NUMERICAL METHODS FOR MATHEMATICS, SCIENCE, AND ENGINEERING

SECOND EDITION

JOHN H. MATHEWS

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Numerical Methods

for Mathematics, Science, and Engineering

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Numerical Methods

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Preface

Numerical Methods for Mathematics, Science, and Engineering, Second Edition, provides a rudimentary introduction to numerical analysis for either a single course or a year-long sequence and is suitable for undergraduate students in mathematics, science, and engineering. Ample material is presented so that instructors will be able to select topics appropriate to their needs. It is assumed that the reader is familiar with calculus and has taken a structured programming language such as BASIC, C, FORTRAN, or Pascal.

Students of all backgrounds enjoy numerical methods and this is kept in mind throughout the book. A variety of examples and problems sharpen one's skill in both the theory and practice of numerical analysis. Computer calculations are presented in the form of tables and graphs whenever possible so that the resulting numerical approximations are easier to interpret. Many figures for this second edition were obtained by using the software Mathematica™. The algorithms for the various numerical processes are given in pseudo-code and are easy for students to translate into BASIC, C, FORTRAN, or Pascal. The structure of the algorithms makes them easy to adapt to a programming environment such as MAPLE, Mathematica™, or MATLAB™.

Emphasis is placed on understanding why numerical methods work and their limitations. This is not easy for a first course; it involves a balance between theory, error analysis, and readability by students. An error analysis for each method is presented in a fashion that is appropriate for the method at hand and yet does not turn off the reader. A mathematical derivation for each method is given that uses elementary results and builds the student's understanding of numerical analysis. Computer assignments implementing the algorithms give students an opportunity to practice their skills at scientific programming.

Shorter numerical exercises can be carried out with a pocket calculator/computer, but others can be done more efficiently by computer. I have tried to be flexible on this issue and do not specify the precise hardware that must be used to solve any given problem. It is left for instructors to guide their students regarding the pedagogical use of numerical computations. Instructors must make assignments that are appropriate to the availability of computing resources for their particular courses.

The use of numerical analysis hardware, software packages, and libraries is encouraged. Sometimes the phrase "use a computer" occurs in an exercise. This must be interpreted in view of a school's particular learning environment. Instructors have the flexibility to permit their students to use the automatic root-finding and numerical integration routines found on some pocket calculator/computers or to use other popular software such as MathCad™, MATLAB™, Mathematica™, and IMSL™. Also, algorithms in the text are available in MATLAB™, FORTRAN, and Pascal and Mathematica™ notebooks for both IBM PC-compatible computers and APPLE Macintosh computers. These materials can be used to assist students in performing their "numerical experiments."

Acknowledgments

I would like to express my gratitude to all the people whose efforts contributed to both the first and second editions of this book. I thank the students at California State University, Fullerton. I thank my colleagues Stephen Goode, Mathew Koshy, Edward Sabotka, Harris Shultz, and Soo Tang Tan for their support in the first edition and Russell Egbert, William Gearhart, Ronald Miller, and John Pierce for their suggestions for the second edition. I also thank James Friel, chairman of the Mathematics Department at CSUF, for his encouragement.

I also express my gratitude to the reviewers who made recommendations for the first edition: Kenneth P. Bube, University of California, Los Angeles; Michael A. Freedman, University of Alaska, Fairbanks; Peter J. Gingo, University of Akron; George B. Miller, Central Connecticut State University; and Walter M. Patterson III, Lander College. For the second edition, I thank Richard T. Bumby, Rutgers University; Robert L. Curry, U.S. Army; Bruce Edwards, University of Florida; and David R. Hill, Temple University.

Finally, I wish to express my appreciation to the staff at Prentice Hall, especially Steven Conmy, mathematics editor, and Kathleen Lafferty, production editor, for their assistance and encouragement.

