Numerical Methods in Scientific Computing

Volume I

Numerical Methods in Scientific Computing

Volume I

Germund Dahlquist
Royal Institute of Technology
Stockholm, Sweden

Åke Björck
Linköping University
Linköping, Sweden

Society for Industrial and Applied Mathematics • Philadelphia

10 9 8 7 6 5 4 3 2 1

Library of Congress Cataloging-in-Publication Data

Dahlquist, Germund.
Numerical methods in scientific computing / Germund Dahlquist, Åke Björck.
p.cm.
Includes bibliographical references and index.
ISBN 978-0-898716-44-3 (v. 1 : alk. paper)
1. Numerical analysis—Data processing. I. Björck, Åke, 1934- II. Title.

QA297.D335 2008
518—dc22 2007061806

To Marianne and Eva

Contents

List of Figures

List of Tables

List of Conventions

Besides the generally accepted mathematical abbreviations and notations (see, e.g., James and James, *Mathematics Dictionary* [1985, pp. 467–471]), the following notations are used in the book:

MATLAB® has been used for this book in testing algorithms. We also use its notations for array operations and the convenient colon notation.

$.*$	$A \,.* \,B$ element-by-element product $A(i,j)B(i,j)$
$./$	$A \,./B$ element-by-element division $A(i,j)/B(i,j)$
$i:k$	same as $i, i+1, \dots, k$ and empty if $i > k$
$i:j:k$	same as $i, i+j, i+2j, \dots, k$
$A(:,k)$, $A(i,:)$	the kth column, ith row of A, respectively
$A(i:k)$	same as $A(i), A(i+1), \dots, A(k)$
$\lfloor x \rfloor$	floor, i.e., the largest integer $\le x$
$\lceil x \rceil$	roof, i.e., the smallest integer $\ge x$
e^x and $\exp(x)$	both denote the exponential function
$fl\,(x+y)$	floating-point operations; see Sec. 2.2.3
$\{x_i\}_{i=0}^n$	denotes the set $\{x_0, x_1, \dots, x_n\}$
$[a,b]$	closed interval $(a \le x \le b)$
(a,b)	open interval $(a < x < b)$
sign (x)	$+1$ if $x \ge 0$, else -1
int $(a,b,c,\dots,w)$	the smallest interval which contains $a, b, c, \dots, w$
$f(x) = O(g(x)),\ x \to a$	$\lvert f(x)/g(x)\rvert$ is bounded as $x \to a$
	(a can be finite, $+\infty$, or $-\infty$)
$f(x) = o(g(x)),\ x \to a$	$\lim_{x\to a} f(x)/g(x) = 0$
$f(x) \sim g(x),\ x \to a$	$\lim_{x\to a} f(x)/g(x) = 1$
$k \le i, j \le n$	means $k \le i \le n$ and $k \le j \le n$
$\mathcal{P}_k$	the set of polynomials of degree *less than* k
(f,g)	scalar product of functions f and g
$\lVert \cdot \rVert_p$	p-norm in a linear vector or function space; see Sec. 4.5.1–4.5.3 and Sec. A.3.3 in Online Appendix A
$E_n(f)$	$\operatorname{dist}(f, \mathcal{P}_n)_{\infty,[a,b]}$; see Definition 4.5.6

The notations $a \approx b$, $a \lessapprox b$, and $a \gtrapprox b$ are defined in Sec. 2.1.2. Matrices and vectors are generally denoted by Roman letters A and b. A^T and b^T denote the transpose of the matrix A and the vector b, respectively. $(A,\ B)$ means a partitioned matrix; see Sec. A.2 in Online Appendix A. Notation for matrix computation can also be found in Online Appendix A. Notations for differences and difference operators, e.g., $\Delta^2 y_n$, $[x_0, x_1, x_2]f$, $\delta^2 y$, are defined in Chapters 3 and 4.

Preface

In 1974 the book by Dahlquist and Björck, *Numerical Methods*, was published in the Prentice–Hall Series in Automatic Computation, edited by George Forsythe. It was an extended and updated English translation of a Swedish undergraduate textbook used at the Royal Institute of Technology (KTH) in Stockholm. This book became one of the most successful titles at Prentice–Hall. It was translated into several other languages and as late as 1990 a Chinese edition appeared. It was reprinted in 2003 by Dover Publications.

In 1984 the authors were invited by Prentice–Hall to prepare a new edition of the book. After some attempts it soon became apparent that, because of the rapid development of the field, one volume would no longer suffice to cover the topics treated in the 1974 book. Thus a large part of the new book would have to be written more or less from scratch. This meant more work than we initially envisaged. Other commitments inevitably interfered, sometimes for years, and the project was delayed. The present volume is the result of several revisions worked out during the past 10 years.

Tragically, my mentor, friend, and coauthor Germund Dahlquist died on February 8, 2005, before this first volume was finished. Fortunately the gaps left in his parts of the manuscript were relatively few. Encouraged by his family, I decided to carry on and I have tried to the best of my ability to fill in the missing parts. I hope that I have managed to convey some of his originality and enthusiasm for his subject. It was a great privilege for me to work with him over many years. It is sad that he could never enjoy the fruits of his labor on this book.

