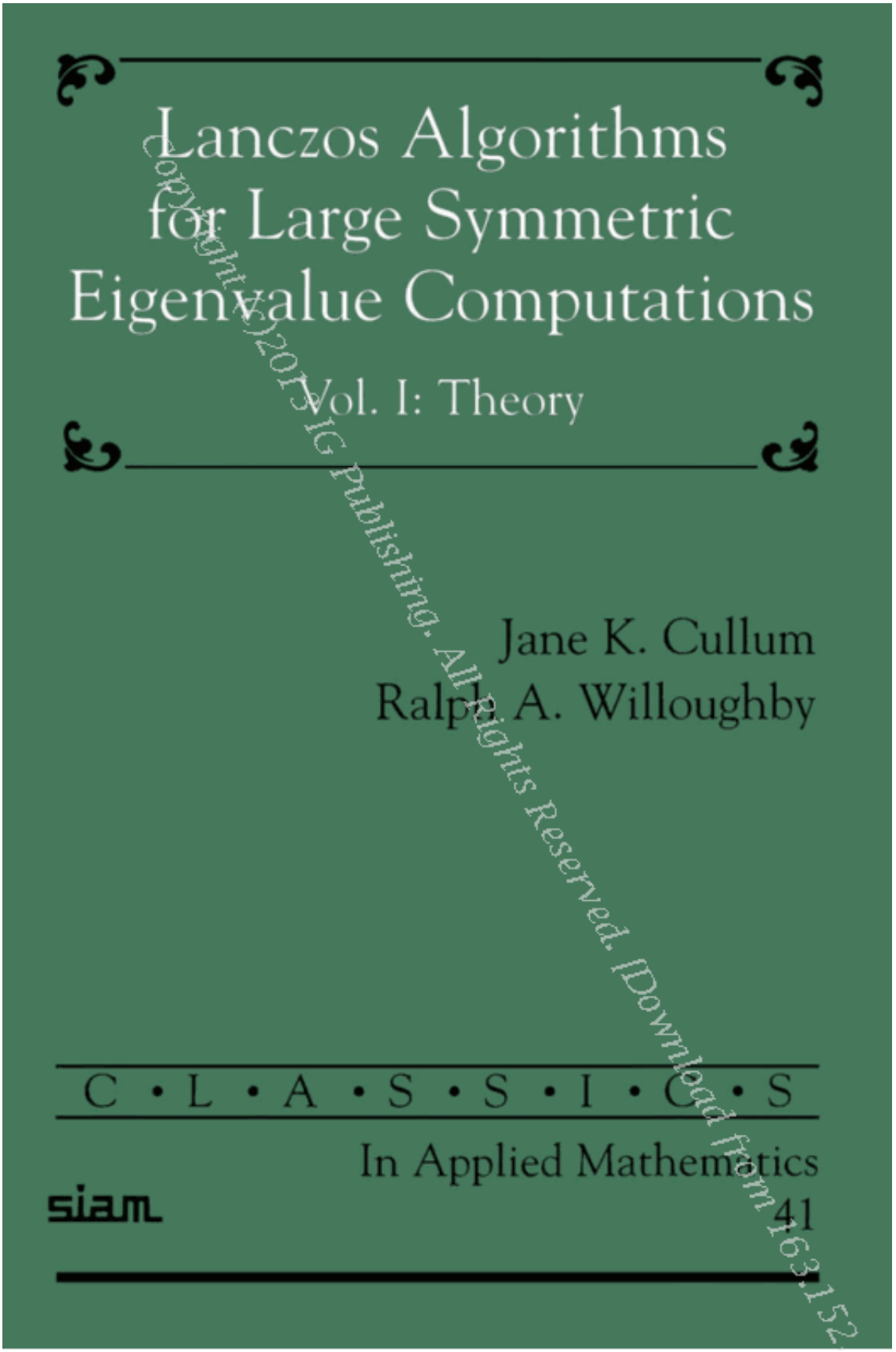

Lanczos Algorithms for Large Symmetric Eigenvalue Computations

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Lanczos Algorithms for Large Symmetric Eigenvalue Computations

Vol. I: Theory

Jane K. Cullum
Ralph A. Willoughby

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Philadelphia

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PREFACE TO THE CLASSICS EDITION

Since 1985, when this book was first published, interest in practical Lanczos algorithms for computing eigenvalues of large scale problems has soared. The developments since 1985 could fill easily a new two-volume book.

The computers of today are many orders of magnitude more powerful than the computers that we used in the early 1980s when the algorithms which are described in this book were developed. In 1984 we labeled problems of size 200 or larger as *large scale* and speculated that our codes should be useful on problems up to size 10,000.

Today, eigenvalue problems that involve *millions* of degrees of freedom are of great interest for many different kinds of scientific and engineering studies, and, in fact, parallel extensions of the real symmetric Lanczos algorithm described in Chapter 4 of this monograph have been used on problems involving more than a million variables.

The focus of this research monograph is on *symmetric* problems. Symmetric does not, however, imply Hermitian. The discussion not only covers real symmetric and Hermitian problems but also covers singular value problems and complex symmetric problems.

This monograph is unique in terms of the types of algorithms that are presented. Most of the numerical analysis community focuses on procedures that are firmly entrenched in the *orthogonal* world where spectral entities of orthogonal projections of operators are used to obtain corresponding approximations for the original problem. The use of orthogonal projections ensures direct relationships between these projections and the original problem. The popular package that is described in [1] utilizes this approach.

The algorithms in Chapters 4, 5, and 6 are based upon a different paradigm. The justification for our approach rests upon the nonintuitive discovery that the real symmetric Lanczos recursion is numerically stable in finite precision arithmetic [2, 3]. The analysis in [2, 3], when combined with our nonintuitive discovery that the eigenvalues of any Lanczos matrix can be *systematically* sorted into distinct subsets of *good* and *spurious* eigenvalues, enabled the development of practical Lanczos eigenvalue algorithms that do not require reorthogonalization. Details are in Chapter 4.

These algorithms function in two stages. Eigenvalues (singular values) are computed separately from corresponding eigenvector (singular vector) approximations. Separating these computations has two significant consequences. First, the amount of memory required for the eigenvalue computations is minimal, only some small multiple of the size of the original problem matrix. The size of this multiplier depends upon what the user wants to compute and upon the distribution of the spectrum of A. With minimal memory requirements, very large problems can be handled on not very large computers, and huge problems can be handled on large computers.

Second, the achievable accuracy of the eigenvalue approximations obtained by one of these algorithms can be greater than that achievable using a classical approach which incorporates reorthogonalization with respect to eigenvector approximations which are accurate to only a few digits. The procedures in Chapters 4, 5, and 6 do not invoke any type of deflation, and as long as the errors in the Lanczos recursions remain small, there is no degradation in the accuracy as more eigenvalue approximations are computed.

The eigenvalue procedures described in Chapters 4, 5, and 6 are simple to parallelize. There are no potential communication bottlenecks associated with a need to reorthogonalize every vector with respect to all vectors previously generated.

The penalty for not being *orthogonal* is that the matrix-vector multiplications required for the Lanczos recursions must be computed consistently at each stage of the Lanczos recursion. This limits the use of these methods in applications where the matrix-vector computations are inexact with varying accuracy. For example, these methods would not work well when these computations are accomplished via finite differences of nonlinear functions or as the numerical solution of a differential equation. In such a situation, the algorithms in Chapters 4, 5, and 6 could be used to obtain limited information about the spectrum but would eventually diverge. An approach based upon orthogonalization, such as in [1], may continue to function in such an environment, but the accuracy of the computed values may be difficult to determine.

Chapters 6 and 7 contain research that is not available in archival journals. In Chapter 6 we demonstrate that much of the analysis for the real symmetric Lanczos algorithm in Chapter 4 can be formally extended to the complex symmetric case.

The algorithms in Chapter 7 differ from those in Chapters 4, 5, and 6 in that they are block methods and belong to the *orthogonal* world. Reorthogonalization of vectors is invoked but in a very limited way. Of primary importance in Chapter 7 is our proposal for the *implicit deflation* of nearly dependent vectors from blocks. This form of deflation accelerates convergence, allows *converged* eigenvector approximation to continue to converge, and mollifies the negative effects which vector deflation can have upon approximations which have not yet converged. Details are in Chapter 7.

Algorithms that are based upon the work in this book, in spite of their relatively advanced age, are still being used. See, for example, [4], which contains numerical comparisons of the algorithm described in Chapter 4 with that in [1].

Volume 2 of this book, which is not being reproduced in the SIAM *Classics in Applied Mathematics* series, contains listings of all of the original implementations of the algorithms that are discussed in this monograph. The text for Volume 2, along with the source code for each of those listings, is available at the numerical analysis community Web repository, *www.netlib.org*, under the name "*lanczos*."

We hope that republication of this book will be of benefit to the computational physics, chemistry, and engineering communities that have shown interest in these types of algorithms. We also hope that students in the numerical linear algebra community will find this book useful as a means for building appreciation for the potential gains that may be achievable by thinking outside of the *orthogonal* box.

