

# RESOURCES IN NUMERICAL ANALYSIS

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## INTRODUCTION

Numerical analysis is the area of mathematics and computer science that creates, analyzes, and implements algorithms for solving numerically the problems of continuous mathematics. Such problems originate generally from real-world applications of algebra, geometry, and calculus, and they involve variables that vary continuously; these problems occur throughout the natural sciences, social sciences, engineering, medicine, and business. During the second half of the twentieth century and continuing up to the present day, digital computers have grown in power and availability. This has led to the use of increasingly realistic mathematical models in science and engineering, and numerical analysis of increasing sophistication has been needed to solve these more sophisticated mathematical models of the world. The formal academic area of numerical analysis varies, from quite foundational mathematical studies to the computer science issues involved in the creation and implementation of algorithms.

In this chapter, we place more emphasis on the theoretical mathematics involved in studying numerical analysis while also discussing more briefly the resources associated with the computer science aspects of the subject. The implementation of numerical algorithms is affected by physical characteristics of the computers being used for the computation, and we consider this in our presentation. In addition, the purpose of most numerical analysis research is to develop actual computer codes to solve real problems; and thus the development of computer software to implement numerical algorithms is an important part of the subject. With the growth in importance of using computers to carry out numerical procedures in solving mathematical models of the world, an area known as "scientific computing" or "computational science" has taken shape during the 1980s and 1990s. This new area looks at the use of numerical analysis from a computer science perspective. It is concerned with using the most powerful tools of numerical analysis, computer graphics, symbolic mathematical computations, and graphical user interfaces to make it easier for a user to set up, solve, and interpret complicated mathematical models of the real world. We will give a few resources for scientific computing, but numerical analysis is the focus of this presentation.

Following is a selection of texts that together provide an overview of numerical analysis, given in order from introductory to specialist.

A Quarteroni, R Sacco, and F Saleri. *Numerical Mathematics*, Springer-Verlag, New York, 2000. This is a current introduction to most topics in numerical analysis, including the numerical solution of partial differential equations. The text is suitable for a beginning graduate student in mathematics.

K Atkinson and W Han. *Theoretical Numerical Analysis*, Springer-Verlag, New York, 2001. This introduces a wide variety of functional analysis tools for studying numerical methods. These are applied to problems in approximation theory, ordinary and partial differential equations, integral equations, and nonlinear variational inequalities.

G Golub and C Van Loan. *Matrix Computations*, 3<sup>rd</sup> ed., John Hopkins University Press, 1996. This is an excellent reference book for a wide variety of topics in numerical linear algebra at all

levels of the subject. It covers the theoretical framework for a variety of linear algebra problems, and it also considers the effects of computer arithmetic and serial vs. parallel computers.

A Iserles. *A First Course in the Numerical Analysis of Differential Equations*, Cambridge University Press, 1996. This is a very nice introductory presentation of the theoretical framework for the numerical analysis for both ordinary and partial differential equations.

## I. General Numerical Analysis

### A. Introductory Sources

The best general introductions to numerical analysis are beginning graduate-level textbooks that cover most of the commonly recognized topics within numerical analysis. A few of my current favorites, listed alphabetically, are the following. Each of them gives an introduction to most of what are considered basic topics in numerical analysis. I include both current texts and classical texts that are still important references.

M Allen III and E Isaacson. *Numerical Analysis for Applied Science*, John Wiley, New York, 1998. A very nice introduction.

K Atkinson. *An Introduction to Numerical Analysis*, 2<sup>nd</sup> ed., John Wiley, New York, 1989. I am the author of this text, and I believe it gives a good introduction to most introductory level topics in numerical analysis.

W Gander and J Hrebicek. *Solving Problems in Scientific Computing Using Maple and Matlab*, 3<sup>rd</sup> ed., Springer, 1997.

W Gautschi. *Numerical Analysis: An Introduction*, Birkhäuser, Boston, 1997.

P Henrici. *Elements of Numerical Analysis*, John Wiley, New York, 1964. This is a classic text by a master of the subject. It contains well-written discussions of a broad set of topics. It is dated in some respects, but still contains much that is useful and interesting.

E Isaacson and H Keller. *Analysis of Numerical Methods*, corrected reprint of the 1966 original, Dover Pub., New York, 1994. This is a classic text covering many topics not covered elsewhere. For example, this text contains a very good introduction to finite difference methods for approximating partial differential equations.

R Kress. *Numerical Analysis*, Springer-Verlag, New York, 1998.

A Quarteroni, R Sacco, and F Saleri. *Numerical Mathematics*, Springer-Verlag, New York, 2000. This was cited earlier in the introduction as giving a very good introduction to the current state of numerical analysis.

J Stoer and R Bulirsch. *Introduction to Numerical Analysis*, 2<sup>nd</sup> ed., Springer-Verlag, New York, 1993. This is a translation of a popular German text.

C Uberhuber. *Numerical Computation: Methods, Software, and Analysis*, Vols. 1 and 2, Springer-Verlag, New York, 1997. This text pays much attention to software and to machine aspects of numerical computing.

#### B. Advanced Introductory Texts with Broad Coverage

In most cases, such texts create a general framework within which to view the numerical analysis of a wide variety of problems and numerical methods. This is usually done using the language of functional analysis; and often it is directed towards solving ordinary differential, partial differential, and integral equations.

K Atkinson and W Han. *Theoretical Numerical Analysis*, Springer-Verlag, New York, 2001. This was cited earlier in the introduction as giving a good introduction to the current state of theoretical numerical analysis at a more abstract level.

L Kantorovich and G Akilov. *Functional Analysis*, 2<sup>nd</sup> ed., Pergamon Press, New York, 1982. This is the second edition of a classic text in the use of functional analysis in studying problems of numerical analysis. L Kantorovich is often credited with originating and popularizing the use of functional analysis, beginning with a seminal 1948 paper. Among the many topics in this volume, there is a very useful introduction to the calculus of nonlinear operators on Banach spaces; and this is used to define and study Newton's method for solving nonlinear operator equations on Banach spaces.