Today mathematics is used in one form or another within most areas of science and industry. Although there has always been a close interaction between mathematics on the one hand and science and technology on the other, there has been a tremendous increase in the use of sophisticated mathematical models in the last decades. Advanced mathematical models and methods are now also used more and more within areas such as medicine, economics, and social sciences. Today, experiment and theory, the two classical elements of the scientific method, are supplemented in many areas by computations that are an equally important component.

The increased use of numerical methods has been caused not only by the continuing advent of faster and larger computers. Gains in problem-solving capabilities through better mathematical algorithms have played an equally important role. In modern scientific computing one can now treat more complex and less simplified problems through massive amounts of numerical calculations.

This volume is suitable for use in a basic introductory course in a graduate program in numerical analysis. Although short introductions to numerical linear algebra and differential equations are included, a more substantial treatment is deferred to later volumes. The book can also be used as a reference for researchers in applied sciences working in scientific computing. Much of the material in the book is derived from graduate courses given by the first author at KTH and Stanford University, and by the second author at Linköping University, mainly during the 1980s and 90s.

We have aimed to make the book as self-contained as possible. The level of presentation ranges from elementary in the first and second chapters to fairly sophisticated in some later parts. For most parts the necessary prerequisites are calculus and linear algebra. For some of the more advanced sections some knowledge of complex analysis and functional analysis is helpful, although all concepts used are explained.

The choice of topics inevitably reflects our own interests. We have included many methods that are important in large-scale computing and the design of algorithms. But the emphasis is on traditional and well-developed topics in numerical analysis. Obvious omissions in the book are wavelets and radial basis functions. Our experience from the 1974 book showed us that the most up-to-date topics are the first to become out of date.

Chapter 1 is on a more elementary level than the rest of the book. It is used to introduce a few general and powerful concepts and ideas that will be used repeatedly. An introduction is given to some basic methods in the numerical solution of linear equations and least squares problems, including the important singular value decomposition. Basic techniques for the numerical solution of initial value problems for ordinary differential equations is illustrated. An introduction to Monte Carlo methods, including a survey of pseudorandom number generators and variance reduction techniques, ends this chapter.

Chapter 2 treats floating-point number systems and estimation and control of errors. It is modeled after the same chapter in the 1974 book, but the IEEE floating-point standard has made possible a much more satisfactory treatment. We are aware of the fact that this aspect of computing is considered by many to be boring. But when things go wrong (and they do!), then some understanding of floating-point arithmetic and condition numbers may be essential. A new feature is a section on interval arithmetic, a topic which recently has seen a revival, partly because the directed rounding incorporated in the IEEE standard simplifies the efficient implementation.

In Chapter 3 different uses of infinite power series for numerical computations are studied, including ill-conditioned and semiconvergent series. Various algorithms for computing the coefficients of power series are given. Formal power series are introduced and their convenient manipulation using triangular Toeplitz matrices is described.

Difference operators are handy tools for the derivation, analysis, and practical application of numerical methods for many tasks such as interpolation, differentiation, and quadrature. A more rigorous treatment of operator series expansions and the use of the Cauchy formula and the fast Fourier transform (FFT) to derive the expansions are original features of this part of Chapter 3.

Methods for convergence acceleration of series (sequences) are covered in detail. For alternating series or series in a complex variable, Aitken extrapolation and Euler's transformation are the most important. Variants of Aitken, Euler–Maclaurin, and Richardson acceleration work for monotonic sequences. A partly new and more rigorous theoretical analysis given for completely monotonic sequences reflects Dahlquist's interest in analytic function theory. Although not intended for the novice, this has been included partly because it illustrates techniques that are of more general interest.

An exposition of continued fractions and Padé approximation, which transform a (formal) power series into a sequence of rational functions, concludes this chapter. This includes the ϵ-algorithm, the most important nonlinear convergence acceleration method, as well as the qd algorithm.

Chapter 4 treats several topics related to interpolation and approximation. Different bases for polynomial interpolation and related interpolation formulas are explained. The advantages of the barycentric form of Lagrange interpolation formula are stressed. Complex analysis is used to derive a general Lagrange–Hermite formula for polynomial interpolation in the complex plane. Algorithms for rational and multidimensional interpolation are briefly surveyed.

Interpolation of an analytic function at an infinite equidistant point set is treated from the point of view of complex analysis. Applications made to the Runge phenomenon and the Shannon sampling theorem. This section is more advanced than the rest of the chapter and can be skipped in a first reading.

Piecewise polynomials have become ubiquitous in computer aided design and computer aided manufacturing. We describe how parametric Bézier curves are constructed from piecewise Bernštein polynomials. A comprehensive treatment of splines is given and the famous recurrence relation of de Boor and Cox for B-splines is derived. The use of B-splines for representing curves and surfaces with given differentiability conditions is illustrated.