Regrettably, my co-author, Ralph Willoughby, passed away in July 2001 prior to the republication of our book in the SIAM *Classics in Applied Mathematics* series.

Ralph and I worked together from 1977 to 1991. Most of our research on "symmetric" problems is contained in this book. From 1984 through 1991 the focus of our work on algorithms for eigenvalue problems moved to nonsymmetric problems and to the extension of many of the ideas in this book to those types of problems.

Our joint publication in 1991 provided strategies for selecting appropriate matrix shifts for use in either symmetric or nonsymmetric shift and invert algorithms.

I wish to express my personal gratitude to Ralph's wife, Nona Willoughby, for her support in the republication of this book.

Jane Cullum
March 2002

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PREFACE

Energy levels, resonances, vibrations, feature extraction, factor analysis - the names vary from discipline to discipline; however, all involve eigenvalue/eigenvector computations. An engineer or physicist who is modeling a physical process, structure, or device is constrained to select a model for which the subsequently-required computations can be performed. This constraint often leads to reduced order or reduced size models which may or may not preserve all of the important characteristics of the system being modeled. Ideally, the modeler should not be forced to make such a priori reductions. It is our intention to provide here procedures which will allow the direct and successful solution of many large 'symmetric' eigenvalue problems, so that at least in problems where the computations are of this type there will be no need for model reduction.

Matrix eigenelement computations can be classified as small, medium, or large scale, in terms of their relative degrees of difficulty as measured by the amount of computer storage and time required to complete the desired computations. A matrix eigenvalue problem is said to be small scale if the given matrix has order smaller than 100. Well-documented and reliable FORTRAN programs exist for small scale eigenelement computations, see in particular EISPACK [1976,1977]. Typically those programs explicitly transform the given matrix into a simpler canonical form. The eigenelement computations are then performed on the canonical form. For the EISPACK programs the storage requirements grow as the square of the order of the matrix being processed and the operation counts grow cubically with the order.

A matrix eigenvalue problem is said to be medium scale if it is real symmetric, and if it is computationally feasible to compute the eigenelements by using Sturm sequencing and bisection in combination with inverse iteration directly on the original matrix. For example, a band matrix with a reasonable band width will be said to be of medium scale.

Matrix eigenvalue computations are said to be large scale if the size of the matrix and the pattern of the nonzeros in the matrix preclude the use of EISPACK-type procedures or of a Sturm sequencing/bisection/inverse iteration approach. For example, if the given matrix has order larger than 200 and is not banded, then we would classify the associated eigenvalue computation for that matrix as large scale. In most of our experiments, large scale has meant of order greater than 500.

We focus on large scale, 'symmetric' matrix eigenelement computations. Symmetric is in quotes because we include a procedure for computing singular values and vectors of real rectangular matrices. In addition we also include a procedure for computing eigenelements of nondefective complex symmetric matrices. Such matrices do not possess the desirable properties of real symmetric matrices, and the amount of computation required to process them can be

significantly more than that required in the real symmetric case. We will not address the general nonsymmetric eigenvalue problem.

This is a research monograph intended for engineers, scientists and mathematicians who are interested in computational procedures for large matrix eigenvalue problems. The discussion focuses on one particular subset of one particular family of procedures for large matrix eigenvalue computations. We are interested in Lanczos procedures.

Lanczos procedures derive their name from a famous (fifteen years ago some people may have been inclined to say infamous) 3-term recursion that was originally proposed as a means of transforming a general real symmetric matrix into a real symmetric tridiagonal matrix. Within the scientific community we find two basic approaches to Lanczos procedures. One approach maintains that 'global orthogonality is crucial' and the other approach maintains that 'local orthogonality is sufficient'. This terminology is explained in Chapter 2, Sections 2.4 and 2.5 where we briefly survey the literature on Lanczos procedures for eigenelement computations.

Our emphasis is on computation. We focus primarily on our research on single-vector Lanczos procedures with no reorthogonalization. These procedures belong to the class of 'local orthogonality is sufficient' procedures. The material is organized into two volumes. This volume contains the material necessary for understanding the proposed Lanczos procedures. The second volume contains the FORTRAN codes and documentation for each of the Lanczos procedures discussed in this volume.

Users with large problems are concerned about the amounts of computer storage and time required by the procedures which they have to use. Our single-vector Lanczos procedures are storage efficient. In most cases they are also time efficient if the matrix, whose eigenvalues (singular values) are to be computed, is such that matrix-vector multiplies can be computed rapidly and accurately. Typically if the given matrix is sparse, in the sense that there are only a few nonzero entries in each row and column, then this can be achieved.

Some of what is presented is new and has not yet been published elsewhere. Much of what is presented has appeared at least in preliminary form in papers and reports published in various places. It is hoped that by bringing all of this material together in one place, that these results will prove useful to a wide variety of users in the engineering and scientific community.

Jane K. Cullum
Ralph A. Willoughby
July 1984

INTRODUCTION

We consider the question of the computation of eigenvalues and eigenvectors of large, 'symmetric' matrices. While in a strictly mathematical sense, the scope of this book is very narrow, the potential applications for the material which is included are important and numerous. Perhaps the most familiar application of eigenvalue and eigenvector computations is to structural analysis, studies of the responses of aircraft, of bridges, or of buildings when they are subjected to different types of disturbances such as air turbulence, various types of loadings, or earthquakes. In each case, the physical system being analyzed varies continuously with time, and its true motion is described by one or more differential equations. Matrix eigenvalue problems and approximations to this motion are obtained by discretizing the system equations in some appropriate way.

For a given matrix A, the 'simple' eigenvalue-eigenvector problem is to determine a scalar λ and a vector $x \neq 0$ such that $Ax = \lambda x$. In structural problems, one typically encounters the generalized eigenvalue problem $Kx = \lambda Mx$, involving 2 different matrices, a mass matrix M and a stiffness matrix K. In fact the problems there can be nonlinear quadratic eigenvalue problems, see for example Abo-Hamd and Utku [1978]. However, the 'solution' of a linearization of one of these quadratic problems is often used as a basis for reducing the given nonlinear eigenvalue problem to a much smaller but dense generalized eigenvalue problem. In such a problem a few of the smallest eigenvalues and corresponding eigenvectors may be required or in some cases in order to determine the response of a given structure to external disturbances it may be necessary to compute eigenvalues and corresponding eigenvectors on some interior interval of the spectrum of the given matrix. In structures the matrices used are typically banded, that is all of the nonzero entries are clustered around the main diagonal of the system matrices. For many years simultaneous iteration techniques have been applied successfully to shifted and inverted matrices $(K - \mu M)$, using equation solving techniques designed for band matrices.

Very large matrix eigenvalue problems also arise in studies in quantum physics and chemistry, see for example Kirkpatrick [1972] and Gehring [1975]. The matrices generated are large and sparse. Typically significant numbers of the eigenvalues of these matrices are required. An entirely different kind of application is the use of eigenvectors in heuristic partitioning algorithms, see for example Barnes [1982]. For the particular application which Barnes considered, the placement of electrical circuits on silicon chips, the goal was to position a large number of circuits on a given number of chips in such a way that the resulting number of external connections between circuits on different chips was minimized.

Other applications for eigenvalue/eigenvector computations occur in quantum chemistry, see for example Nesbet [1981]; in power system analysis, see for example Van Ness [1980]; in

oceanography, see for example Winant [1975] and Platzman [1978]; in magnetohydrodynamics, see for example Gerlakh [1978]; in nuclear reactor studies, see for example Geogakis [1977]; in helicopter stability studies, see for example Hodges [1979]; and in geophysics, see for example Kupchinov [1973].

As we said earlier we are considering the question of computing eigenvalues and eigenvectors of large 'symmetric' matrices which arise in various applications. The word symmetric is in quotes because we also present procedures for two types of matrix computations which are not symmetric in the ordinary sense. The basic ideas which we discuss are equally applicable to any matrix problem which is equivalent to a real symmetric eigenvalue/eigenvector problem. We consider several such equivalences. These include Hermitian matrices, certain real symmetric generalized eigenvalue problems, and singular value and singular vector computations for real, rectangular matrices. We also consider complex symmetric matrices which are not equivalent to real symmetric matrices.

The actual scope of this book is limited to a particular family of algorithms for large scale eigenvalue problems, the Lanczos procedures. Other types of eigenelement procedures suitable for large matrices exist, most of which are based upon either simultaneous iterations or upon Rayleigh quotient iterations, see Bathe and Wilson [1976] and Jennings [1977] for complete and very readable discussions of simultaneous iteration procedures. The research on Rayleigh quotient iteration procedures is scattered. Parlett [1980, Chapter 4] discusses the theoretical properties of such procedures and gives references for interested readers. We do not cover any of the non-Lanczos procedures in our discussions.

