hand sides are involved since each solution proceeds independently and r solutions involve r times as much work. With Cholesky type methods the factorization of A is required only once, however many right-hand sides are involved.

4. Non-Positive Definite Symmetric Matrices

There are no algorithms in this volume designed to take advantage of symmetry in the solution of dense symmetric matrices and they must be solved using the procedures described in later sections. The two sets of procedures *bandet1*, *bansol1* and *bandet2*, *bansol2* may be used to deal with symmetric band matrices

but they do not take advantage of symmetry and indeed this is destroyed during the factorization. Either of the procedures *bandet1, 2* may be used to factorize A and to find its determinant and subsequently *bansol1, 2* may be used to solve sets of equations having A as the matrix of coefficients. The first set of procedures is appreciably more efficient than the second, but *when A is symmetric, bandet2 also computes the number of positive eigenvalues.* It can therefore be used to find the number of eigenvalues greater than a given value p by working with $A - pI$.

5. Non-Hermitian Matrices

The solution of a system of equations having a dense non-Hermitian matrix of coefficients is a more severe problem than that for a symmetric positive definite system of equations. In particular the problem of scaling presents difficulties which have not been solved in an entirely satisfactory way. The procedures given here are in this respect something of a compromise between what is desirable and what is readily attainable.

5.1. Dense Matrices (Real and Complex)

The procedures depend on the LU factorization of the matrix A, where L is lower triangular and U is unit upper triangular. *Partial pivoting* is used in the factorization so that the algorithms effectively "correspond" to Gaussian elimination in which the pivotal element at each stage is chosen to be the largest element in the leading column of the remaining matrix, though this would give rise to a unit lower triangular L.

The procedure *unsymdet* produces the LU factorization of a real dense matrix A and produces the determinant as a by-product; subsequently any number of linear systems having A as the matrix of coefficients may be solved by using the procedure *unsymsol*. The procedures *compdet* and *compsol* perform the analogous operations for a complex matrix A.

To cover the cases when A is too ill-conditioned for the computed solution to be sufficiently accurate the procedures *unsym acc solve* and *cx acc solve* perform iterative refinement of the solution, using the initial factorization of A given by *unsymdet* or *compdet* respectively. Provided A is not almost singular to working accuracy iterative refinement will ultimately give a solution $\bar{x}$ which is correct to working accuracy, i.e. such that $\|x - \bar{x}\|_\infty / \|x\|_\infty \leq k \times macheps$, where *macheps* is the machine precision and k is a constant of order unity. Notice that "small" components of x may well have a low relative accuracy. We stress once again that one step of iterative refinement is of great value in giving an estimate of the sensitivity of the system of equations. If $\bar{x}^{(1)}$ and $\bar{x}^{(2)}$ are the first two solutions, then $\bar{x}^{(2)} - \bar{x}^{(1)}$ usually gives a good estimate of the effect of end figure changes in the data. (See earlier comments in 3.1(a).)

5.2. Unsymmetric Band Matrices

The procedures *bandet1* and *bansol1* are designed to deal with real unsymmetric matrices of band form. They deal efficiently with banded matrices having a different number of non-zero diagonal columns on the two sides. An