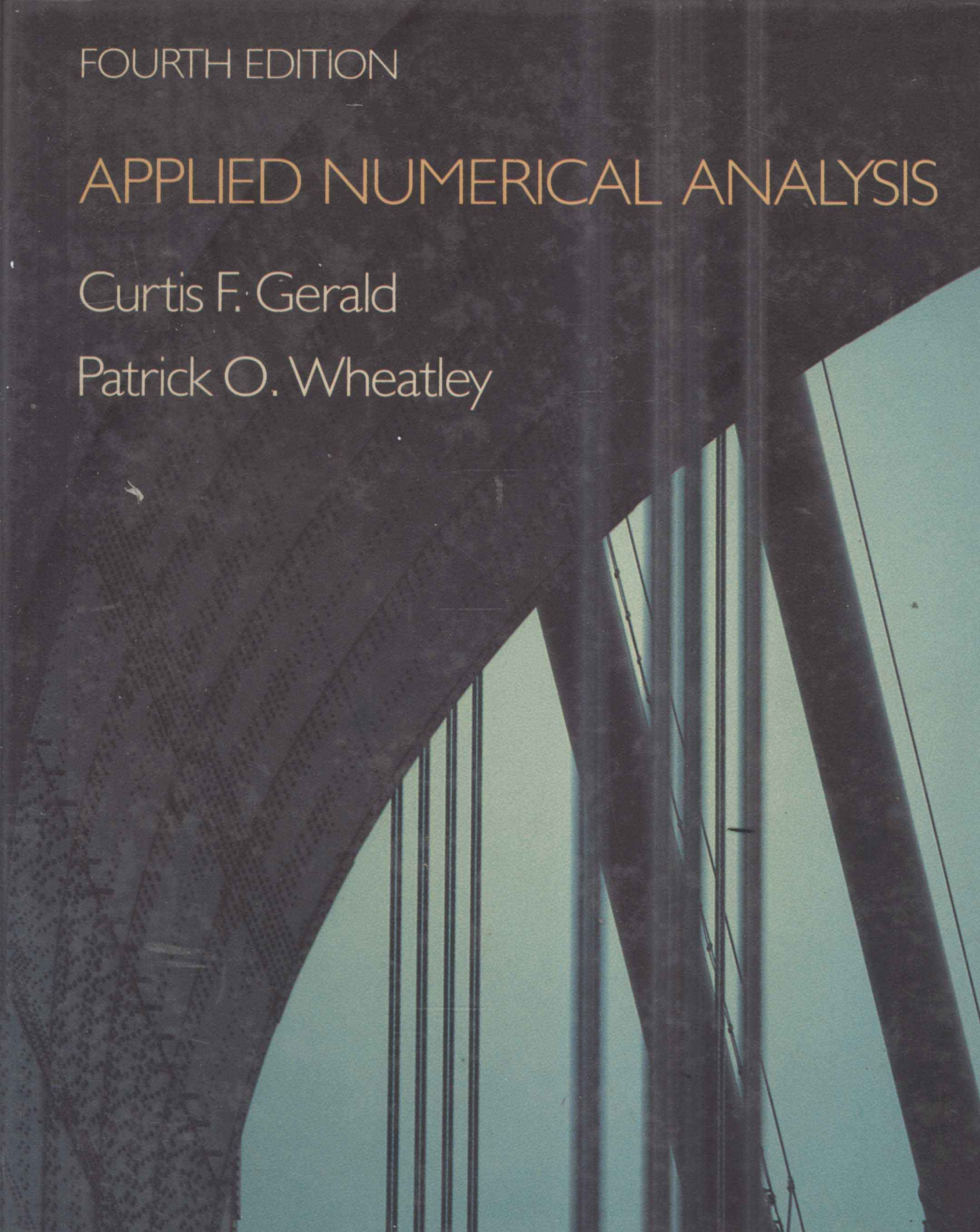
FOURTH EDITION

APPLIED NUMERICAL ANALYSIS

Curtis F. Gerald

Patrick O. Wheatley



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California Polytechnic State University
San Luis Obispo

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To my wife, Elsie, who has been
a sustaining influence from the beginning
C.F.G.