The research on Lanczos procedures for eigenelement computations (and for solving systems of equations) continues. Although many interesting results have been obtained, many of the theoretical questions concerning Lanczos procedures have not been satisfactorily resolved. Much of the existing literature on Lanczos procedures has not adequately incorporated the effects of roundoff errors due to the inexactness of the computer arithmetic. Numerical experiments with various Lanczos procedures have however clearly demonstrated their advantages and capabilities. Many different people have contributed to this research, and we apologize if we have neglected to mention one or more of these authors in our discussions or if for the authors we do mention we have not referenced all of their papers on this subject.

The demonstrated computational efficiences and excellent convergence properties which can be achieved by Lanczos procedures, have generated much interest in the scientific and engineering communities. Parlett [1980] is primarily devoted to discussions of small to medium size real symmetric eigenvalue problems where other type of eigenelement procedures are applicable. However, Chapter 13 of that book is devoted to Lanczos procedures for large matrices, but that discussion focuses on the 'global orthogonality is crucial' approach to Lanczos procedures and there is not much discussion of the 'local orthogonality is sufficient' approach

which we use in our single-vector Lanczos procedures. Specific comments regarding the differences between these two approaches are given in Sections 2.4 and 2.5 of Chapter 2. We focus primarily on one subset of the Lanczos eigenelement procedures, the single-vector Lanczos procedures which do not use any reorthogonalization. Iterative block Lanczos procedures with limited reorthogonalization are also discussed but to a lesser extent.

This book is divided into two volumes. This volume provides the background material necessary for understanding the Lanczos procedures which we have developed and gives some perspective of the existing research on Lanczos procedures for eigenvalue or singular value computations. The second volume contains FORTRAN programs for each of the Lanczos procedures discussed in this volume. We have tried to make these volumes self-contained by including the material from matrix theory which is necessary for following the arguments given. Both volumes of this book should be accessible to engineers and scientists who have some knowledge of matrix eigenvalue problems. References are given to other books and papers where the interested reader can pursue various topics discussed.

Chapter 0 is intended as a reference chapter for the reader. Basic definitions and concepts from matrix theory which are used throughout the book are listed. Our notation is specified and special types of matrices are defined, along with special types of matrix transformations and projections.

Chapter 1 contains brief summaries of fundamental results from matrix theory which are needed in later chapters. Properties of real symmetric matrices, of Hermitian matrices, and of real symmetric generalized eigenvalue problems are summarized. Sparse matrices are discussed along with sparse matrix factorizations.

Chapter 2 begins with a description of a basic single-vector Lanczos procedure for computing eigenelements of real symmetric matrices. Properties of this procedure are derived, assuming that the computations are being performed in exact arithmetic. However, we are interested in Lanczos procedures which do not use any reorthogonalization and must therefore be concerned with what happens in finite precision arithmetic. In Section 2.3 we summarize the results obtained by Paige [1971,1972,1976,1980], assuming finite precision arithmetic. These results are the basis for the arguments which are given in Chapter 4 to justify our Lanczos procedures with no reorthogonalization. In Section 2.4 we discuss the question of constructing practical Lanczos procedures, that is, procedures which are numerically-stable in finite precision arithmetic. Section 2.5 consists of a survey of the literature on Lanczos procedures.

Chapter 3 contains proofs of several basic properties of general tridiagonal matrices, including determinant recursions and formulas for computing eigenvectors from the determinants of the matrix, along with comments on inverse iteration computations. We need these properties in Chapters 4, 5, and 6.

Chapter 4 is the main chapter of this volume. Here we develop the single-vector Lanczos procedure with no reorthogonalization for real symmetric matrices. Included is a discussion of the relationships between Lanczos tridiagonalization and the conjugate gradient method for solving systems of equations. This relationship is used to construct a plausibility argument for the belief that the 'local orthogonality is sufficient' approach is legitimate. The key to the success of these types of eigenvalue procedures, an identification test which sorts the 'good' eigenvalues from the 'spurious' ones, is developed in Section 4.5. This test is justified heuristically using the connection of the Lanczos recursion with conjugate gradient iterations. Results of numerical experiments are used to demonstrate the performance of this procedure on different types of matrices. FORTRAN code for this procedure is given in Chapter 2 of Volume 2. Chapters 3, 4, and 5 of Volume 2 contain respectively, FORTRAN codes for corresponding Lanczos procedures for Hermitian matrices, for factored inverses of real symmetric matrices, and for certain real symmetric generalized eigenvalue problems.

Chapter 5 addresses the question of constructing a single-vector Lanczos procedure for computing singular values and singular vectors of real rectangular matrices. A general discussion of basic properties of singular values and singular vectors and of the relationships between singular values and eigenvalues is given. Section 5.3 contains a very brief discussion of several applications of singular values and vectors. Section 5.4 centers on our single-vector Lanczos procedure with no reorthogonalization. Results of numerical experiments are included to demonstrate the performance of this procedure. FORTRAN code for this procedure is given in Chapter 6 of Volume 2.

Chapter 6 addresses the question of constructing a single-vector Lanczos procedure for diagonalizable complex symmetric matrices. This class of matrices is genuinely nonsymmetric, possessing none of the desirable properties of real symmetric matrices. Relevant properties of complex symmetric matrices are included. The Lanczos procedure which is proposed maps the given complex symmetric matrix into a family of complex symmetric tridiagonal matrices. FORTRAN code for this procedure is given in Chapter 7 of Volume 2.

Chapter 7 addresses the question of iterative block Lanczos procedures. First a practical implementation of the block Lanczos procedure given in Cullum and Donath [1974] is discussed. We then describe a recently-developed hybrid procedure which combines ideas from the single-vector Lanczos procedures and from the iterative block procedure. FORTRAN code for this hybrid procedure is given in Chapter 8 of Volume 2.

CHAPTER 0
PRELIMINARIES: NOTATION AND DEFINITIONS

In this preliminary chapter we have included a summary of the notation and of the basic mathematical quantities which are used repeatedly throughout this book. Many of these definitions will also be given somewhere else in this book. However they are provided here in a contiguous fashion as an aid to the reader. Additional information on these quantities may be found in basic textbooks on matrix theory, for example Stewart [1973] and Parlett [1980]. No attempt is made to provide complete coverage of the basic notions of matrix theory. Only those concepts which are actually used in the discussions in this book are included.

SECTION 0.1 NOTATION

We are dealing with finite-dimensional matrices and therefore all of the vectors and subspaces which are used are also finite-dimensional.

SCALARS Scalar integers will be denoted by lower case Roman letters such as i, j, k, ℓ, m, and n. Non-integer scalars will be denoted by either lower case Roman letters other than i, j, k, ℓ, m, or n, or by lower case Greek letters such as α, β, ϵ, λ, and σ. The complex conjugate of a complex scalar b will be denoted by $\bar{b}$.

VECTORS Vectors will be denoted by lower case Roman letters such as x and v. If the vector x is a column vector, then x^T denotes the corresponding row vector and x^H denotes the corresponding row vector whose components are complex conjugates of the components of x. We call x^H the complex conjugate transpose of x. For a real vector $x^T = x^H$. The ith component of a vector x will be denoted by x(i).

The real and the Hermitian vector norm will be defined by

$$\|x\|_2 \equiv \left(\sum_{k=1}^{n} |x(k)|^2\right)^{1/2}. \tag{0.1.1}$$

$|x(k)|$ denotes the absolute value of the kth component x(k). If x is a real vector then we have that

$$\|x\|_2^2 \equiv x^T x \equiv x^H x \equiv \sum_{k=1}^{n} [x(k)]^2. \tag{0.1.2}$$

If x is a complex vector then we have that

$$\|x\|_2^2 \equiv x^H x \equiv \sum_{k=1}^{n} \bar{x}(k)x(k) \tag{0.1.3}$$

Thus, we use the same symbol to denote the vector norm for both real and for complex vectors. If x is a complex vector then clearly

$$x^H x \neq x^T x. \tag{0.1.4}$$

The inner product of two real vectors x and y will be defined by $x^T y$. The inner product of two vectors x and y, at least one of which is complex, will be defined by $x^H y$. We note however that in Chapter 6 where we discuss complex symmetric matrices, we will be using the real inner product when x and y are complex vectors. In this case of course it is no longer an inner product since there are complex vectors $x \neq 0$ such that $x^T x = 0$.

We denote an ordered set of vectors $\{x_1,...,x_k\}$ by X_k and denote the span of this set of vectors by $\mathscr{X}^k \equiv sp\{X_k\}$. A vector $y \in \mathscr{X}^k$ if and only if $y = X_k u$ for some vector u. A set of vectors $X_k \equiv \{x_1, ..., x_k\}$ will be said to be an orthogonal set of vectors if and only if $x_j^T x_\ell = 0$ for $j \neq \ell$. We denote Euclidean n-space by E^n, and the corresponding complex n-space by $\mathscr{C}^n$.