Function spaces are introduced in Chapter 4 and the concepts of linear operator and operator norm are extended to general infinite-dimensional vector spaces. The norm and distance formula, which gives a convenient error bound for general approximation problems, is presented. Inner product spaces, orthogonal systems, and the least squares approximation problem are treated next. The importance of the three-term recurrence formula and the Stieltjes procedure for numerical calculations is stressed. Chebyshev systems and theory and algorithms for approximation in maximum norm are surveyed.

Basic formulas and theorems for Fourier series and Fourier transforms are discussed next. Periodic continuation, sampled data and aliasing, and the Gibbs phenomenon are treated. In applications such as digital signal and image processing, and time-series analysis, the FFT algorithm (already used in Chapter 3) is an important tool. A separate section is therefore devoted to a matrix-oriented treatment of the FFT, including fast trigonometric transforms.

In Chapter 5 the classical Newton–Cotes rules for equidistant nodes and the Clenshaw–Curtis interpolatory rules for numerical integration are first treated. Next, extrapolation methods such as Romberg's method and the use of the ϵ-algorithm are described. The superconvergence of the trapezoidal rule in special cases and special Filon-type methods for oscillating integrands are discussed. A short section on adaptive quadrature follows.

Quadrature rules with both free and prescribed nodes are important in many contexts. A general technique of deriving formulas using the method of undetermined coefficients is given first. Next, Gauss–Christoffel quadrature rules and their properties are treated, and Gauss–Lobatto, Gauss–Radau, and Gauss–Kronrod rules are introduced. A more advanced exposition of relations between moments, tridiagonal matrices, and Gauss quadrature is included, but this part can be skipped at first reading.

Product rules for multidimensional integration formulas use simple generalizations of univariate rules and are applicable to rectangular domains. For more general domains, integration using irregular triangular grids is more suitable. The basic linear and quadratic interpolation formulas on such grids are derived. Together with a simple correction for curved boundaries these formulas are also very suitable for use in the finite element method. A discussion of Monte Carlo and quasi–Monte Carlo methods and their advantages for high-dimensional integration ends Chapter 5.

Chapter 6 starts with the bisection method. Next, fixed-point iterations are introduced and the contraction mapping theorem proved. Convergence order and the efficiency index are discussed. Newton's method is treated also for complex-valued equations and an interval Newton method is described. A discussion of higher-order methods, including the Schröder family of methods, is featured in this chapter.

Because of their importance for the matrix eigenproblem, algebraic equations are treated at length. The frequent ill-conditioning of roots is illustrated. Several classical methods are described, as well as an efficient and robust modified Newton method due to Madsen and Reid. Further, we describe the progressive qd algorithm and Sturm sequence methods, both of which are also of interest for the tridiagonal eigenproblem.

Three Online Appendices are available from the Web page of the book, `www.siam.org/books/ot103`. Appendix A is a compact survey of notations and some frequently used results in numerical linear algebra. Volume II will contain a full treatment of these topics. Online Appendix B describes Mulprec, a collection of MATLAB m-files for (almost) unlimited high precision calculation. This package can also be downloaded from the Web page. Online Appendix C is a more complete guide to literature, where advice is given on not only general textbooks in numerical analysis but also handbooks, encyclopedias, tables, software, and journals.

An important feature of the book is the large collection of problems and computer exercises included. This draws from the authors' 40+ year of experience in teaching courses in numerical analysis. It is highly recommended that a modern interactive system such as MATLAB is available to the reader for working out these assignments. The 1974 book also contained answers and solutions to most problems. It has not been possible to retain this feature because of the much greater number and complexity of the problems in the present book.

We have aimed to make and the bibliography as comprehensive and up-to-date as possible. A Notes and References section containing historical comments and additional references concludes each chapter. To remind the reader of the fact that much of the theory and many methods date one or several hundred years back in time, we have included more than 60 short biographical notes on mathematicians who have made significant contributions. These notes would not have been possible without the invaluable use of the biographies compiled at the School of Mathematics and Statistics, University of St Andrews, Scotland (`www-history.mcs.st.andrews.ac.uk`). Many of these full biographies are fascinating to read.

I am very grateful for the encouragement received from Marianne and Martin Dahlquist, who graciously allowed me to access computer files from Germund Dahlquist's personal computer. Without their support the completion of this book would not have been possible.

Many people read early drafts at various stages of the evolution of this book and contributed many corrections and constructive comments. I am particularly grateful to Nick Higham, Lothar Reichel, Zdenek Strakos, and several anonymous referees whose suggestions led to several major improvements. Other people who helped with proofreading include Bo Einarsson, Tommy Elfving, Pablo Guerrero-Garcia, Sven-Åke Gustafsson, and

Per Lötstedt. Thank you all for your interest in the book and for giving so much of your valuable time!

The book was typeset in LaTeX the references were prepared in BibTeX, and the index with MakeIndex. These are all wonderful tools and my thanks goes to Donald Knuth for his gift to mathematics. Thanks also to Cleve Moler for MATLAB, which was used in working out examples and for generating figures.

It is a pleasure to thank Elizabeth Greenspan, Sarah Murphy, and other staff at SIAM for their cheerful and professional support during all phases of the acquisition and production of the book.

Åke Björck
Linköping, July 2007