To my wife, Jo Ann,
and my son, Patrick
P.O.W.

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Preface

Applied Numerical Analysis is written for sophomores and juniors in engineering, science, mathematics, and computer science. It is also valuable as a sourcebook for practicing engineers and scientists who need to use numerical procedures to solve problems. We have been gratified to find that many who purchased this book as students keep it as a permanent part of their reference library because its readability and breadth allow them to expand their knowledge of the subject by self-study.

While it is assumed that the reader has a good knowledge of calculus, appropriate topics are reviewed in the context of their use, and an appendix gives a summary of the most important items that are used to develop and analyze numerical procedures. The mathematical notation is purposely kept simple for clarity.

PURPOSE

The purpose of this fourth edition is the same as in previous editions: to give a broad coverage of the field of numerical analysis, emphasizing its practical applications rather than theory. At the same time, methods are compared, errors are analyzed, and relationships to the fundamental mathematical basis for the procedures are presented so that a true understanding of the subject is attained. Clarity of exposition, development through examples, and logical arrangement of topics aid the student to become more and more adept at applying the methods.

CONTENT FEATURES

Applied Numerical Analysis has enjoyed significant success because of several outstanding features. These are retained and amplified in this fourth edition:

- The unusually large number of exercises allows the instructor to select those that are appropriate for the background and interests of the students. These are keyed to the corresponding section of the chapter to assist in this. When the reader is using the book for self-study, the many exercises are an important supplement to the text. In addition to the practice exercises, each chapter has "Applied Problems and Projects" that are more challenging and that illustrate many fields of application of the various numerical procedures.
- By solving the same problem with several different methods, the relative efficiency and effectiveness of the methods become clear (pp. 11, 12, 13, and 27; pp. 98 and 111; pp. 350, 353, 358, 362, 365, and 368).
- A short summary of its contents is given at the beginning of each chapter to provide a preview of what is coming (pp. 1, 86, 180, 264, 347, and so on).
- Most chapters are introduced with an easily understood example that applies the material of the chapter. This motivates the student and shows that the material is of real utility (pp. 2, 87, 181, 349, 472, and so forth).
- Each chapter ends with a summary that reminds the student of what has been covered and suggests that appropriate review be done to ensure that nothing has been overlooked or not learned (pp. 49, 147, 235, 321, and so on).
- The coverage of partial-differential equations in an easily understood manner is unusual in a book at this level.
- Postponing the treatment of computer arithmetic and errors until after the student has been exposed to some numerical methods puts this important topic into proper context and helps in the appreciation of its significance as one factor in the accuracy of the computed result (p. 38).
- Computer programs in FORTRAN are given at the conclusion of each chapter. These implement the more important algorithms and serve as easily understood examples of how the computer can be used to carry out the computations. They do not pretend to be at a professional level of programming, because their purpose is illustrative and clarity would otherwise be sacrificed. We recognize that many instructors prefer a more structured language, but the presence of many subroutines in FORTRAN dictates our choice. We do provide a Pascal version of the programs in the supplements to the text; both versions are provided on diskettes for ease of entering into the local computer system.

FEATURES OF THIS EDITION

We have benefited by suggestions from those who have used the book in its previous editions. Significant new material has been added, and some chapters have been improved through rearrangement or rewriting. The format of the book has been improved. The use of a second color highlights important items and adds interest and variety to the text.

Important revisions include the following:

- The section on Muller's method in Chapter 1 has been moved up, and the difference between this and methods based on a linear approximation to the function has been emphasized (p. 18).