MATRICES Matrices are denoted by capital Roman letters such as A, T, and X except for diagonal matrices whose diagonal entries are eigenvalues or singular values. Such diagonal matrices will be denoted by capital Greek letters such as Σ or Λ. Diagonal matrices may also be denoted by $diag\{d_1, ..., d_n\}$.

The notation

$$A = (a_{ij}) \quad \text{where} \quad 1 \leq i \leq m, \; 1 \leq j \leq n \tag{0.1.5}$$

denotes a rectangular matrix with m rows and n columns whose (i,j)-th entry is a_{ij}. The entries a_{ij} may be real-valued or complex-valued. Hermitian and complex symmetric matrices will have one or more entries which are complex. Except in our discussions of singular value/vector computations we will always be talking about square matrices. That is, m = n. In some cases we use A(i,j) to denote the (i,j)-th element in a matrix A. Thus, for any matrix A we have the following notational equivalence.

$$a_{ij} \equiv A(i,j), \quad 1 \leq i \leq m, \; 1 \leq j \leq n. \tag{0.1.6}$$

The determinant of a square matrix A will be denoted by det(A).

The matrix norms corresponding to the vector norms in Eqn(0.1.1) are defined by

$$\|A\|_2 \equiv \max_{u \neq 0} \|Au\|_2 / \|u\|_2. \tag{0.1.7}$$

We note that if the vector u is real then $\|u\|_2$ denotes $u^T u$, and if u is complex, it denotes $u^H u$. For any A we have that $\|A\|_2 = \sigma_1(A)$ where $\sigma_1(A)$ denotes the largest singular value of A.

The transpose of an mxn matrix A is denoted by A^T. If $A \equiv (a_{ij})$ then the transpose is the nxm matrix

$$A^T \equiv (a_{ji}) \tag{0.1.8}$$

obtained from A by interchanging the rows and the columns of A. The Hermitian transpose of an mxn matrix A is denoted by A^H and is defined by

$$A^H \equiv (\bar{a}_{ji}) \tag{0.1.9}$$

where the bar denotes the complex conjugate of a_{ji}. We denote the nxn identity matrix by I_n.

APPROXIMATIONS Given a function f(z) where z is a vector and f(z) may be a scalar or a vector-valued function, we use the notation $f(z) = O(\varepsilon^q)$ to mean that there exists a constant C such that $\|f(z)\|_2 \leq C\varepsilon^q$. If f is a scalar-valued function the norm reduces to the absolute value of f. Similarly, we use the notation $f(z) = o(\varepsilon^q)$ to mean that there exists a $\delta>0$ such that $f(z) = O(\varepsilon^{q+\delta})$.

SECTION 0.2 SPECIAL TYPES OF MATRICES

Throughout the discussions in this book we refer repeatedly to several different types of matrices. In this section definitions of each of these types of matrices are provided.

SPARSE MATRIX An mxn matrix A will be said to be a sparse matrix if and only if each row of the matrix contains at most a few entries which are not zero. Typically in the applications, the matrices are very large, several hundred to several thousand or more in size, and sparse.

REAL SYMMETRIC MATRIX An nxn matrix A is real symmetric if and only if A is real and it is equal to its transpose. That is, $A^T = A$.

COMPLEX SYMMETRIC MATRIX An nxn matrix A is complex symmetric if and only if A is complex and symmetric. That is, $A^T = A$ and at least one of the entries in A is complex-valued. The main topic of discussion in this book is real 'symmetric' problems. However, Chapter 6 of Volume 1 and Chapter 7 of Volume 2 deal with complex symmetric matrices and single-vector Lanczos procedures with no reorthogonalization for such matrices. The spectral properties of real symmetric matrices and those of complex symmetric matrices bear little resemblance to each other as we will see in Chapter 6 of this volume.

HERMITIAN MATRICES An nxn complex matrix A is Hermitian if and only if $A^H = A$. That is, for each $1 \leq i,j \leq n$, $a_{ij} = \bar{a}_{ji}$. Therefore, the diagonal entries of any Hermitian matrix must be real. Hermitian matrices possess essentially the same spectral properties as real symmetric matrices. More will be said about this in Section 1.5 of Chapter 1.

TRIDIAGONAL MATRICES A nxn matrix $T \equiv (t_{ij})$ is tridiagonal if and only if

$$t_{ij} \equiv 0 \text{ for all } 1 \le i,j \le n \text{ and } |i - j| > 1. \tag{0.2.1}$$

That is, only the main diagonal, the first superdiagonal and the first subdiagonal may contain nonzero entries. The single-vector Lanczos procedures which we discuss will replace the given matrix problem by 'equivalent' tridiagonal problems. If T is an mxm symmetric tridiagonal matrix we denote its nonzero entries as follows. Define $\beta_1 \equiv 0$. Then define

$$\begin{aligned} &\alpha_k \equiv T(k,k), \text{ for } 1 \le k \le m \text{ and} \\ &\beta_{k+1} \equiv T(k+1,k) \equiv T(k,k+1) \text{ for } 1 \le k \le m-1 \end{aligned} \tag{0.2.2}$$

UNITARY MATRICES A nxn matrix W is a unitary matrix if and only if W is complex and the Hermitian transpose of W is the inverse of W. That is,

$$W \text{ is complex and } W^H W = I_n. \tag{0.2.3}$$

If we write a unitary matrix W as $W = (w_1, w_2, \ldots, w_n)$ where w_j is the jth column of W, then we have the following orthogonality relationships. For $1 \le j,k \le n$,

$$w_j^H w_k = \delta_{jk} \text{ where } \delta_{jk} = 0 \text{ if } j \ne k \text{ and } \delta_{jj} = 1. \tag{0.2.4}$$

We call δ_{jk} the Kronecker delta. Typically whenever we discuss orthogonal sets of vectors we will use the Kronecker delta notation.

ORTHOGONAL MATRIX A nxn matrix Q is an orthogonal matrix if and only if Q is real and the transpose of Q is its inverse. That is,

$$Q \text{ is real and } Q^T Q = I_n. \tag{0.2.5}$$

REAL ORTHOGONAL MATRIX A nxn matrix Q is a real orthogonal matrix if and only if Q is a complex matrix and its transpose is its inverse. That is,

$$Q \text{ is complex and } Q^T Q = I. \tag{0.2.6}$$

The class of real orthogonal matrices plays a fundamental role in the construction of our Lanczos procedures for complex symmetric matrices. These procedures (see Chapter 6) generate complex symmetric tridiagonal matrices. Real orthogonal transformations are used to obtain a storage efficient procedure for computing the eigenvalues of these complex symmetric tridiagonal matrices.

PERMUTATION MATRIX A nxn matrix P is a permutation matrix if and only if each column of P is some column of the identity matrix I_n, and every column of I_n appears as some column

of P. Specifically, there exists a permutation p(i) of the integers i=1,2,...,n such that for each i

$$Pe_i = e_{p(i)}, \tag{0.2.7}$$

where e_i is the ith column of I_n and {p(1),p(2),..,p(n)} is a permutation of the numbers {1,2,...,n}.

Permutation matrices will be useful in our discussions of generalized eigenvalue problems. Generalized eigenvalue problems involve two matrices. Our Lanczos procedures will require the factorization of one of the two matrices involved. In many cases the sparsity of a given matrix can be preserved in its factorization if the matrix is permuted prior to its factorization. Permutation matrices have the property that

$$P^T \equiv P^{-1}. \tag{0.2.8}$$

Therefore, the eigenvalues of a given matrix are preserved under the mapping of A into P^TAP. The eigenvectors of the permuted matrix are simply permutations of the eigenvectors of A.

UPPER HESSENBERG MATRICES A nxn matrix H is an upper Hessenberg matrix if and only if all of its entries below the main subdiagonal are zero. That is, if $H \equiv (h_{ij})$ then

$$h_{ij} \equiv 0, \quad \text{for} \quad i > j + 1 \quad \text{and} \quad 1 \le i, j \le n. \tag{0.2.9}$$

In our discussions we will not have any direct need for Hessenberg matrices because even in the complex symmetric case the Lanczos matrices which we generate will be tridiagonal. In this latter situation however the EISPACK Library [1976,1977] uses Hessenberg matrices, and we will be referring to this fact in our discussions.

UPPER AND LOWER TRIANGULAR MATRICES An nxn matrix A is upper triangular if and only if all the nonzero entries of A are on or above the main diagonal of A. An nxn matrix A is lower triangular if and only if all the nonzero entries of A are on or below the main diagonal of A. We will encounter such matrices when we are discussing factorizations of matrices. An upper or lower triangular matrix is unit upper or unit lower triangular if and only if all of the diagonal entries are 1.