Software disks for both IBM and Macintosh computers are available to instructors who adopt the textbook. They include Pascal, FORTRAN and Matlab source code and Mathematica notebooks for all the algorithms. Inquires about the availability can be made to Prentice Hall, Inc. or the author. Comments and suggestions for improvements to the book and supporting software are welcome and can be made directly to me at (714) 773-3631 or via E-mail:
MATHEWS@FULLERTON.EDU.

John H. Mathews

Contents

1

Preliminaries

Consider the function $f(x) = \cos(x)$, its derivative $f'(x) = -\sin(x)$, and the integral $F(x) = \sin(x)$. These formulas were studied in calculus. The former is used to determine the slope $m = f'(x_0)$ of the curve $y = f(x)$ at a point $(x_0, f(x_0))$, and the latter is used to compute the area under the curve for $a \le x \le b$.

The slope at the point $(\pi/2, 0)$ is $m = f'(\pi/2) = -1$ and can be used to find the tangent line at this point [Figure 1.1(a)]:

$$y_{\tan} = m\left(x - \frac{\pi}{2}\right) + 0 = f'\left(\frac{\pi}{2}\right)\left(x - \frac{\pi}{2}\right) = -x + \frac{\pi}{2}.$$

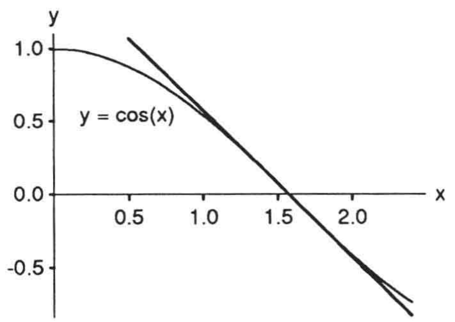

Figure 1.1 (a) The tangent line to the curve $y = \cos(x)$ at the point $(\pi/2, 0)$.

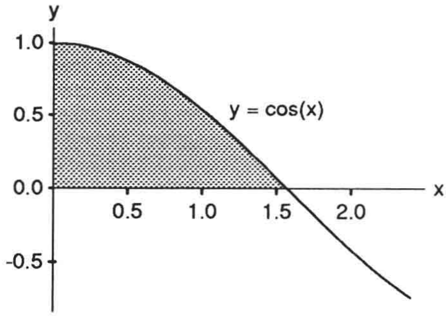

Figure 1.1 (b) The area under the curve $y = \cos(x)$ over the interval $[0, \pi/2]$.

The area under the curve for $0 \le x \le \pi/2$ is computed using an integral [Figure 1.1(b)]:

$$\text{area} = \int_0^{\pi/2} \cos(x)\,dx = F\left(\frac{\pi}{2}\right) - F(0) = \sin\left(\frac{\pi}{2}\right) - 0 = 1.$$

These are some of the results that we will need to use from calculus.

1.1 REVIEW OF CALCULUS

It is assumed that the reader is familiar with the notation and subject matter covered in the undergraduate calculus sequence. This included the topics real and complex numbers, continuity, limits, differentiation, integration, sequences, and series. Throughout the book we refer to the following results. They are illustrated with numerical examples that are characteristic of the study of numerical analysis.

Limits and Continuity

Definition 1.1. Assume that $f(x)$ is defined on the set S of real numbers. Then f is said to have the **limit** L at $x = x_0$, and we write

$$\lim_{x \to x_0} f(x) = L, \tag{1}$$

if given any $\epsilon > 0$, there exists a $\delta > 0$ such that whenever $x \in S$,

$$0 < |x - x_0| < \delta \quad \text{implies that} \quad |f(x) - L| < \epsilon.$$