L Collatz. *Functional Analysis and Numerical Mathematics*, Academic Press, New York, 1966. This contains a functional analysis framework for a variety of problems. Especially notable is the use of partially ordered functions spaces and norms whose values belong to the positive cone of a partially order space.

J-P Aubin. *Applied Functional Analysis*, 2<sup>nd</sup> ed., John Wiley, New York, 2000. This contains developments of tools for studying numerical methods for partial differential equations and also for optimization problems and convex analysis.

#### C. Books With a Sampling of Introductory Topics

For a classic look at numerical analysis, one that also give some "flavor" of the subject, see the following collection.

G Golub, ed. *Studies in Numerical Analysis*, Vol. 24, MAA Studies in Mathematics, 1984. This is a splendid collection of articles on special topics, beginning with the very nice article "The Perfidious Polynomial" by James Wilkinson.

#### D. Major Journals and Serial Publications

There are over fifty journals devoted to various aspects of numerical analysis; and in addition, many other mathematics journals contain articles on numerical analysis. Also, many areas of business, engineering, and the sciences are closely tied to numerical analysis, and much of the published research in those areas is about numerical methods of solving problems for the area of application. We highlight here some of the major journals and serial publications in numerical analysis.

## 1. General surveys

*Acta Numerica* (ISSN 0962-4929) published by Cambridge University Press, is an annual collection of survey articles in a variety of areas of numerical analysis, beginning in 1992. Articles in this annual publication are intended to contain new research results and to also survey the state of the field as regards current research at its leading edge. If you are seeking information on the current state of art in some area of numerical analysis, I recommend you begin by looking at the table of contents of all of the issues of this annual publication. This is an excellent collection of articles!

*The State of the Art in Numerical Analysis* is the name of a research conference held every ten years in the United Kingdom, and it is also the name of the accompanying volume of the survey talks presented at the conference. The most recent such conference was in 1996; and there have been four such conferences. The most recent volume is referenced as follows.

I Duff and G Watson, editors. *The State of the Art in Numerical Analysis*, Oxford University Press, Oxford, 1997.

I strongly recommend the articles in these volumes as introductions to many areas of numerical analysis.

*SIAM Review* (ISSN 0036-1445) is the flagship journal for the Society of Industrial and Applied Mathematics, and it is published quarterly. The first part of the journal contains survey articles, and a number of these are survey articles on the current state of the research in some area of numerical analysis.

## 2. Leading journals with a general coverage in numerical analysis.

SIAM (Society of Industrial and Applied Mathematics) has a number of journals which are devoted to various aspects of numerical analysis. The *SIAM Journal on Numerical Analysis* (ISSN 0036-1429) is probably the most popular and referenced journal in numerical analysis. Its coverage is all of numerical analysis. Other SIAM journals that deal with special areas of numerical analysis are *SIAM Journal on Scientific Computing* (ISSN 1064-8275), *SIAM Journal on Matrix Analysis* (ISSN 0895-4798), and *SIAM Journal on Optimization* (ISSN 1052-6234). These are all well-referenced journals. In addition, important review articles for topics in

numerical analysis appear regularly in *SIAM Review*, as mentioned earlier. Other SIAM journals also contain a number of articles related to numerical analysis.

*Numerische Mathematik* (ISSN 0029-599X) is the flagship journal in numerical analysis from Springer-Verlag. For a number of years, virtually all of its papers have been written in English. It has excellent articles in a wide variety of areas.

*Mathematics of Computation* (ISSN 0025-5718) is published by the American Mathematical Society, and it dates back to 1940; it is the oldest journal devoted to numerical computation. In addition to articles on numerical analysis, it also contains articles on computational number theory.

*IMA Journal of Numerical Analysis* (ISSN 0272-4979) is published by the British counterpart to SIAM, the Institute of Mathematics and Its Applications.

3. Other journals with a general coverage in numerical analysis.

The following is only a partial list of the journals with a general coverage of numerical analysis. The list is alphabetical.

*ACM Transactions on Mathematical Software* (ISSN 0098-3500) is published by the ACM (Association for Computing Machinery), one of the major professional associations for computer science, especially within academia and research institutes. This journal deals principally with issues of implementation of numerical algorithms as computer software. It includes the *Collected Algorithms of the ACM*, a large collection of refereed numerical analysis software.

*Advances in Computational Mathematics* (ISSN1019-7168), Kluwer Academic Pub. This is of more recent origin. It considers all types of computational mathematics, although most papers are from numerical analysis.

*BIT: Numerical Mathematics* (ISSN 0006-3835) dates from 1961, and it is sponsored by numerical analysts in The Netherlands and the various Scandinavian countries. This is published by Swets & Zeitlinger of The Netherlands.

*Computing* (ISSN0010-485X), Springer-Verlag. This contains numerical analysis papers that are more computationally oriented or deal with computer science issues linked to numerical computation.

*Electronic Transactions on Numerical Analysis* (ISSN 1068-9613) began publication in 1993. It is a fully refereed journal that appears only in electronic form. Its URL is <http://etna.mcs.kent.edu/>

The journal is published by the Kent State University Library in conjunction with the Institute of Computational Mathematics at Kent State University, Kent, Ohio.

*Foundations of Computational Mathematics* (ISSN 1615-3375), Springer-Verlag. This is a new journal focusing on the interface of computer science with mathematics, especially numerical analysis and forms of computational mathematics.

*Journal of Computational and Applied Mathematics* (ISSN 0377-0427), Elsevier Science Pub. This is a popular journal, publishing a wide variety of papers, conference proceedings, and survey articles.

*Journal of Computational Physics* (ISSN 0021-9991), Academic press. This journal treats the computational aspects of physical problems, presenting techniques for the numerical solution of mathematical equations arising in all areas of physics. Many experimental numerical procedures are discussed here.