- Sections on computer arithmetic and errors have been rewritten and expanded (pp. 38–46).
- The use of matrix algebra has been broadened throughout the book. This is especially apparent in the discussion of iterative methods in Chapters 2 and 6.
- The relation between Gauss, Gauss–Jordan, and other *LU* methods has been clarified (p. 106).
- The chapter on interpolation has been streamlined and the use of divided differences has been emphasized.
- Other spline-based methods have been added and their use in approximating surfaces has been discussed (pp. 217 and 233).
- The section on adaptive integration has been improved (p. 305).
- We have given more modern versions of higher-order Runge–Kutta methods (p. 358).
- A most significant addition has been an elementary treatment of the finite-element method. This is introduced by an explanation of variational methods in one-dimensional boundary-value problems (p. 426). Finite elements are then applied to elliptic equations (p. 512) and to parabolic equations (p. 573).
- A discussion of the *QR* method for finding eigenvalues is included in Chapter 6.
- The section on fast Fourier transforms has been rewritten and expanded (p. 652).
- More of the programs at the end of each chapter have sample output for the reader to examine. Moreover, we have included new programs that implement adaptive integration, divided differences, the Runge–Kutta–Fehlberg method, and the *QR* technique. We have replaced a program in Chapter 2 with one that implements the *LU* decomposition method for Gaussian elimination.
- The appendix that describes software packages has been updated to cover some newer software, especially that for personal computers.

PEDAGOGICAL FEATURES

We recognize that the student is the most important part of the teaching/learning system and have tried to facilitate his or her understanding by several items, some of which are new in this edition:

- Sections that preview the material lead off each chapter.
- A chapter summary at the end of each chapter reminds the student of what should have been learned.
- The second color makes it easier to recognize the more important equations and algorithms. Color in the illustrations adds interest and makes their message clearer.
- The sections that have been rewritten eliminate some items that may have caused confusion for some students.
- The bibliography has been updated, and selected references have been given at the end of each chapter. This makes it easy for the student to find other treatments of the material, some of which go into more detail than we are able to.

SUPPLEMENTS

A number of supplements are available to assist the instructor:

- A *Solutions Manual* gives the answers to nearly all the exercises and to some of the "Applied Problems and Projects." Hints for other problems or projects are also provided.
- Copies of the programs, both in the FORTRAN version that is printed in the text and in an equivalent Pascal version, are available to adopters. These are on diskettes in IBM PC–compatible form so that they can readily be entered into the local computer system if the instructor wishes to make them available to the student on-line. Alternatively, copies can be provided to students when personal computers are to be used.
- The *Solutions Manual* gives suggestions for how the instructor can select from the text when he or she does not have time to cover all of it. Since our coverage of topics in numerical analysis is unusually broad, such selection is frequently necessary.

ACKNOWLEDGMENTS

We especially want to thank the multitude of our own students whose feedback has helped us to improve over previous editions. Our wives have been supportive during this revision and have helped us with proofreading. Many instructors have given valuable suggestions and constructive criticism.

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C.F.G.
P.O.W.

Contents

2 Solving Sets of Equations 86

3 Interpolating Polynomials 180

4 Numerical Differentiation and Numerical Integration 264

9 Hyperbolic Partial-Differential Equations 592

10 Curve-fitting and Approximation of Functions 624

Appendixes A-1

References A-22

Answers to Selected Exercises A-25

Index I-1

1

Solving Nonlinear Equations

1.0 CONTENTS OF THIS CHAPTER

Chapter 1 introduces you to numerical analysis by explaining how methods of successive approximations can find the solution of a single nonlinear equation. It explains how computer programs can be written to obtain such solutions and gives numerous examples that implement the methods of the chapter.

1.1 THE LADDER IN THE MINE

Illustrates how the methods of the chapter are applied to a realistic problem.

1.2 METHOD OF HALVING THE INTERVAL

Describes an ancient and simple method.

1.3 METHOD OF LINEAR INTERPOLATION

Presents two improvements on halving of intervals; it solves $f(x) = 0$ by using a secant line.

1.4 NEWTON'S METHOD

Is a widely used and rapidly convergent method that uses a tangent line to find a root.

1.5 MULLER'S METHOD

Uses a parabola to approximate the function.

1.6 USE OF $x = g(x)$ METHOD

Departs from the previous techniques and establishes some theory that is used in analyzing the various methods and in setting up for accelerating convergence.

1.1 THE LADDER IN THE MINE

In this book we will begin most chapters with an example that illustrates the application of the numerical techniques covered in the chapter. We will frame these in the context of the real world but simplified. This first example is typical and defines the problem, describes how it can be solved, and ends by pointing out how numerical methods are useful in getting the solution.