When the h-increment notation $x = x_0 + h$ is used, equation (1) is equivalent to

$$\lim_{h \to 0} f(x_0 + h) = L. \tag{2}$$

Definition 1.2. Assume that $f(x)$ is defined on a set S of real numbers and let $x_0 \in S$. Then f is said to be **continuous** at $x = x_0$ if

$$\lim_{x \to x_0} f(x) = f(x_0). \tag{3}$$

The function f is said to be continuous on S if it is continuous at each point $x \in S$. The notation $C(S)$ stands for the set of all functions continuous on S. When S is an interval, the parentheses in this notation are omitted (e.g., the set of all functions continuous on the closed interval $[a, b]$ is denoted $C[a, b]$). When the h-increment notation $x = x_0 + h$ is used, equation (3) is equivalent to

$$\lim_{h \to 0} f(x_0 + h) = f(x_0). \tag{4}$$

For example, consider $f(x) = \cos(x) - \sqrt{2}/2$ over $[0, 0.6]$ and the value $x_0 = 0.4$ with the corresponding function value $y_0 = f(x_0) = f(0.4) = 0.21395$. For illustration, let us choose the tolerance as $\epsilon = 0.04$ and determine the corresponding δ. If x is restricted to lie in the interval $0.27998 < x < 0.49270$, the function value satisfy

$$f(x_0) - \epsilon = 0.17395 < f(x) < 0.25395 = f(x_0) + \epsilon.$$

Thus for $\epsilon = 0.04$ we choose $\delta = \min\{0.4 - 0.27998, 0.49270 - 0.4\} = \min\{0.12002, 0.09270\} = 0.09270$. Points on the portion of the graph $y = f(x)$ above the interval $[x_0 - \delta, x_0 + \delta] = [0.30730, 0.49270]$ will have y-coordinates that lie in $[y_0 - \epsilon, y_0 + \epsilon] = [0.17395, 0.25395]$. This portion of the graph is highlighted in Figure 1.2.

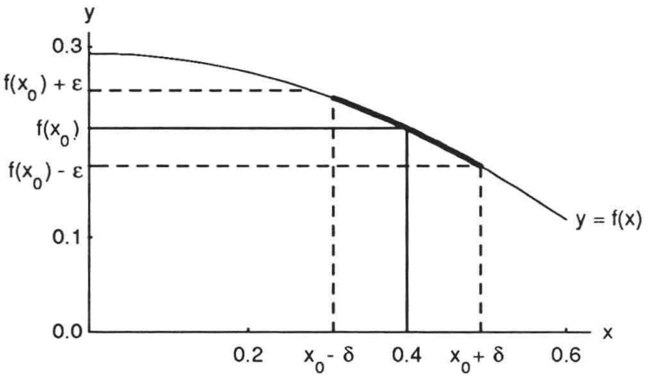

Figure 1.2 Investigating the continuity of $f(x) = \cos(x) - \sqrt{2}/2$ at $x_0 = 0.4$

Definition 1.3. Suppose that $\{x_n\}_{n=1}^{\infty}$ is an infinite sequence. Then the sequence is said to have the limit L, and we write

$$\lim_{n \to \infty} x_n = L, \tag{5}$$

if given any $\epsilon > 0$, there exists a positive integer $N = N(\epsilon)$ such that

$$n > N \quad \text{implies that} \quad |x_n - L| < \epsilon.$$

When a sequence has a limit, we say that it is a **convergent sequence**. Another popular notation is that $x_n \to L$ as $n \to \infty$. Equation (5) is equivalent to

$$\lim_{n \to \infty} (L - x_n) = 0. \tag{6}$$

Thus we can view the sequence $\epsilon_n = L - x_n$ as an **error sequence**.

For example, if $x_n = [2n^3 + n\sin(n)]/(n^3 + 3n + 1)$, then $\lim_{n\to\infty} x_n = 2$, so that $L = 2$. The error sequence $\epsilon_n = 2 - x_n$ tends to zero as $n \to \infty$. Figures 1.3(a) and (b) shows the behavior of $\{x_n\}$ and $\{\epsilon_n\}$.