DIAGONAL MATRIX A nxn matrix D is diagonal if and only if all of the nonzero entries of D are on the main diagonal of D. That is, if

$$D \equiv (d_{ij}), \text{ then for all } 1 \le i \ne j \le n, \quad d_{ij} \equiv 0. \tag{0.2.10}$$

We may denote a diagonal matrix D by $D = \text{diag}\{d_1,d_2,...,d_n\}$ where d_k is used here to denote the d_{kk} entry of D. This may be somewhat confusing because we also may use the notation $A = (a_1,...,a_n)$ to denote a matrix A. Typically however, the diagonal matrices used in our discussions will be matrices whose entries are either eigenvalues or singular values. In these cases we use lower case Greek letters to denote the nonzero entries in the matrix which itself

would be denoted by a capital Greek letter, and no confusion should result. For example the diagonal matrix could be denoted by Λ and its nonzero entries by λ_k. Thus, $\Lambda = \text{diag}\{\lambda_1,...,\lambda_n\}$.

SKEW SYMMETRIC MATRIX An nxn matrix $A \equiv (a_{ij})$ is skew symmetric if and only if A is real and $A^T = -A$. That is,

$$\text{for } 1 \le i,j \le n, \quad a_{ij} = -a_{ji}. \tag{0.2.11}$$

In particular, the diagonal entries of any skew symmetric matrix must all be zero, and any skew symmetric matrix of odd order must be singular. The nonzero eigenvalues of a skew symmetric matrix are pure imaginary pairs, i.e. of the form $\pm ir$ where r is real and positive. Therefore the related matrix iA has all real roots; in fact it is a Hermitian matrix.

ADJOINT OF A MATRIX If A is a nxn matrix then its adjoint Adj(A) is defined by the following relationships.

$$\text{Adj}(A)A = A\text{Adj}(A) \equiv \det(A)I_n. \tag{0.2.12}$$

If A is nonsingular so that $\det(A) \neq 0$, then $A^{-1} \equiv \text{Adj}(A)/\det(A)$. If the matrix A is real symmetric and has rank (n-1) and u is a n-vector such that $u \neq 0$ but $Au = 0$, then $\text{Adj}(A) = \gamma uu^T$ for some scalar multiple γ. In particular if λ is an eigenvalue of A and the matrix $(A - \lambda I)$ has rank (n-1), then the corresponding eigenvector x of A is in the null space of this matrix. Thus, we have that

$$\text{Adj}(A - \lambda I) = \gamma xx^T. \tag{0.2.13}$$

We will need this property in Chapter 3 in our discussions of tridiagonal matrices. It will prove to be very valuable in some of our arguments justifying our approach to single-vector Lanczos procedures with no reorthogonalization.

PRINCIPAL SUBMATRIX OF A MATRIX Given a nxn matrix A, a kxk matrix B is a principal submatrix of A of order k if and only if B is the submatrix which consists of all of the elements of A which are simultaneously in both the rows and the columns $i_1 < i_2 < \ldots < i_k$ of A.

LEADING PRINCIPAL SUBMATRIX OF A MATRIX Given a nxn matrix A, a kxk matrix B is the leading principal submatrix of A of order k if and only if B is the submatrix which consists of all of those elements of A which are simultaneously in both the first k rows and the first k columns of A. Leading principal submatrices are central to the Sturm sequencing computations used to compute eigenvalues of real symmetric tridiagonal matrices.

SECTION 0.3 SPECTRAL QUANTITIES

In this section we summarize the basic definitions needed in discussing eigenvalue and eigenvector problems for matrices, as well as those needed for the discussions of singular value and vector problems given in Chapter 5 of Volume 1 and Chapter 6 of Volume 2.

EIGENVALUES AND EIGENVECTORS Given any nxn matrix A, a scalar λ and nonzero vector x are called an eigenvalue and corresponding right eigenvector of A if

$$Ax = \lambda x. \tag{0.3.1}$$

Similarly, a nonzero vector y is called a left eigenvector associated with the eigenvalue λ if

$$A^T y = \lambda y. \tag{0.3.2}$$

Any nxn matrix has n eigenvalues, they may not all be distinct. However, a matrix need not have a full set of right and left eigenvectors. If A is a real symmetric matrix, then its left and right eigenvectors are identical and A has a full complement of eigenvectors. In fact for any real symmetric matrix there is an orthonormal set of eigenvectors which is a basis for the entire space E^n.

Given any two nxn matrices A and B we can define the generalized eigenvalue problem as follows. Determine scalars λ and nonzero vectors x such that

$$Ax \equiv \lambda Bx. \tag{0.3.3}$$

Such problems are considered briefly in Chapter 1 and Chapter 4 but only for the case when A and B are both real symmetric matrices and either A or B is a positive definite matrix. Volume 2 Chapter 5 contains a single-vector Lanczos procedure for such problems which is applicable whenever the Cholesky factorization $B = LL^T$ is available.

SPECTRUM OF A MATRIX The set of eigenvalues of any given nxn matrix A is called the spectrum of A. If a matrix has all real eigenvalues, then the extreme eigenvalues of A are defined as those eigenvalues which are the algebraically-largest or the algebraically-smallest. Typically for such a matrix we write the eigenvalues as

$$\{\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n\} \tag{0.3.4}$$

with the algebraically-largest eigenvalues assigned low indices and the algebraically-smallest eigenvalues assigned the highest indices.

POSITIVE DEFINITE MATRICES An nxn real symmetric or Hermitian matrix A is said to be positive definite if and only if all of its eigenvalues are positive. If all of its eigenvalues are nonnegative then it is said to be positive semidefinite. There are analogous definitions for negative definite and negative semidefinite matrices. Matrices which are not definite or semidefinite are called indefinite.

NONDEFECTIVE MATRIX An nxn matrix A is said to be a nondefective matrix if and only if it is diagonalizable. That is there exists a nonsingular matrix X and a diagonal matrix $\Lambda = \text{diag}\{\lambda_1,\lambda_2,..,\lambda_n\}$ such that

$$A \equiv X\Lambda X^{-1}. \tag{0.3.5}$$

If this is the case then clearly $AX = X\Lambda$ and $A^TX^{-T} = X^{-T}\Lambda$. Therefore, the columns of X must be right eigenvectors of A, the columns of X^{-T} must be left eigenvectors of A, and the λ_i are the eigenvalues of A. Any real symmetric, Hermitian, or skew symmetric matrix is nondefective. Furthermore, any nxn matrix with n distinct eigenvalues is nondefective (diagonalizable).

SPECTRAL DECOMPOSITION OF A MATRIX If A is a nxn nondefective matrix then from Eqn(0.3.5) we have the following decomposition of A into a sum of rank 1 matrices.

$$A \equiv \sum_{k=1}^{n} \lambda_k x_k y_k^T \text{ where } Y^T = X^{-1}. \tag{0.3.6}$$

If the matrix A is real symmetric, then X can be taken to be an orthogonal matrix and $A = X\Lambda X^T$. If the matrix A is Hermitian, then X can be taken to be a unitary matrix and $A = X\Lambda X^H$.

RAYLEIGH QUOTIENTS Let A be a nxn real symmetric (Hermitian) matrix with eigenvalues $\{\lambda_1, ..., \lambda_n\}$ and let $X \equiv \{x_1, ..., x_n\}$ be a corresponding orthonormal (unitary) basis of eigenvectors. For a real symmetric matrix A and any nonzero vector x we define the Rayleigh quotient $\rho(x,A)$ of A and x as follows.

$$\rho(x,A) \equiv (x^TAx)/(x^Tx). \tag{0.3.7}$$

If A is Hermitian we replace the real inner products in Eqn(0.3.7) by the corresponding complex inner product. We may use $\rho(x)$ to denote the Rayleigh quotient when it is clear from the context which matrix A is being used. For any nonzero vector x we have that

$$\lambda_n(A) \le \rho(x,A) \le \lambda_1(A). \tag{0.3.8}$$

For any eigenvalue-eigenvector pair (λ_j,x_j), $\rho(x_j) = \lambda_j$.

The eigenvalues of a given real symmetric or Hermitian matrix A have the following minmax characterization as the minimums of the maximums of Rayleigh quotients over certain size subspaces. In Eqn(0.3.9) $z \neq 0$ and $1 \le j \le n$.

$$\lambda_{n-j+1} = \min_{\mathcal{X}^j} \max_{z \in \mathcal{X}^j} \rho(z) \tag{0.3.9}$$

where $\mathcal{X}^j$ denotes an arbitrary j-dimensional subspace. There is an analogous characterization using the max-min and subspaces $\mathcal{X}^{(n-j+1)}$. See for example, Stewart [Chapter 6, 1973] for a proof of this well-known result.

If for some vector y and some eigenvector x_j corresponding to an eigenvalue λ_j we have that

$$y = x_j + O(\epsilon) \text{ then } \rho(y) = \lambda_j + O(\epsilon^2). \tag{0.3.10}$$

Eqn(0.3.10) states that if we have an eigenvector approximation y of order ϵ, then the corresponding Rayleigh quotient is an approximation to the corresponding eigenvalue of order ϵ^2. This property has been used to justify Rayleigh-Ritz methods for computing eigenvalues and eigenvectors of real symmetric or Hermitian matrices. Such methods are iterative and on each iteration include the computation of an approximate eigenvector (typically obtained using some form of inverse iteration with the current eigenvalue approximation) followed by the subsequent computation of the corresponding Rayleigh quotient which then becomes the updated approximation to the eigenvalue. The single-vector Lanczos procedures which we describe in Chapters 4, 5 and 6 are not Rayleigh-Ritz type algorithms. However, the iterative block Lanczos procedures which we describe in Chapter 7 can be interpreted as block analogs of Rayleigh-Ritz procedures.