*Numerical Algorithms* (ISSN 1017-1398), Kluwer Academic Pub. The journal is devoted to all aspects of the study of numerical algorithms.

*SIAM Journal on Scientific Computing* (ISSN 1064-8275), SIAM Pub. This is quite similar to the SIAM Journal on Numerical Analysis, but articles in it are to be tied more closely to actual numerical computation, with possibly more consideration given to questions of implementation.

#### E. Other Printed Resources

*Handbook of Numerical Analysis*, ed. by P. Ciarlet & J. Lions. This a multi-volume work, giving advanced level and extensive introductions to major topics in numerical analysis. Six volumes have been written to date, and most have connections to partial differential equations, with several main articles devoted to numerical analysis aspects of some problems from continuum mechanics. The publishers are Elsevier Science Pub.

*Numerical Recipes*, authored by W. Press, S. Teukolsky, W. Vetterling, and B. Flannery, Cambridge University Press. This is published in several versions based on different computer languages, including Fortran, C, and Pascal. This work is extremely wide-ranging in its coverage, including a sampling of essentially every area of numerical analysis. The book is popular among users of numerical analysis in the sciences and engineering, as it gives a quick and useful introduction to a topic, accompanied with computer codes. I recommend it as one possible introduction to a topic of interest, but I also recommend that it be followed by a more extensive introduction to examine additional nuances of the subject.

#### F. Online Resources

Numerical analysis was among the earliest of areas in mathematics to make extensive use of computers, and much of the early history of computing is linked to the intended application of the computers to solving problems involving numerical analysis. For that reason, it is not surprising that numerical analysts are at the leading edge as regards using computers to make resources available online, both reference material and computer

software. We list here a few online resources that contain information on numerical analysis and associated software; and there are many sites we do not list.

*sci.math.num-analysis*. This is a popular Usenet bulletin board devoted to numerical analysis.

*Netlib* (<http://www.netlib.org/>). This is the most extensive online library of numerical analysis software. It is operated jointly by Oak Ridge National Laboratory and the University of Tennessee. Many important software projects are available through this site; for example, LINPACK, EISPACK, and LAPACK are important numerical linear algebra packages which now form the core of most numerical analysis libraries in the linear algebra. The Collected Algorithms of the ACM are also available here, while first being published in the *ACM Transactions on Mathematical Software*.

*NIST GAMS* (<http://gams.nist.gov/>). This acronym denotes the National Institute for Science and Technology Guide to Available Mathematical Software. It is an excellent guide to numerical analysis software, some of which is free through Netlib. In addition, the site <http://math.nist.gov/> provides links to other areas of numerical computation.

*The Mathematical Atlas*.

([http://www.math.niu.edu/~rusin/known-math/index/tour\\_na.html](http://www.math.niu.edu/~rusin/known-math/index/tour_na.html)). This is a general look at all of mathematics, and numerical analysis is one of the options provided. The sponsor is Northern Illinois University.

*Scientific Computing FAQ*

(<http://www.mathcom.com/corpdir/techinfo.mdir/scifaq/index.html>). The acronym translates to "Frequently Asked questions". It lists a large amount of information on numerical analysis and associated areas within Scientific Computing. The sponsor is MathCom Inc.

## II. Numerical Linear Algebra, Nonlinear Algebra, and Optimization

This refers to problems involving the solution of systems of linear and nonlinear equations and the related problem of optimizing a function of several variables; often the number of variables is quite large.

### A. Numerical Linear Algebra

Many problems in applied mathematics involve solving systems of linear equations, with the linear system occurring naturally in some cases and as a part of the solution process in other cases. Linear systems are usually written using matrix-vector notation,  $A\mathbf{x}=\mathbf{b}$  with  $A$  the matrix of coefficients for the system,  $\mathbf{x}$  the column vector of the unknown variables, and  $\mathbf{b}$  a given column vector. Solving linear systems with up to  $n=1000$  variables is now considered relatively straightforward in most cases. For small to moderate sized linear systems (say  $n \leq 1000$ ), the favorite numerical method is *Gaussian elimination* and its variants; this is simply a precisely stated algorithmic variant of the method of elimination

of variables that students first encounter in elementary algebra. The *QR*-method is another direct method, often used with ill-conditioned problems.

For larger linear systems, there are a variety of approaches, depending on the structure of the coefficient matrix  $A$ . *Direct methods* lead to a theoretically exact solution  $\mathbf{x}$  in a finite number of steps, with Gaussian elimination the best-known example. There are errors, however, in the computed value of  $\mathbf{x}$  due to rounding errors in the computation, arising from the finite length of numbers in standard computer arithmetic. *Iterative methods* are approximate methods that create a sequence of approximating solutions of increasing accuracy. Linear systems are categorized according to many properties (e.g.  $A$  may be *symmetric* about its main diagonal), and specialized methods have been developed for problems with these special properties.

## 1. General references

There are a large number of excellent references on numerical linear algebra. We list only a few of the better known ones here. We begin our list of resources and references with two specialist journals.

*Linear Algebra and its Applications* (ISSN 0024-3795), North-Holland, Elsevier Science. Many articles involve questions of numerical linear algebra.

*SIAM Journal on Matrix Analysis* (ISSN 0895-4798), SIAM Pub. As the title implies, this specializes in numerical linear algebra.

G Golub and C Van Loan. *Matrix Computations*, 3<sup>rd</sup> ed., John Hopkins University Press, 1996. This was cited earlier in the introduction as giving a very good overview of the current state of numerical linear algebra.

N Higham. *Accuracy and Stability of Numerical Algorithms*, SIAM Pub., 1996. This contains an excellent discussion of error and stability analyses in numerical analysis, with numerical linear algebra a favored topic.

The following two texts furnish an excellent introduction to numerical linear algebra, suitable for use in teaching a first year graduate course.

J Demmel. *Applied Numerical Linear Algebra*, SIAM Pub., 1997.

L Trefethen and D Bau. *Numerical Linear Algebra*, SIAM Pub., 1997.