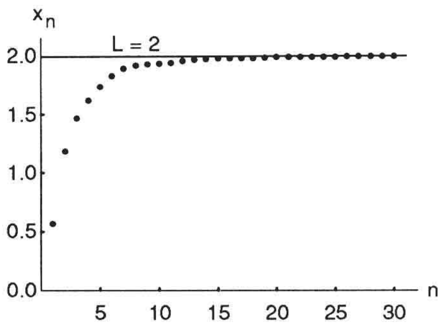

Figure 1.3 (a) A sequence $\{x_n\}$ where $L = 2 = \lim_{n\to\infty} x_n$.

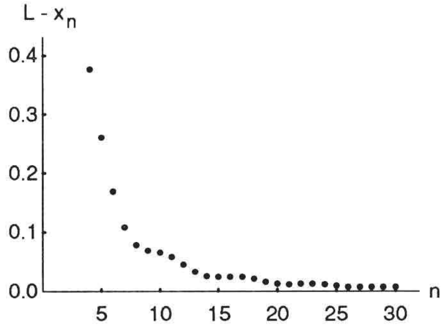

Figure 1.3 (b) The error sequence $\{\epsilon_n\} = \{L - x_n\}$ where $\lim_{n\to\infty} \epsilon_n = \lim_{n\to\infty} L - x_n = 0$.

Theorem 1.1. Assume that $f(x)$ is defined on the set S and $x_0 \in S$. The following statements are equivalent:

$$\text{The function } f \text{ is continuous at } x_0. \tag{7}$$

$$\text{If } \lim_{n\to\infty} x_n = x_0, \text{ then } \lim_{n\to\infty} f(x_n) = f(x_0). \tag{8}$$

Theorem 1.2 (Intermediate Value Theorem). Assume that $f \in C[a, b]$ and L is any number between $f(a)$ and $f(b)$. Then there exists a value c with $a < c < b$ such that $f(c) = L$.

For example, consider $f(x) = \cos(x - 1)$ over $[0, 1]$ and the constant $L = 0.8$. Then the solution to $f(x) = 0.8$ over $[0, 1]$ is $c_1 = 0.356499$. In the interval $[1, 2.5]$ the solution to $f(x) = 0.8$ is $c_2 = 1.643502$. These two cases are shown in Figure 1.4.

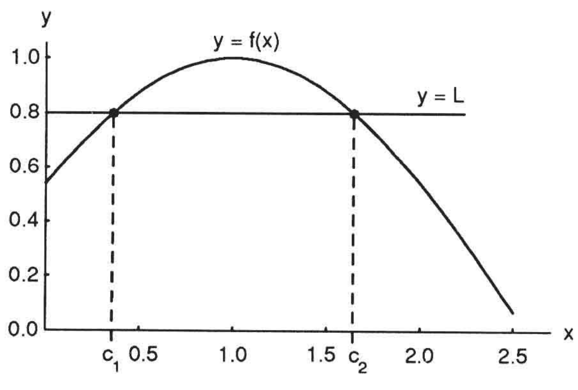

Figure 1.4 The intermediate value theorem applied to the function $f(x) = \cos(x - 1)$ over $[0, 1]$ and over the interval $[1, 2.5]$.

Theorem 1.3 (Extreme Value Theorem for a Continuous Function). Assume that $f \in C[a, b]$. Then there exists a lower bound M_1 and an upper bound M_2 and two numbers $x_1, x_2 \in [a, b]$ such that

$$M_1 = f(x_1) \le f(x) \le f(x_2) = M_2 \qquad \text{whenever} \quad x \in [a, b]. \tag{9}$$

We sometimes express this by writing

$$M_1 = f(x_1) = \min_{a \le x \le b} \{f(x)\} \qquad \text{and} \qquad M_2 = f(x_2) = \max_{a \le x \le b} \{f(x)\}. \tag{10}$$

Differentiable Functions

Definition 1.4. Assume that $f(x)$ is defined on an open interval containing x_0. Then f is said to be differentiable at x_0 if

$$\lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0} = f'(x_0) \tag{11}$$

exists. When this limit exists it is denoted by $f'(x_0)$ and is called the **derivative** of f at x_0. An equivalent way to express this limit is to use the h-increment notation:

$$\lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0). \tag{12}$$

A function that has a derivative at each point in S is said to be **differentiable** on S. The number $m = f'(x_0)$ is the slope of the tangent line to the curve $y = f(x)$ at $(x_0, f(x_0))$.