It is not uncommon, in applied mathematics, to have to solve a nonlinear equation. If you worked for a mining company the following might be a typical problem.

EXAMPLE There are two intersecting mine shafts that meet at an angle of 123°, as shown in Fig. 1.1. The straight shaft has a width of 7 ft, while the entrance shaft is 9 ft wide. What is the longest ladder that can negotiate the turn? You can neglect the thickness of the ladder members and assume it is not tipped as it is maneuvered around the corner. Your solution should provide for the general case in which the angle A is a variable, as well as for the widths of the shafts.

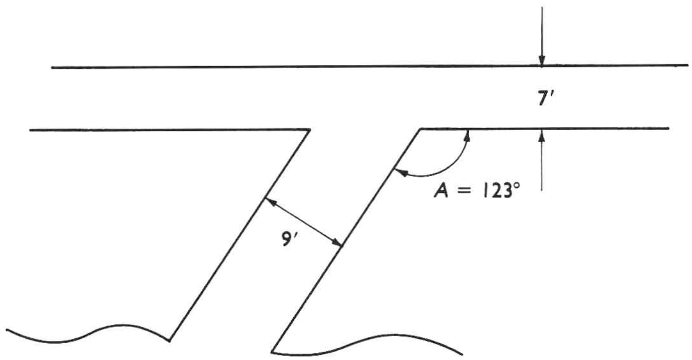

Figure 1.1 ■

Whenever a scientific or engineering problem is solved, there are four general steps to be followed:

1. State the problem clearly, including any simplifying assumptions.
2. Develop a mathematical statement of the problem in a form that can be solved for a numerical answer. This may involve, as in the present case, the use of calculus. In other situations, other mathematical procedures may be employed.
3. Solve the equation(s) that result from step 2. Sometimes this is a method from algebra, but frequently more advanced methods will be needed. The subject matter of this text is numerical procedures that are quite powerful and of general applicability. The result of this step is a numerical answer or set of answers.
4. Interpret the numerical result to arrive at a decision. This will require experience and an understanding of the situation in which the problem was embedded. This interpretation is the hardest part of solving problems and must be learned on the job. This book will emphasize step 3 and will deal to some extent with steps 1 and 2, but step 4 cannot be meaningfully treated in the classroom.

The above description of the problem has taken care of step 1. Now for step 2:

Here is one way to analyze our ladder problem. Visualize the ladder in successive locations as we carry it around the corner; there will be a critical position in which the two ends of the ladder touch the walls while a point along the ladder touches the corner where the two shafts intersect. (See Fig. 1.2.) Let C be the angle between the ladder and the wall when in this critical position. It is usually preferable to solve problems in general terms, so we work with variables C, A, B, w_1, and w_2.

Consider a series of lines drawn in this critical position—their lengths vary with the angle C, and the following relations hold (angles are expressed in radian measure):

$$\ell_1 = \frac{w_2}{\sin B}; \qquad \ell_2 = \frac{w_1}{\sin C};$$

$$B = \pi - A - C;$$

$$\ell = \ell_1 + \ell_2 = \frac{w_2}{\sin(\pi - A - C)} + \frac{w_1}{\sin C}.$$

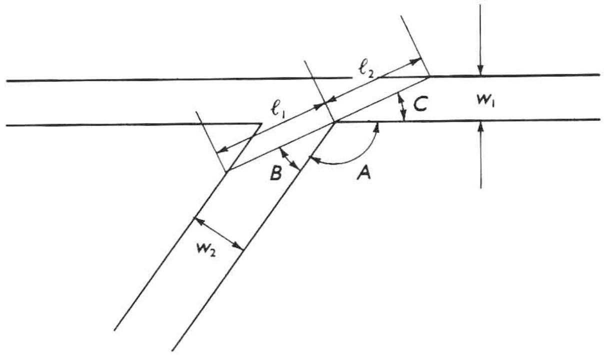

Figure 1.2

The maximum length of ladder that can negotiate the turn is the minimum of ℓ as a function of angle C. We hence set $d\ell/dC = 0$.