## 2. Eigenvalue problems

B Parlett. *The Symmetric Eigenvalue Problem*, Classics in Applied Mathematics, SIAM Pub., 1998. This is a reprint, with corrections, of a classic text that appeared in 1980. It provides an excellent introduction to the problem of the title.

J Wilkinson. *The Algebraic Eigenvalue Problem*, Oxford University Press, 1965. This is a classic text for numerical linear algebra, especially the eigenvalue problem, written by the Dean of researchers in this area.

### 3. Iterative methods

There are many approaches to developing iterative methods for solving linear systems, and they usually depend heavily on the "structure" of the matrix in the system under consideration. Most linear systems solved using iteration are "sparse systems" in which most of the elements in the coefficient matrix are zero. Such systems arise commonly when discretizing partial differential equations in order to solve them numerically. As one consequence, there are many texts on iterative methods for linear systems, and we list only a few of them here. Work of the past two decades has been along two principal lines. First, there has been a generalization of the "Conjugate Gradient method", and this has led to what are called "Krylov subspace iterative methods". Second, work on solving discretizations of partial differential equations has led to what is called multigrid iteration. We list a few recent important texts on iterative methods.

A Greenbaum. *Iterative Methods for Solving Linear Systems*, SIAM Pub., 1997. This work discusses Krylov subspace methods, especially their application to solving discretizations of partial differential equations.

O Axelsson. *Iterative Solution Methods*, Cambridge University Press, 1994. This is an extensive treatment of most iterative methods, both classical methods that are still popular and more recently developed methods.

R Barrett, M Berry, T Chan, et al. *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM Pub., 1994.

W Hackbusch. *Iterative Solution of Large Sparse Systems of Equations*, Springer-Verlag, 1994.

Y Saad. *Iterative Methods for Sparse Linear Systems*, PWS Pub., 1996. This contains a comprehensive introduction to iterative methods, including the use of parallel computing.

### 4. Applications on parallel and vector computers

J Demmel, M Heath, and H van der Vorst. *Parallel Numerical Linear Algebra*, Acta Numerica (1993), pp. 111-198.

J Dongarra, I Duff, D Sorensen, and H van der Vorst. *Numerical Linear Algebra for High-Performance Computers*, SIAM Pub., 1998. Solving linear systems on high-performance computers requires use of special procedures to make optimal use of the computer. That is the focus of this book.

J Dongarra, I Duff, D Sorensen, & H van der Vorst. *Solving Linear Systems on Vector and Shared Memory Computers*, SIAM Pub., 1991. This discusses the general problems involved in solving linear systems on parallel and vector pipeline computers.

## 5. Over-determined linear systems

Another important type of linear system to solve is the "over-determined linear system". The most popular method for solving such systems is called the "method of least squares". This refers to solving linear systems  $A\mathbf{x}=\mathbf{b}$  in which the matrix  $A$  is of order  $m \times n$ , usually with  $m$  much larger than  $n$ . Then a "solution" is found by attempting to minimize the Euclidean size of the vector  $A\mathbf{x}-\mathbf{b}$ . This is a difficult and important problem that occurs regularly in nonlinear regression analysis in statistics. For an up-to-date accounting of this problem and its solution, see the following text.

A Bjorck. *Numerical Methods for Least Squares Problems*, SIAM Pub., 1996.

## B. Numerical Solution of Nonlinear Systems

Solving nonlinear equations is often treated numerically by reducing the solution process to that of solving a sequence of linear problems. As a simple but important example, consider the problem of solving a nonlinear equation  $f(x)=0$ . Given an estimate  $\alpha$  of the root, approximate the graph of  $y=f(x)$  by the tangent line at  $\alpha$ ; and then use the root of the tangent line to obtain an improved estimate of the root of the original nonlinear function  $f(x)$ . This is called *Newton's method* for rootfinding.

This procedure generalizes to handling systems of nonlinear equations. Let  $\mathbf{f}(\mathbf{x})=\mathbf{0}$  denote a system of  $n$  nonlinear equations in the  $n$  unknown components of  $\mathbf{x}$ . In this, the role of the derivative is played by  $\mathbf{f}'(\mathbf{x})$ , the Jacobian matrix of  $\mathbf{f}(\mathbf{x})$ . To find the root of the approximating linear approximation, we must solve a linear system  $\mathbf{f}'(\alpha)\delta=-\mathbf{f}(\alpha)$ , a linear system of order  $n$ . There is a large literature on Newton's method for nonlinear systems and on ways to increase its efficiency. There are numerous other approaches to solving nonlinear systems, most based on using some type of approximation by linear functions.

### 1. Single equations

For solving a single equation of one variable,  $f(x)=0$ , see the following books.

J Traub. *Iterative Methods for the Solution of Equations*, Prentice-Hall, 1964. This is a classic text that examines this problem from almost every imaginable perspective.

A Householder. *The Numerical Treatment of a Single Nonlinear Equation*, McGraw-Hill, New York, 1970. This is a classic treatment of the quite old, but still interesting, problem of finding the roots of a nonlinear equation. Included are special methods for polynomial rootfinding.

## 2. Multivariate problems

For introductions to the numerical solution of nonlinear systems, see the following texts.

J Ortega & W Rheinboldt. *Iterative Solution of Nonlinear Equations in Several Variables*, Academic Press, 1970. This is a classic text on the subject. It covers many types of methods in great detail, and it also presents the mathematical tools needed to work in this area.

C Kelley, *Iterative Methods for Linear and Nonlinear Equations*, SIAM Pub., 1995. This is an excellent introduction to the general area of solving nonlinear systems.

In addition, the solution of nonlinear systems for particular types of problems is often discussed in the intended area of application. For example, discretizations of nonlinear partial differential equations leads to special types of nonlinear systems, and special types of methods have been developed for solving these systems. The solution of such nonlinear systems is discussed at length in the literature for solving partial differential equations.