INVERSE ITERATION Let A be a nxn matrix. Given any scalar λ which is a good approximation to a simple eigenvalue of A, the method of inverse iteration provides a mechanism for computing an approximation to the corresponding eigenvector of A. For any such λ and any given random n-vector w, the following ill-conditioned set of equations is solved for z.

$$(A - \lambda I)z = w. \tag{0.3.11}$$

The starting vector w is scaled so that $\sum_{k=1}^{n} |w(k)| = \gamma\epsilon_{mach}$ where ϵ_{mach} is the machine epsilon for the computer being used and γ is a scaling obtained from A. (The machine espilon is the smallest positive number such that $1.0 + \epsilon_{mach} \neq 1.0$). If the computed vector z satisfies the condition $\sum_{k=1}^{n} |z(k)| \geq 1$, then z is accepted as an approximate eigenvector associated with λ and the approximate eigenvector $y \equiv z/\|z\|_2$. Otherwise z replaces w in Eqn(0.3.11), normalized as before, and another step of inverse iteration is performed. Only a small number of iterations is allowed. Typically one iteration is sufficient.

INVARIANT SUBSPACES Let $\mathscr{X}^k \equiv sp\{X_k\}$, then $\mathscr{X}^k$ is an invariant subspace of a given matrix A if and only if for any $x \in \mathscr{X}^k$ and the corresponding $y = Ax$, we have that $y \in \mathscr{X}^k$. For any set of eigenvectors $X_k \equiv \{x_1, ..., x_k\}$ of a matrix A the corresponding subspace $\mathscr{X}^k$ is an invariant subspace of A.

SINGULAR VALUES OF MATRICES Let A be a real ℓxn matrix with $\ell \geq n$. A scalar σ and two nonzero vectors x and y are respectively a singular value, a right singular vector and a left singular vector of A if and only if

$$Ax = \sigma y, \text{ and } A^T y = \sigma x. \tag{0.3.12}$$

If A is complex then A^T has to be replaced by A^H in Eqn(0.3.12). Typically we label the singular values as follows $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n$, and denote corresponding right and left singular vectors by $X \equiv \{x_1, \ldots, x_n\}$ and $Y \equiv \{y_1, \ldots, y_\ell\}$.

We have the following singular value decomposition for any ℓxn matrix. There exists an ℓxℓ unitary matrix Y of left eigenvectors and a nxn unitary matrix X of right eigenvectors such that

$$A \equiv Y\Sigma X^H \text{ where } \Sigma = \begin{bmatrix} \Sigma_1 \\ 0 \end{bmatrix} \tag{0.3.13}$$

with $\Sigma_1 = \text{diag}\{\sigma_1, \ldots, \sigma_n\}$. When A is a real matrix X and Y are orthogonal matrices. This is the generalization of the spectral decomposition for diagonalizable matrices given in Eqn(0.3.5) to an arbitrary matrix. Observe that $\|A\|_2 \equiv \sigma_1(A)$.

ILL-CONDITIONED MATRIX An nxn nonsingular matrix A is said to be ill-conditioned if small changes in a vector b cause relatively large changes in the solution x of the corresponding system of equations Ax = b. One commonly-used measure of ill-conditioning is the ratio of the largest to the smallest singular value of A, $\sigma_1(A)/\sigma_n(A)$. This measure applies equally well to a mxn rectangular matrix where this ratio uses the smallest nonzero singular value.

SECTION 0.4 TYPES OF MATRIX TRANSFORMATIONS

In this section we briefly describe each type of matrix transformation which will be used somewhere in this book.

UNITARY TRANSFORMATION Given a nxn matrix A and a nxn unitary matrix U, the matrix

$$A' \equiv U^H A U \tag{0.4.1}$$

obtained from A is called a unitary transformation of A. Unitary transformations preserve the norms of the vectors they are transforming. This property is very desirable numerically because it controls the sizes of the quantities encountered. Many of the eigenelement procedures in the EISPACK Library [1976,1977] are primarily sequences of unitary or orthogonal transformations.

ORTHOGONAL TRANSFORMATION Given a nxn matrix A and a nxn orthogonal matrix W, the matrix

$$A' \equiv W^T A W \tag{0.4.2}$$

obtained from A is called an orthogonal transformation of A. Unitary and orthogonal transformations preserve eigenvalues and singular values. In either case the resulting transformed

matrix A' has the same eigenvalues and singular values as the original matrix. This is important for both numerical and theoretical considerations.

SIMILARITY TRANSFORMATION Given a nxn matrix A and a nxn nonsingular matrix S, the matrix

$$A' \equiv S^{-1}AS \tag{0.4.3}$$

obtained from A is called a similarity transformation of A. Similarity transformations preserve the eigenvalues of the given matrix. Furthermore, we have that for any eigenvalue and eigenvector pair (λ,x) of A that $(\lambda, S^{-1}x)$ is an eigenvalue and eigenvector pair of A'.

ROW PERMUTATION Given a nxn matrix A and a nxn permutation matrix P, the matrix

$$A' \equiv PA \tag{0.4.4}$$

obtained from A is called a row permutation of A. That is, the rows of A' are simply a permutation of the rows of A. Specifically, P defines some permutation p(i) of the integers $1 \le i \le n$, and the ith row of A' is simply the p(i)-th row of A.

COLUMN PERMUTATION Given a nxn matrix A and a nxn permutation matrix P, the matrix

$$A' \equiv AP \tag{0.4.5}$$

obtained from A is called a column permutation of A. That is, the columns of A' are simply a permutation of the columns of A. Specifically, P defines some permutation p(i) of the integers $1 \le i \le n$ and the ith column of A' is simply the p(i)-th column of A.

PLANE ROTATION Let A be a nxn real symmetric matrix. Select real scalars c and s such that $c^2 + s^2 = 1$. Select integers k and ℓ such that $1 \le k < \ell \le n$. Define the associated plane rotation matrix $R \equiv (r_{ij})$ as follows.

$$\begin{aligned} r_{kk} &\equiv r_{\ell\ell} \equiv c, \\ r_{\ell k} &\equiv -r_{k\ell} \equiv s, \\ r_{ij} &\equiv \delta_{ij}, \quad \text{for } i, j \neq k, \ell. \end{aligned} \tag{0.4.6}$$

The matrix

$$A' = R^T AR, \tag{0.4.7}$$

is called a plane rotation of the matrix A. Observe that only rows and columns k and ℓ of A

are modified. Specifically we have that

$$\begin{aligned} a'_{ik} &= a'_{ki} = ca_{ki} + sa_{\ell i} \\ a'_{i\ell} &= a'_{\ell i} = ca_{\ell i} - sa_{ki} \\ a'_{kk} &= a_{kk} + sb, \quad a'_{\ell\ell} = a_{\ell\ell} - sb \\ a'_{k\ell} &= a'_{\ell k} = -a_{k\ell} + cb \\ \text{where } b &= 2ca_{k\ell} + s(a_{\ell\ell} - a_{kk}). \end{aligned} \tag{0.4.8}$$

Any plane rotation matrix R is real symmetric and orthogonal. In Chapter 6 in our discussion of Lanczos methods for complex symmetric matrices we find it necessary to use a complex generalization of these real plane rotation matrices. There we consider 'rotation' matrices defined by the following equations.

$$\begin{aligned} r_{\ell\ell} &\equiv -r_{kk} \equiv c, \\ r_{\ell k} &\equiv r_{k\ell} \equiv s, \\ r_{ij} &\equiv \delta_{ij}, \quad \text{for } i, j \neq k, \ell. \end{aligned} \tag{0.4.9}$$

where the scalars c and s are complex-valued. These matrices are complex symmetric and real orthogonal. See Chapter 6 for more details.

TRIANGULAR FACTORIZATION Given a nxn matrix A we define the triangular factorization A = LU of A where L is a lower triangular matrix and U is a unit upper triangular matrix. The entries in L and U are defined by the following recursions. For each k=1,2,...,n compute

$$\begin{aligned} \ell_{ik} &\equiv a_{ik} - \sum_{j=1}^{k-1} \ell_{ij} u_{jk}, \quad \text{for } k \le i \le n \\ u_{ki} &\equiv (a_{ki} - \sum_{j=1}^{k-1} \ell_{kj} u_{ji}) / \ell_{kk}, \quad \text{for } k+1 \le i \le n. \end{aligned} \tag{0.4.10}$$

There are matrices for which this factorization is not well-defined. However, if we assume that all of the leading principal submatrices of A are nonsingular, then this triangularization is well-defined. If for each k = 1,...,n we denote the kxk leading principal submatrix of A, L, and U by respectively, A_k, L_k, and U_k, then we have that for each k, $A_k = L_k U_k$. That is, the factors of the leading principal submatrices of A are obtained from the leading principal submatrices of the factors of A. An alternative form for the factorization is $A = \bar{L}DU$ where $\bar{L}$ is a unit lower triangular matrix. This form can be obtained by replacing ℓ_{ik} in Eqn(0.4.10) by ℓ_{ik}/ℓ_{kk} and defining $D \equiv \text{diag}\{\ell_{11}, \ldots, \ell_{nn}\}$. If A is a symmetric matrix then $U = \bar{L}^T$.