$$\frac{d\ell}{dC} = \frac{w_2 \cos(\pi - A - C)}{\sin^2(\pi - A - C)} - \frac{w_1 \cos C}{\sin^2 C} = 0.$$

We can solve the general problem if we can find the value of C that satisfies this equation. With the critical angle determined, the ladder length is given by

$$\ell = \frac{w_2}{\sin(\pi - \mathrm{A} - \mathrm{C})} + \frac{w_1}{\sin C}.$$

As this analysis shows, to solve the specific problem we must solve a transcendental equation for the value of C:

$$\frac{9 \cos(\pi - 2.147 - C)}{\sin^2(\pi - 2.2147 - C)} - \frac{7 \cos C}{\sin C} = 0,$$

and then substitute C into

$$\ell = \frac{9}{\sin(\pi - 2.2147 - C)} + \frac{7}{\sin C},$$

where we have converted 123° into 2.147 radians.

Finding the solution to an algebraic or transcendental equation, as we must do here, is the topic of this first chapter.

In this chapter we study methods to find the roots of an equation, such as in our ladder-in-the-mine example. Much of algebra is devoted to the "solution of equations." In simple situations, this consists of a rearrangement to exhibit the value of the unknown variable as a simple arithmetic combination of the constants of the equation. For second-degree polynomials, this can be expressed by the familiar quadratic formula. For third- and fourth-degree polynomials, formulas exist but are so complex as to be rarely used; for higher-degree equations it has been proved that finding the solution through a formula is impossible. Most transcendental equations (involving trigonometric or exponential functions) are likewise intractable.

Even though it is difficult if not impossible to exhibit the solution of such equations in explicit form, numerical analysis provides a means where a solution may be found, or at least approximated as closely as desired. Many of these numerical procedures follow a scheme that may be thought of as providing a series of successive approximations, each more precise than the previous one, so that enough repetitions of the procedure eventually give an approximation that differs from the true value by less than some arbitrary error tolerance. Numerical procedures are thus seen to resemble the limit concept of mathematical analysis.

When a numerical solution that satisfies the transcendental equation above has been obtained, we have completed step 3 of the general procedure. The rest of this chapter treats several methods for doing this. We will not do step 4, but in this case it would consist of deciding if the maximum-length ladder that can be carried into the mine is long enough. If it is not, a decision must be made about the remedy. Perhaps this would be to use an extension ladder or to cut a notch in the corner of the wall.

This example shows how important calculus can be in solving practical problems. You will also find that calculus is a critical component in the analysis of numerical methods. Appendix A provides a summary of some of the most important elements of calculus. Look this over now to see if there are items that you should review.

1.2 METHOD OF HALVING THE INTERVAL

This first chapter describes methods for solving equations; that is, given an equation of the form $f(x) = 0$, what value(s) of x satisfy the equation? There are several obvious possibilities that we will not cover, such as trial and error (trying various values of x until we discover one that works) and drawing a graph of values of $f(x)$ versus x-values, seeing where the plot crosses the x-axis. Our methods will be more systematic than these, although a rough graph is frequently helpful in understanding the nature of the function and approximately where the function has roots.

The first numerical procedure that we will study is that of *interval halving*.* Consider the cubic

$$f(x) = x^3 + x^2 - 3x - 3 = 0.$$

At $x = 1$, f has the value -4. At $x = 2$, f has the value $+3$. Since the function is continuous, it is obvious that the change in sign of the function between $x = 1$ and $x = 2$ guarantees at least one root on the interval (1, 2). (See Fig. 1.3.)

Suppose we now evaluate the function at $x = 1.5$ and compare the result to the function values at $x = 1$ and $x = 2$. Since the function changes sign between $x = 1.5$ and $x = 2$, a root lies between these values. We can obviously continue this interval halving to determine a smaller and smaller interval within which a root must lie. For this example, continuing the process leads eventually to an approximation to the root at $x = \sqrt{3} = 1.7320508075\ldots$ The process is illustrated in Fig. 1.4.

*The method, also known as the *Bolzano method*, is of ancient origin. Some authors call it the *bisection method*.