## C. Optimization

An important related class of problems occurs under the heading of optimization, sometimes considered as a sub-area of "operations research". Given a real-valued function  $f(\mathbf{x})$  with  $\mathbf{x}$  a vector of unknowns, we wish to find a value of  $\mathbf{x}$  which minimizes  $f(\mathbf{x})$ . In some cases  $\mathbf{x}$  is allowed to vary freely, and in other cases there are constraints on the values of  $\mathbf{x}$  that can be considered. Such problems occur frequently in business and engineering applications. This is an enormously popular area of research, with many new methods having been developed recently, both for classic problems such as that of linear programming and for previously unsolvable problems. In many ways, this area needs a chapter of its own; and in the classification scheme for *Mathematical Reviews*, it has a category (MR90) separate from that of numerical analysis (MR65).

For introductions with a strongly mathematical flavor, see the following, listed alphabetically. Most of these books also address the practical problems of implementation.

We begin our list of resources and references with a specialist journal; otherwise, the list is alphabetical.

*SIAM Journal on Optimization* (ISSN 1052-6234), SIAM Pub. An important journal for articles on optimization theory, especially from a numerical analysis perspective.

D Bertsekas. *Nonlinear Programming*, Athena Scientific Pub., 1995.

J Dennis and R Schnabel. *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice-Hall, 1983. A classic text in the numerical analysis aspects of optimization theory.

R Fletcher. *Practical Methods of Optimization*, 2<sup>nd</sup> ed., John Wiley, 1987. A classic text.

P Gill, W Murray, and M Wright. *Numerical Linear Algebra and Optimization*, Vol. I, Addison-Wesley, 1991.

C Kelley, *Iterative Methods for Optimization*, SIAM Pub., 1999. A very useful introduction. It includes optimization of functions which are "noisy", meaning they are known subject to data noise of some kind, and it includes derivative-free methods, e.g. the Nelder-Mead algorithm.

D Luenberger. *Linear and Nonlinear Programming*, 2<sup>nd</sup> ed., Addison-Wesley, 1984. A very nice introduction to the classical theory for optimization.

J Nocedal and S Wright, *Numerical Optimization*, Springer-Verlag, 1999. This is an up-to-date introduction that covers a wide variety of methods, including the important interior point methods. It also discusses the use of automatic differentiation, and it allows an easier implementation of methods that use derivatives of the function being optimized.

Y Ye. *Interior Point Algorithms: Theory and Analysis*, John Wiley, 1997. This is an advanced level text that covers all aspects of the use and analysis of interior point methods.

### III. Approximation Theory

This category covers the approximation of functions and methods based on using such approximations. When evaluating a function  $f(x)$  with  $x$  a real or complex number, a computer or calculator can only do a finite number of numerical operations. Moreover, these operations are the basic arithmetic operations of addition, subtraction, multiplication, and division, together with comparison operations such as determining whether  $x > y$  is true or false. With the four basic arithmetic operations, we can evaluate polynomials and rational functions, polynomials divided by polynomials. Including the comparison operations, we can evaluate different polynomials or rational functions on different sets of real or complex numbers  $x$ . The evaluation of all other functions, e.g.  $f(x)=\sqrt{x}$  or  $\cos x$ , must be reduced to the evaluation of a polynomial or rational function that approximates the given function with sufficient accuracy. All function evaluations on calculators and computers are accomplished in this manner. This topic is known as approximation theory, and it is a well-developed area of mathematics.

#### A. General Approximation Theory

Approximation theory using polynomials, rational functions, and trigonometric polynomials goes back many centuries, but much of the theory for functions of one variable was developed during the period of 1850 to 1950.

## 1. General references

Some classic introductions are the following.

We begin our list of resources and references with a specialist journal; otherwise, the list is alphabetical.

*Journal of Approximation Theory* (ISSN 0021-9045), Academic Press. This is the leading journal for research articles on approximation theory.

P Davis. *Interpolation and Approximation*, Blaisdell Pub., 1963. This is a well-written classic text. I highly recommend it.

N Akhiezer. *Theory of Approximation*, transl. by C. Hyman, Frederick Ungar Pub. Co., 1956. This too is a well-known text, written at a higher level than the preceding book by Davis.

M Powell. *Approximation Theory and Methods*, Cambridge University Press, 1981. This is a very well-written and general introduction to approximation theory. It includes several chapters on approximation and interpolation by spline functions, a development of the period from 1950 to the present day.

T Rivlin. *An Introduction to the Approximation of Functions*, Blaisdell Pub., 1969. This is available as a Dover Pub. reprint.

## 2. Algorithms and software

For creating approximations suitable for use on computers, see the following books.

M Abramowitz and I Stegun (eds.). *Handbook of Mathematical Functions*, Dover Pub., 1964. This is the classic book on approximation of the special functions of mathematics and physics. It gives theoretical results on a variety of special functions, it gives tables of values, and it gives approximations of these functions in order to compute them more easily.

W Cody and W Waite. *Software Manual for the Elementary Functions*, Prentice-Hall, 1980.

Y Luke. *Mathematical Functions and Their Approximations*, Academic Press, 1975.

J Muller. *Elementary Functions: Algorithms and Implementation*, Birkhaeuser Pub., 1997.

### 3. Special topics

G Baker and P Graves-Morris. *Pade Approximants*, 2<sup>nd</sup> ed., Cambridge University Press, 1996.

T Rivlin. *Chebyshev Polynomials*, John Wiley, 1974.

G Szego. *Orthogonal Polynomials*, 3<sup>rd</sup> ed., American Mathematical Society, 1967.

A Zygmund. *Trigonometric Series*, Vols. I and II, Cambridge University Press, 1959.

### 4. Multivariate approximation theory

In the not too distant past, most approximation theory dealt with functions of one variable, whereas now there is a greater interest in functions of several variables. For example, see the following references to the current literature on multivariate approximation theory.

C de Boor. *Multivariate Piecewise Polynomials*, Acta Numerica (1993), pp. 65-110.