For example, let $f(x) = \ln(x)$, then $f'(x) = 1/x$. For $x_0 = 2$ and $h = 0.01$ we have the approximation

$$f'(x_0) = \frac{1}{2} \approx 0.4988 = \frac{0.698135 - 0.693147}{0.01} = \frac{f(2.01) - f(2.00)}{0.01}$$
$$= \frac{f(x_0 + h) - f(x_0)}{h}.$$

Theorem 1.4. If $f(x)$ is differentiable at $x = x_0$, then $f(x)$ is continuous at $x = x_0$.

Theorem 1.5 (Rolle's Theorem). Assume that $f \in C[a, b]$ and $f'(x)$ exists for all $a < x < b$. If $f(a) = f(b) = 0$, then there exists a value c, with $a < c < b$, such that $f'(c) = 0$.

Theorem 1.6 (Mean Value Theorem). Assume that $f \in C[a, b]$ and $f'(x)$ exists for all $a < x < b$. Then there exists a number c, with $a < c < b$, such that

$$f'(c) = \frac{f(b) - f(a)}{b - a} = m. \tag{13}$$

For example, consider $f(x) = \sin(x)$ over $[a, b] = [0.1, 2.1]$. Then

$$m = \frac{f(b) - f(a)}{b - a} = \frac{f(2.1) - f(0.1)}{2.1 - 0.1} = \frac{0.863209 - 0.099833}{2.1 - 0.1} = 0.381688.$$

Using $f'(x) = \cos(x)$, the solution to $f'(c) = \cos(c) = 0.381688 = m$ is $c = 1.179174$. The line that goes through the points $(a, f(a))$ and $(b, f(b))$ is $y = 0.0998334 + 0.381688(x - 0.1) = 0.0616646 + 0.381688x$ and the line tangent to the curve at the point $(c, f(c))$ is $y = 0.924291 + 0.381688(x - 1.179174) = 0.474215 + 0.381688x$. The graphs of $f(x)$ and these two lines are shown in Figure 1.5.

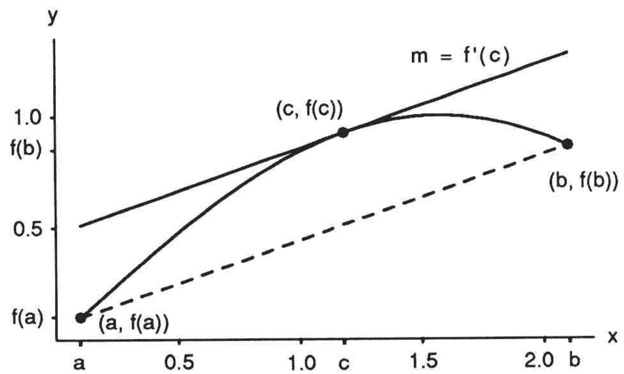

Figure 1.5 The mean value theorem applied to $f(x) = \sin(x)$ over the interval $[0.1, 2.1]$.

Theorem 1.7 (Extreme Value Theorem for a Diffentiable Function). Assume that $f \in C[a, b]$ and $f'(x)$ exists for all $a < x < b$. Then there exists a lower bound M_1 and an upper bound M_2 and two numbers $x_1, x_2 \in [a, b]$ such that

$$M_1 = f(x_1) \le f(x) \le f(x_2) = M_2 \qquad \text{whenever } x \in [a, b]. \tag{14}$$

The numbers x_1 and x_2 occur either at endpoints of $[a, b]$ or where $f'(x) = 0$.