CHOLESKY FACTORIZATION For any positive definite symmetric matrix A the triangular factorization of A is called the Cholesky factorization. In this case the formulas in Eqn(0.4.10)

reduce to the following. For each $k=1,2,\ldots,n$ compute

$$\ell_{kk} \equiv (a_{kk} - \sum_{j=1}^{k-1} \ell_{kj}^2)^{1/2} > 0 \quad \text{and}$$
$$\ell_{ik} \equiv (a_{ik} - \sum_{j=1}^{k-1} \ell_{ij}\ell_{kj}) / \ell_{kk}, \quad \text{for} \quad k<i\leq n. \tag{0.4.11}$$

The associated factorization is $A = LL^T$ where $L \equiv (\ell_{ik})$ defined in Eqn(0.4.11).

HOUSEHOLDER TRANSFORMATION Let u be a n-vector such that $u^H u = 1$. Then

$$Q \equiv I - 2uu^H \tag{0.4.12}$$

is called a Householder transformation matrix. Q is a Hermitian unitary matrix. That is, $Q^H = Q^{-1} = Q$. If u is a real vector then u^T is used and Q is real symmetric and orthogonal. For any such Q, the corresponding matrix $A' \equiv QAQ$ has the same eigenvalues as A. Given any complex nxn matrix A, a sequence of n Householder transformations can be used to reduce A to upper Hessenberg form. If the matrix A is Hermitian or real symmetric, then the resulting matrix can be made to be real symmetric and tridiagonal. Householder transformations are used in many of the EISPACK Library programs [1976,1977].

GRAM-SCHMIDT ORTHOGONALIZATION Let $Z \equiv \{z_1, z_2, \ldots, z_n\}$ be a set of linearly independent mx1 real vectors. The Gram-Schmidt orthogonalization procedure generates a corresponding orthogonal set of vectors $Q = \{q_1, q_2, \ldots, q_n\}$ such that

$$sp\{Q\} \equiv sp\{Z\}, \tag{0.4.13}$$

and $Z = QR$ where $R \equiv (r_{ij})$ is a unit upper triangular matrix. The vectors q_k and the matrix R are defined recursively by the following equations. Define $q_1 \equiv z_1$. Then for each $k=2,\ldots,n$ define

$$q_k = z_k - \sum_{i=1}^{k-1} r_{ki} q_i, \quad \text{where}$$
$$r_{ki} \equiv z_k^T q_i / d_i, \quad \text{and} \quad d_i \equiv q_i^T q_i. \tag{0.4.14}$$

Observe that $Q^T Q = D \equiv \text{diag}\{d_1, \ldots, d_n\}$. The error propagation which occurs when Eqns(0.4.14) are implemented on a computer is such that they are seldom used in practice. See for example Bjorck [1967] for a discussion of this problem. Typically the modified form of the Gram-Schmidt orthogonalization which is defined in the next paragraph is used.

MODIFIED GRAM-SCHMIDT The following modification of the basic Gram-Schmidt procedure yields an orthogonalization procedure with better numerical stability than the Gram-Schmidt procedure as defined in Eqns(0.4.14). Let $Z = \{z_1, \ldots, z_n\}$ be a set of linearly independent mx1 real vectors. The modified Gram-Schmidt orthogonalization procedure generates a corresponding orthogonal set of vectors $Q = \{q_1, q_2, \ldots, q_n\}$ such that

$sp\{Q\} \equiv sp\{Z\}$. using the following recursions. The vectors q_k and the matrix R are defined recursively by the following equations.

$$\begin{aligned} &\text{For each k define } q_k = z_k^{(k)} \text{ where} \\ &z_j^{(k+1)} \equiv z_j^{(k)} - r_{kj}q_k, \text{ for } j>k. \\ &r_{kj} \equiv q_k^T z_j^{(k)}/d_k \text{ and } d_k \equiv q_k^T q_k. \end{aligned} \tag{0.4.15}$$

Column interchanges (pivoting) can be used in the orthogonalization process. In particular at any stage in the process the vector in the remaining subset of vectors which has maximal norm can be normalized. That is at stage k, choose vector $z_s^{(k)}$ such that

$$\|z_s^{(k)}\|_2 = \max_{k\le j\le n} \|z_j^{(k)}\|_2. \tag{0.4.16}$$

SECTION 0.5 SUBSPACES, PROJECTIONS, AND RITZ VECTORS

The terms Lanczos recursion, Krylov subspaces, projections of matrices, and Ritz vectors and values are used repeatedly throughout this book. In this section we give basic definitions for each of these concepts.

KRYLOV SUBSPACES Given a nxn matrix A and a vector v_1 we define the family of Krylov subspaces $\mathscr{K}^k$, k = 1,2,...,n, as follows.

$$\mathscr{K}^k \equiv sp\{v_1, Av_1, A^2v_1, ..., A^{k-1}v_1\}. \tag{0.5.1}$$

As we will see in Chapter 2, theoretically for any given real symmetric matrix A, the real symmetric Lanczos recursion defined below in Eqn(0.5.3) generates orthonormal bases for the Krylov subspaces corresponding to the starting vector v_1 used in the Lanczos recursion. (In practical implementations of this recursion this will not be true. We discuss the numerical problems in Section 2.3 in Chapter 2.)

ORTHOGONAL PROJECTIONS OF MATRICES Let A be a real nxn matrix. Let V be a nxm matrix whose columns are orthonormal. Then the matrix

$$B \equiv V^T AV \tag{0.5.2}$$

is an orthogonal projection of A onto the space spanned by the columns of V. Theoretically, for a given real symmetric matrix A the Lanczos recursion in Eqn(0.5.3) generates tridiagonal matrices which are the orthogonal projections of A onto the corresponding subspaces $sp\{V_m\}$, spanned by the Lanczos vectors generated. These subspaces are in fact Krylov subspaces. In particular $sp\{V_m\} = \mathscr{K}^m(v_1,A)$. See Eqns(0.5.3) below.

BASIC LANCZOS RECURSION Let A be a nxn real symmetric matrix. Let v_1 be a starting vector. Define Lanczos vectors v_j, j = 2,...,m and Lanczos matrices T_m for m = 1,2,...,M as follows. Define $\beta_1 \equiv 0$, and $v_0 \equiv 0$. Then for k=1,2,...,M

$$\begin{aligned} \beta_{k+1}v_{k+1} &= Av_k - \alpha_k v_k - \beta_k v_{k-1}, \\ \alpha_k &= v_k^T A v_k \text{ and } \beta_{k+1} = v_{k+1}^T A v_k \end{aligned} \tag{0.5.3}$$

Let $V_m \equiv (v_1, v_2, \ldots v_m)$ be the matrices of Lanczos vectors generated. Then in matrix form Eqn(0.5.3) becomes

$$AV_m = V_m T_m + \beta_{m+1} v_{m+1} e_m^T \tag{0.5.4}$$

where T_m is the real symmetric, tridiagonal Lanczos matrix of order m generated. We have that

$$\begin{aligned} &T_m(k,k) \equiv \alpha_k, \text{ for } 1 \le k \le m \\ &T_m(k,k+1) \equiv T_m(k+1,k) \equiv \beta_{k+1} \text{ for } 1 \le k \le m-1. \end{aligned}$$

LANCZOS/RITZ VECTORS Let A be a nxn real symmetric matrix. Refer to Eqns(0.5.3) for the definition of the basic single-vector Lanczos recursion. If the basic Lanczos recursion for k=1,...,m or a variant of it is used to generate a Lanczos tridiagonal matrix T_m, then for any eigenvalue-eigenvector pair (μ,u) of T_m we define a corresponding Ritz vector

$$y \equiv V_m u. \tag{0.5.5}$$

Eigenvalues of any Lanczos matrix will be called Ritz values for the corresponding matrix A and the vectors obtained as in Eqn(0.5.5) from the corresponding eigenvectors of the Lanczos matrix will be called Ritz vectors for A. It is important to note that for the single-vector Lanczos procedures presented in Chapter 4 it will not be the case that every eigenvalue-eigenvector pair of every Lanczos matrix generated yields a Ritz value and Ritz vector which are approximations to eigenvalues and eigenvectors of A. We will see that in general it is only appropriate to use certain subsets of the eigenvalues of the Lanczos matrices as approximations to eigenvalues of A. Please see Chapter 4 for detailed comments.