C Chui. *Multivariate Splines*, SIAM Pub., 1988.

M Sabin. *Numerical Geometry of Surfaces*, Acta Numerica (1994), pp. 411-466.

### 5. Wavelets

"Wavelets" furnish a means to combine the separate advantages of Fourier analysis and piecewise polynomial approximation. Although the first example of wavelets, the Haar function, goes back to 1910, much of the research on wavelets and their application is from 1980 onwards. Connected to wavelets is the idea of "multiresolution analysis", a decomposition of a function or a process into different levels of precision. Wavelets and multiresolution analysis is a very active area at present, and we give only some of the better known references on it.

C Chui. *An Introduction to Wavelets*, Academic Press, 1992.

I Daubechies. *Ten Lectures on Wavelets*, SIAM Pub., 1992.

R DeVore and B Lucier. *Wavelets*, Acta Numerica (1992), pp. 1-56. This gives an approximation theoretic perspective of wavelets and multiresolution. It is a tightly written article, and it has a good bibliography.

S Mallat. *Multiresolution Approximation and Wavelet Orthonormal Bases of  $L^2(\mathbf{R})$* , Transactions of the Amer. Math. Soc. **315** (1989), pp. 69-87.

Y Meyer. *Wavelets and Operators*, Cambridge University Press, 1992.

P Wojtaszczyk. *A Mathematical Introduction to Wavelets*, Cambridge University Press, 1997.

## B. Interpolation Theory

One method of approximation is called *interpolation*. Consider being given a finite set of points  $(x_i, y_i)$  in the  $xy$ -plane; then find a polynomial  $p(x)$  whose graph passes through the given points,  $p(x_i) = y_i$ . The polynomial  $p(x)$  is said to interpolate the given data points. Interpolation can be performed with functions other than polynomials (although these are the most popular category of interpolating functions), with important cases being rational functions, trigonometric polynomials, and spline functions. Interpolation has a number of applications. If a function  $f(x)$  is known only at a discrete set of  $n$  data points, then interpolation can be used to extend the definition to nearby points  $x$ . If  $n$  is even moderately large, then spline functions are preferable to polynomials for this purpose. Spline functions are smooth piecewise polynomial functions with minimal oscillation as regards interpolation, and they are used commonly in computer graphics, statistics, and other applications.

Good introductions to polynomial interpolation theory for functions of one variable are given in most introductory textbooks on numerical analysis, e.g. the texts cited earlier in the Introduction and under I-A.

### 1. Multivariable interpolation

For multivariable polynomial interpolation, most presentations are given in association with the intended area of application. This includes applications to the finite element discretization of partial differential equations, the numerical solution of integral equations, and the construction of surfaces in computer graphics. We give only a few examples.

S Brenner and R Scott. *The Mathematical Theory of Finite Element Methods*, Springer-Verlag, 1994. This contains many results on the theory of multivariable approximation using polynomials.

G Strang and G Fix. *An Analysis of the Finite Element Method*, Prentice-Hall, 1973. This is a classic text for the finite element method, and it contains useful information on multivariable polynomial interpolation and approximation.

P Lancaster and K Salkaukas. *Curve and Surface Fitting: An Introduction*, Academic Press, 1986. This gives multivariate interpolation over varied regions in the context of computer graphics.

### 2. Spline functions

Spline functions are an important particular form of piecewise polynomial functions. They are a very flexible tool that is used throughout the sciences and engineering. The theory of one variable spline functions is well-developed, while that of multivariable spline functions is an important current area of research.

C de Boor. *A Practical Guide to Splines*, Springer-Verlag, 1978. This is a classic text, developing both the theoretical side of the subject and giving practical software to make it easier to use spline functions. Much of the current spline function software is based on what is given in this text.

C de Boor. *Multivariate Piecewise Polynomials*, Acta Numerica (1993), pp. 65-110.

C Chui. *Multivariate Splines*, SIAM Pub., 1988.

L Schumaker. *Spline Functions: Basic Theory*, John Wiley, 1981. This is a complete and well-written presentation of the theory of spline functions.

P Dierckx. *Curve and Surface Fitting with Splines*, Oxford University Press, 1993. This looks at spline functions in the context of the needs of computer graphics.

## C. Numerical Integration and Differentiation

After obtaining approximations of a given function  $f(x)$ , integrals and derivatives of  $f(x)$  can be obtained by replacing  $f(x)$  with its approximation in the integral or derivative. Most methods for numerical integration and differentiation can be obtained by this means. Similarly, approximation theory is basic to developing methods for approximating differential and integral equations.

### 1. General references

Numerical integration for functions of a single variable has been the principal focus of research in numerical integration. Most introductory textbooks on numerical analysis contain good introductions. In addition, see the following.

P Davis and P Rabinowitz. *Methods of Numerical Integration*, 2<sup>nd</sup> ed., Academic Press, 1984.

W Gautschi, F Marcellan, and L Reichel (eds). *Numerical Analysis 2000. Vol. V. Quadrature and Orthogonal Polynomials*, Journal of Computational and Applied Mathematics **127**, 2001, no. 1-2. A collection of papers on the current state of the art between numerical integration and orthogonal polynomials.

A Krommer and C Ueberhuber. *Computational Integration*, SIAM Pub., 1998.

D Laurie and R Cools (eds). *Numerical Evaluation of Integrals*, Journal of Computational and Applied Mathematics **112**, 1999, no. 1-2. A collection of papers on the current state of the art in numerical integration.

## 2. Multivariate numerical integration

For some of the current literature on multivariate numerical integration, see the following.

A Stroud. *Approximate Calculation of Multiple Integrals*, Prentice-Hall, 1971. This is an old book, but is still the main reference for multivariate numerical integration.

R Cools. *Constructing Cubature Formulae: The Science Behind the Art*, Acta Numerica (1997), pp. 1-54. This gives a current perspective on constructing multivariate numerical integration formulas.

H Niederreiter. *Random Number Generation and Quasi-Monte Carlo Methods*, SIAM Pub., 1992.