For example, consider $f(x) = 35 + 59.5x - 66.5x^2 + 15x^3$ over $[0, 3]$. Then $f'(x) = 59.5 - 133x + 45x^2$ and the solutions to $f'(x) = 0$ are $x_1 = 0.54955101$ and $x_2 = 2.4060045$. The minimum and maximum values of f over $[0, 3]$ are:

$$\min\{f(a), f(b), f(x_1), f(x_2)\} = \min\{35, 20, 50.104383, 2.118497\} = 2.118497$$

and

$$\max\{f(a), f(b), f(x_1), f(x_2)\} = \max\{35, 20, 50.104383, 2.118497\} = 50.104383,$$

respectively. The situation is shown in Figure 1.6.

Theorem 1.8 (Generalized Rolle's Theorem). Assume that $f \in C[a, b]$ and that $f'(x), f''(x), \ldots, f^{(n)}(x)$ exist over (a, b) and $x_0, x_1, \ldots, x_n \in [a, b]$. If $f(x_j) = 0$ for $j = 0, 1, \ldots, n$, then there exists a value c, with $a < c < b$, such that

$$f^{(n)}(c) = 0. \tag{15}$$

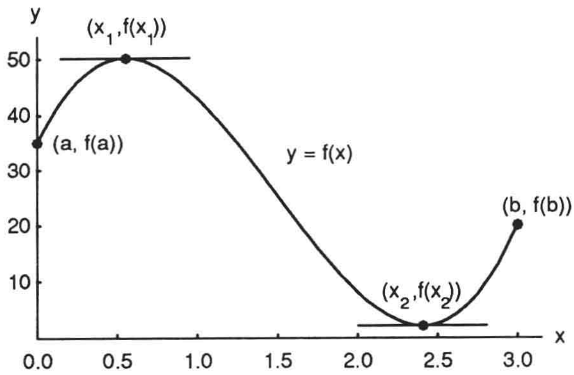

Figure 1.6 The extreme value theorem applied to the function $f(x) = 35 + 59.5x - 66.5x^2 + 15x^3$ over the interval $[0, 3]$.

Integrals

Theorem 1.9 (First Fundamental Theorem). If f is continuous over $[a, b]$, then there exists a function F, called the **antiderivative** of f, such that

$$\int_a^b f(x)\,dx = F(b) - F(a) \qquad \text{where} \quad F'(x) = f(x). \tag{16}$$

Theorem 1.10 (Second Fundamental Theorem). If f is continuous over $[a, b]$ and $a < x < b$, then

$$\frac{d}{dx}\int_a^x f(t)\,dt = f(x). \tag{17}$$

Theorem 1.11 (Mean Value Theorem for Integrals). Assume that $f \in C[a, b]$ for $a \leq x \leq b$. Then there exists a number c with $a < c < b$ such that

$$\frac{1}{b-a}\int_a^b f(x)\,dx = f(c). \tag{18}$$

For example, consider $f(x) = \sin(x) + \frac{1}{3}\sin(3x)$ over the interval $[a, b] = [0, 2.5]$. The indefinite integral is $F(x) = -\cos(x) - \frac{1}{9}\cos(3x)$. The average value for the integral is:

$$\frac{1}{2.5 - 0}\int_0^{2.5} f(x)\,dx = \frac{F(2.5) - F(0.0)}{2.5} = \frac{0.762629 - (-1.111111)}{2.5} = \frac{1.873740}{2.5}$$
$$= 0.749496.$$

There are three solutions to the equation $f(c) = 0.749496$ over the interval $[0, 2.5]$: $c_1 = 0.440565$, $c_2 = 1.268010$, and $c_3 = 1.873583$. The area of the rectangle with base $b - a = 2.5$ and height $f(c_j) = 0.749496$ is $(b - a)f(c_j) = 1.873740$ and has the same