SECTION 0.6 MISCELLANEOUS DEFINITIONS

In this section we include a definition which does not fit naturally into the earlier sections.

CHEBYSHEV POLYNOMIALS Error estimates for various Lanczos procedures can be obtained (at least in the case when we assume that we are using infinite precision arithmetic) by using the special properties of the Krylov subspaces generated by the Lanczos recursions. These estimates utilize the Chebyshev polynomials, $\mathcal{T}_k$, k = 1, ..., m. These polynomials are defined as follows. For any k>0,

$$\begin{aligned} &\mathcal{T}_k(x) \equiv \cos(k \arccos x), \text{ for } |x| \le 1, \\ &\mathcal{T}_k(x) \equiv \cosh(k \operatorname{arccosh} x) \text{ for } |x| \ge 1. \end{aligned} \tag{0.6.1}$$

Chebyshev polynomials satisfy the following recursion. (This is actually a trigonometric identity.)

$$\mathcal{T}_{k+1}(x) = 2x\mathcal{T}_k(x) - \mathcal{T}_{k-1}(x). \tag{0.6.2}$$

These polynomials have the special property that if we define the corresponding polynomials $p_k(x) \equiv \mathcal{T}_k(x)/2^{k-1}$, then $p_k(x)$ is the monic polynomial of degree k with the smallest maximum absolute value over the interval $[-1,1]$. This maximum is simply $1/2^{k-1}$. The error estimates obtained using these polynomials are so-called 'worst' case estimates. That is, they provide estimates of the maximum error which can occur and do not necessarily give indications of the average error incurred. For more details about Chebyshev polynomials, see for example, Hamming [Chapter 28, 1973] and Parlett [Appendix B, 1980].

CHAPTER 1
REAL 'SYMMETRIC' PROBLEMS

SECTION 1.1 REAL SYMMETRIC MATRICES

This book focuses on the solution of real symmetric eigenvalue problems. This includes not only real symmetric matrices but also includes other classes of problems which are equivalent to eigenvalue problems for real symmetric matrices. One primary example of such an equivalence is the computation of singular values and vectors of real rectangular matrices. Lanczos [1961] suggested a simple mechanism for obtaining a real symmetric eigenvalue problem from any real rectangular singular value problem, and we take advantage of this mechanism to obtain a single-vector Lanczos procedure for computing singular values and vectors of such matrices. This is discussed in Chapter 5. Hermitian matrices provide another example. As the reader will see in Chapter 4, it is possible to define a Lanczos procedure which reduces the required Hermitian computations to computations on real symmetric tridiagonal matrices.

A is a real symmetric nxn matrix if and only if it is real and symmetric. That is $A^T = A$. This class of matrices is the most well-behaved and thus the 'easiest' to handle numerically. All of the eigenvalues of a real symmetric matrix are real and all of the eigenvectors are real. We denote the eigenvalues of A by $\{\lambda_1 \geq \lambda_1 \geq \ldots \geq \lambda_n\}$ and denote any corresponding set of eigenvectors by $X = \{x_1, x_2, \ldots, x_n\}$. For any real symmetric (or Hermitian) matrix $\|A\|_2 = \max\{|\lambda_1|, |\lambda_n|\}$.

Real symmetric matrices are discussed in detail in Stewart [1973] and Parlett [1980]. There are three principal properties of real symmetric matrices which we will need in our discussions. First, real symmetric matrices have complete eigensystems. The dimension of the eigenspace corresponding to each eigenvalue of the matrix A is the same as the multiplicity of that eigenvalue as a root of the characteristic polynomial of A. Second, for any two distinct eigenvalues λ and μ of A and corresponding eigenvectors x and y, $x^T y = 0$. Thus, eigenvectors corresponding to different eigenvalues are orthogonal, and we can therefore construct an eigenvector basis which is orthonormal. Third, small symmetric perturbations in any real symmetric matrix cause only small perturbations in the eigenvalues. Corresponding perturbations in the eigenvectors must be viewed in terms of perturbations on eigenspaces not as perturbations on individual vectors. If there exists a decent gap between two eigenvalues λ_j and λ_{j+1} of A, then small symmetric perturbations in A will yield small perturbations in the eigenspaces corresponding to the two sets of eigenvalues $\Lambda_1 \equiv \{\lambda_1, \ldots, \lambda_j\}$ and $\Lambda_2 \equiv \{\lambda_{j+1}, \ldots, \lambda_n\}$.

We are interested in very large real symmetric matrices. Such matrices arise in a variety of applications. The following incomplete list indicates how diverse the application areas are.

CLUSTERING ANALYSIS

1. Computation of eigenvectors for use in constructing a model of a power system for use in transient stability studies. See for example, Chow et al [1984].

2. Calculation of eigenvectors for use in the partitioning of graphs which represent the interconnections between electrical circuits which are to be placed upon a silicon chip for use in an electronic device. The objective is to partition the graph (i.e. circuits) in such a way as to minimize the number of edges (connections between the circuits) which connect the resulting subgraphs of the partition to each other. See for example Barnes [1982].

PHYSICS

1. Computation of eigenvalues and eigenvectors of the Schrodinger equation for use in the comparison of various theories of quantum mechanical interactions with experimental observations. See for example, Haydock [1980].

2. Eigenvalue and eigenvector computations for matrices which model the arrangement of atoms in a disordered material. The objective is to determine various physical properties of such materials. See for example Kirkpatrick [1979], Dean [1972], and Stein and Krey [1979].

3. Eigenvalue and eigenvector computations used in attempts to understand the Jahn-Teller effect. This effect depends upon the coupling between electronic and nuclear (vibrational) motion within the nucleus of an atom. See for example, Sears et al [1981].

4. Eigenvalue and eigenvector computations used in studies of the many-body nuclear system of an atom. See for example Whitehead et al [1977].

5. Eigenvalue and eigenvector computations used to estimate the atomic densities of states near the surfaces in semiconductors. See for example Pandey [1983].

CHEMISTRY

1. Eigenvalue computations for the calculation of bond energies in molecules. See for example, Nesbet [1981] and Davidson [1983].

STRUCTURAL MECHANICS

1. Eigenvalue and eigenvector computations for the vibrational or the buckling analysis of structures. Typically these problems are generalized eigenvalue problems. See for example Jennings [1977] and NASTRAN [1977].

OCEANOGRAPHY

1. Eigenvalue computations for the analysis of models of ocean tides. See for example Platzman [1978] and Cline et al [1976].

The power systems application in Chow et al [1984] requires the computation of a number of the algebraically-smallest eigenvalues and corresponding eigenvectors of a large sparse real symmetric matrix which describes the power system being analyzed. The computed eigenvectors are used to partition the network of electric generators and buses in such a way that the connections between the resulting disjoint subsets of machines and buses are weak. The objective is to obtain a subdivision such that if an electrical fault occurs within one of the subgroups, the effects of this fault can be studied by modelling that subgroup in detail but treating each of the other subgroups (in terms of their interactions with the subgroup where the fault occurred) as simple average 'machines'. In Chow et al [1984] a matrix of size 2161 was used to model a hypothetical but realistic grid of generators and buses for the Western United States. The eigenvectors required for the analysis in Chow et al [1984] were computed using the version of our single-vector Lanczos procedure given in Volume 2, Chapter 4.

SECTION 1.2 PERTURBATION THEORY

We simply restate three well-known results. See Stewart [Chapter 6, 1973] for more details.

THEOREM 1.2.1 Stewart [Chapter 6, 1973] Let A be a nxn Hermitian (real symmetric) matrix. Let $A' \equiv A + E$ where E is a Hermitian (real symmetric) perturbation of A. Define the eigenvalues of A as $\{\lambda_1 \geq \ldots \geq \lambda_n\}$ and the eigenvalues of A' by $\{\lambda'_1 \geq \ldots \geq \lambda'_n\}$. Then for each i=1,2,...,n we have that

$$\lambda_i - \|E\|_2 \leq \lambda'_i \leq \lambda_i + \|E\|_2 \qquad (1.2.1)$$

We have that $\|E\|_2 = \max\{|\lambda_1(E)|, |\lambda_n(E)|\}$ for any Hermitian or real symmetric matrix E. Therefore, the eigenvalues of a matrix resulting from such a perturbation of a Hermitian or of a real symmetric matrix cannot differ from the eigenvalues of the original matrix by more than the largest eigenvalue of the perturbation matrix E. Thus if the norm of the perturbation matrix is small compared to the norm of A, the changes in the eigenvalues must also be small. Note that these are absolute changes not relative changes. If a matrix has both very large and very small eigenvalues, then the relative changes in the smaller eigenvalues may be large.

Stewart [Chapter 6, 1973] gives the following theorem for the perturbations in the corresponding eigenvectors. Davis and Kahan [1970] provide generalizations of this result to subspaces of eigenvectors of A and A'. These generalizations do not look at changes in