I Sloan and S Joe. *Lattice Methods for Multiple Integration*, Oxford University Press, 1994.

## IV. Solving Differential and Integral Equations

Most mathematical models used in the natural sciences and engineering are based on ordinary differential equations, partial differential equations, and integral equations. The reader should also refer to the chapter on differential equations for information on some of these topics.

The numerical methods for these equations are primarily of two types. The first type approximates the unknown function in the equation by a simpler function, often a polynomial or piecewise polynomial function, choosing it so as to satisfy the original equation approximately. Among the best known of such methods is the "finite element method" for solving partial differential equations. Such methods are often called "projection methods" because of the tools used in the underlying mathematical theory. The second type of numerical method approximates the derivatives or integrals in the equation of interest, generally solving approximately for the solution function at a discrete set of points. Most initial value problems for ordinary differential equations and partial differential equations are solved in this way, and the numerical procedures are often called "finite difference methods", primarily for historical reasons.

The same subdivision of methods also applies to the numerical solution of integral equations, although the names differ somewhat. Most numerical methods for solving differential and integral equations also involve both approximation theory and the solution of quite large linear and/or nonlinear systems.

## A. Ordinary Differential Equations

There are two principal types of problems associated with ordinary differential equations (ODE): the initial value problem and the boundary value problem. The numerical methods are quite different for these two types of problems, although many of the same tools from approximation theory are used in designing numerical methods for them. In recent years, there has also been much work on specialized forms of ODE. There are many books available for these problems, and many of them cover more than one problem.

U Ascher, R Mattheij, and R Russell. *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations*, Prentice-Hall, 1988. This is a classic text on this topic.

U Ascher and L Petzold. *Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations*, SIAM Pub., 1998.

K Brenan, S Campbell, and L Petzold. *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*, 2<sup>nd</sup> SIAM Pub., 1996. Differential-algebraic equations have become an important form of mathematical model for many problems in mechanical engineering. One solves differential equations subject to algebraic constraints on the unknowns.

K Burrage. *Parallel and Sequential Methods for Ordinary Differential Equations*, Oxford University Press, 1995. An introductory presentation of solving ODE on parallel and serial computers.

J Butcher. *The Numerical Analysis of Ordinary Differential Equations*, John Wiley, 1987. The author is a major figure in the development of the modern theory of Runge-Kutta methods.

C Gear. *Numerical Initial Value Problems in Ordinary Differential Equations*, Prentice-Hall, 1971. This is the classic work which initiated the study of variable stepsize, variable order methods.

E Hairer, S Norsett, and G Wanner. *Solving Ordinary Differential Equations - I: Nonstiff Problems*, 2<sup>nd</sup> ed., Springer-Verlag, 1993. This and the following volume give a complete coverage of the modern theory of the numerical analysis of initial value problems for ordinary differential equations.

E Hairer and G Wanner. *Solving Ordinary Differential Equations - II: Stiff and Differential-Algebraic Problems*, 2<sup>nd</sup> ed., Springer-Verlag, 1996.

A Iserles. *A First Course in the Numerical Analysis of Differential Equations*, Cambridge University Press, 1996. This was cited earlier in the introduction as giving a

good introduction to the theory of numerical methods for solving ordinary differential equations.

J Sanz-Serna and M Calvo. *Numerical Hamiltonian Problems*, Chapman & Hall, 1994.

L Shampine. *Numerical Solution of Ordinary Differential Equations*, Chapman & Hall, 1994. An excellent text with good coverage of questions of software implementation, by one of the foremost designers of such software.

## B. Partial Differential Equations

This is a truly enormous subject, on the same scale as the entire general area of algebra. It encompasses many types of linear and nonlinear partial differential equations (PDE); and the various types of applications lead to other areas of specialization in studying the mathematics, e.g. the mathematics of fluid flow and the study of the Navier-Stokes equation. Among the most important linear PDE are those of order two; they are classified as elliptic, parabolic, and hyperbolic, and these correspond to different types of physical phenomena. There are important equations of orders other than two, especially of order one; and many of the most important PDE are nonlinear.

Numerical methods are similarly quite varied, and we can merely skim the surface with our references. With hyperbolic problems, finite difference methods are the dominant form of discretization, with some aspects of the treatment of elliptic problems used as tools. Elliptic problems are solved principally using finite difference and finite element methods, with boundary element methods also important. Parabolic problems (linear and nonlinear) were solved traditionally by finite difference methods, but the "method of lines" has become a favored treatment in the past 30 years. We give a sampling of books and apologize for what the reader may consider to be major omissions.

We begin our list of resources and references with a specialist journal; otherwise, the list is alphabetical.

*Numerical Methods for Partial Differential Equations* (ISSN 0749-159X), John Wiley. This is an important journal for research on the numerical solution of partial differential equations.

D Braess. *Finite Elements*, Cambridge University Press, 1997. A good introduction to finite element methods.

F Brezzi and M Fortin. *Mixed and Hybrid Finite Element Methods*, Springer-Verlag, 1991.

W Briggs, V-E Henson, S McCormick. *A Multigrid Tutorial*, 2<sup>nd</sup> ed., SIAM Pub., 2000. The multigrid method is the most powerful iteration method for solving discretizations of elliptic PDE, and this is an up-to-date and well-written introduction to that method.

G Chen and J Zhou. *Boundary Element Methods*, Academic Press, 1992.

P Ciarlet. *The Finite Element Method for Elliptic Problems*, North-Holland, 1978. This is a very complete accounting of the theory underlying the finite element method, together with applications to important physical problems.

V Girault and P-A Raviart. *Finite Element Methods for Navier-Stokes Equations*, Springer-Verlag, 1986. This is a comprehensive reference on the analysis of finite element methods for solving Stokes and Navier-Stokes equations.

A Iserles. *A First Course in the Numerical Analysis of Differential Equations*, Cambridge University Press, 1996. This was cited earlier in the introduction as giving a good introduction to the theory of numerical methods for solving partial differential equations.

C Johnson. *Numerical Solution of Partial Differential Equations by the Finite Element Method*, Cambridge University Press, 1987.

L Lapidus and G Pinder. *Numerical Solution of Partial Differential Equations in Science and Engineering*, John Wiley, 1982. This is an encyclopedic account of the subject.

K Morton and D Mayers. *Numerical Solution of Partial Differential Equations*, Cambridge University Press, 1994.

A Quarteroni and A Valli. *Numerical Approximation of Partial Differential Equations*, Springer-Verlag, 1994. This book covers numerous popular methods for solving various types of PDE (including elliptic, parabolic, hyperbolic, advection-diffusion, Stokes, and Navier-Stokes problems).

Ch Schwab. *p- and hp-Finite Element Methods. Theory and Applications in Solid and Fluid Mechanics*, Oxford University Press, 1998. This discusses variable stepsize variable order finite element methods for solving elliptic PDE.

J Strikwerda. *Finite Difference Schemes and Partial Differential Equations*, Wadsworth, 1989. A very nice general introduction that is well embedded in applications.

J Thomas. *Numerical Partial Differential Equations: Finite Difference Methods*, Springer-Verlag, 1995.

J Thomas. *Numerical Partial Differential Equations: Conservation Laws and Elliptic Equations*, Springer-Verlag, 1999.

V Thomee. *Galerkin Finite Element Methods for Parabolic Problems*, Springer-Verlag, 1997. Finite element methods originated with solving elliptic PDE, and this is an excellent presentation of its extension to parabolic PDE.

## C. Integral equations

Integral equations arise directly and as reformulations of ordinary and partial differential equations. Boundary value problems for differential equations can be reformulated as Fredholm integral equations, and initial value problems can be reformulated as Volterra integral equations. Both of these types of integral equations are more general than the reformulations, and most Fredholm and Volterra integral equations cannot, in turn, be returned to a differential equation formulation. There are also integral equations of many other types, including Cauchy singular integral equations and hypersingular integral equations. All of these have important applications in the natural sciences and engineering.

We begin our list of resources and references with a specialist journal; otherwise, the list is alphabetical.

*Journal of Integral Equations and Applications* (ISSN 0897-3962), Rocky Mountain Mathematics Consortium. This journal is devoted to the study of integral equations, especially to the numerical analysis for them and to applications of them.

K Atkinson. *The Numerical Solution of Integral Equations of the Second Kind*, Cambridge University Press. This is a comprehensive look at linear integral equations of Fredholm type. Chapters 7-9 give an introduction to boundary integral equations and their numerical solution.

C Baker. *The Numerical Treatment of Integral Equations*, Oxford University Press, 1977. This is a classic text that ranges widely in discussing most types of integral equations.

H Brunner and P van der Houwen. *The Numerical Solution of Volterra Equations*, North-Holland Pub., 1986. This summarizes well the literature on solving Volterra integral equations. In more recent years, researchers have extended these results to Volterra integro-differential equations.

D Colton and R Kress. *Inverse Acoustic and Electromagnetic Scattering Theory*, 2<sup>nd</sup> ed., Springer-Verlag, 1998. An excellent presentation of the subject in the title.

C Groetsch. *Inverse Problems in the Mathematical Sciences*, Friedr. Vieweg & Sohn, Braunschweig, 1993. This is a very good introduction to ill-posed inverse problems and their numerical solution. Many such problems are posed as integral equations, and that is the author's focus in this book.

W Hackbusch. *Integral Equations: Theory and Numerical Treatment*, Birkhaeuser Verlag, 1995. This gives a general look at integral equations and their numerical analysis.

R Kress. *Linear Integral Equations*, 2<sup>nd</sup> ed., Springer-Verlag, 1999. This is a masterfully written introduction to the theory of integral equations. In addition, it has several well-written chapters on the numerical solution of integral equations.

P Linz. *Analytical and Numerical Methods for Volterra Equations*, SIAM Pub., 1985.

S Proessdorf and B Silbermann. *Numerical Analysis for Integral and Related Operator Equations*, Birkhaeuser Verlag, 1991. This book gives a quite abstract, and important, framework for the singular integral equations associated with many boundary integral equation reformulations of PDE.

## V. Miscellaneous Important References

There are a number of important references that do not fit easily into the above schemata. We present some of those here.

P Henrici. *Applied and Computational Complex Analysis*, Vols. I, II, and III, John Wiley, 1974-1986. These volumes contain a wealth of information on complex analysis and its application to a wide variety of mathematical problems.

M Overton. *Numerical Computing with IEEE Floating Point Arithmetic*, SIAM Pub., 2001. This is an excellent discussion of floating-point arithmetic for numerical computations, carried out for the format of such arithmetic used on most digital computers.

F Stenger. *Numerical Methods Based on Sinc and Analytic Functions*, Springer-Verlag, 1993. This develops the theory of the sinc function and applies it to a wide variety of problems.

## VI. History of Numerical Analysis

Numerical analysis is both quite old and quite young. It is old in that most people doing mathematics in the past, including the quite distant past, did numerical calculations and developed numerical algorithms. It is young in that much of what we study today has been a consequence of the use of digital computers, and computers continue to shape the area today.

H Goldstine. *A History of Numerical Analysis: From the 16th Through the 19th Century*, Springer-Verlag, 1977. This is a very good presentation of the development of numerical algorithms, beginning with logarithms, looking in depth at the contributions of Newton, and going onto the contributions of Euler and others up through the end of the 1800s.

J-L Chabert, et al.. *A History of Algorithms: From the Pebble to the Microchip*, Springer-Verlag, 1999. This is a history of computing from the perspective of developing algorithms, but it has a significant overlap with numerical computing.

S Nash (editor). *A History of Scientific Computing*, ACM Press, 1990. This is a collection of articles discussing numerical analysis, especially in association with the use of digital computers. It fills in some of the history of numerical analysis in the 20th Century.