Numerical Methods Using MATLAB Third Edition

Numerical Methods

Using MATLAB

Third Edition

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Preface

This book provides a fundamental introduction to numerical analysis suitable for undergraduate students in mathematics, computer science, physical sciences, and engineering. It is assumed that the reader is familiar with calculus and has taken a structured programming course. The text has enough material fitted modularly for either a single-term course or a year sequence. In short, the book contains enough material so instructors will be able to select topics appropriate to their needs.

Students of various backgrounds should find numerical methods quite interesting and useful, and this is kept in mind throughout the book. Thus, there is a wide variety of examples and problems that help to 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 visualize and interpret. MATLAB programs are the vehicle for presenting the underlying numerical algorithms.

Emphasis is placed on understanding why numerical methods work and their limitations. This is challenging and involves a balance between theory, error analysis, and readability. An error analysis for each method is presented in a fashion that is appropriate for the method at hand, 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 calculus. Computer assignments using MATLAB give students an opportunity to practice their skills at scientific programming.

Shorter numerical exercises can be carried out with a pocket calculator/computer, and the longer ones can be done using MATLAB subroutines. It is left for the instructor to guide the students regarding the pedagogical use of numerical computations. Each instructor can make assignments that are appropriate to the available computing resources. Experimentation with the MATLAB subroutine libraries is encouraged. These materials can be used to assist students in the completion of the numerical analysis component of computer laboratory exercises.

This Third Edition grows out of much polishing of the narrative for the Second Edition. For example, the QR method has been added to the chapter on Eigenvalues and Eigenvectors. New to this edition is the explicit use of the software MATLAB. An appendix gives an introduction to MATLAB syntax. Examples have been added throughout the text with MATLAB and complete MATLAB programs are given in each section. An instructor's disk is available upon request from the publisher.

Previously we took the attitude that any software program that students mastered would work fine. However, many students entering this course have yet to master a programming language (computer science students excepted). MATLAB has become the tool of nearly all engineers and applied mathematicians, and its newest versions have improved the programming aspects. So we think that students will have an easier and more productive time in this MATLAB version of our text.

Acknowledgments

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Suggestions for improvements and additions to the book are always welcome and can be made by corresponding directly with the authors.

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Preliminaries

Consider the function $f(x) = \cos(x)$, its derivative $f'(x) = -\sin(x)$, and its antiderivative $F(x) = \sin(x) + C$. 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 (see Figure 1.1(a)):

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

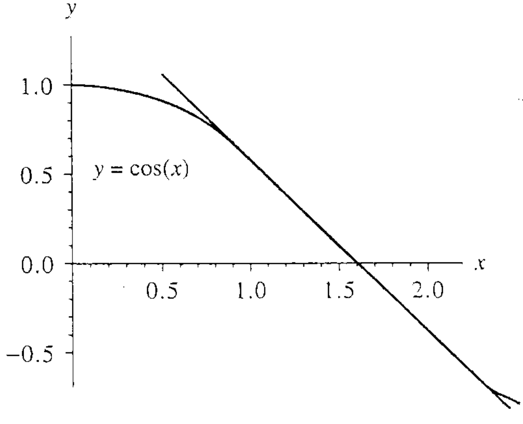

Figure 1.1 (a) The tangent line to the curve $y = \cos(x)$ at the point $(\pi/2, 0)$.

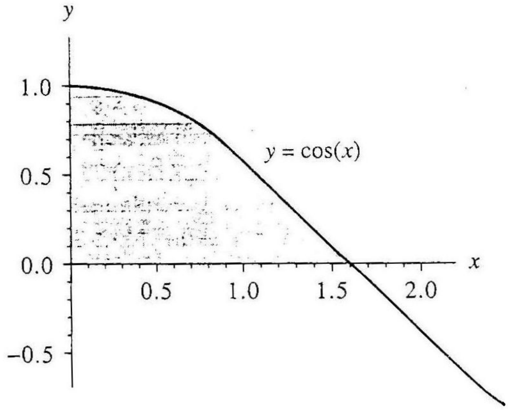

Figure 1.1 (b) The area under the curve $y = \cos(x)$ over the interval $[0, \pi/2]$.

The area under the curve for $0 \leq x \leq \pi/2$ is computed using an integral (see 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 should have included the topics of limits, continuity, differentiation, integration, sequences, and series. Throughout the book we refer to the following results.

Limits and Continuity

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

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

if, given any $\epsilon > 0$, there exists a $\delta > 0$ such that, whenever $x \in S$, $0 < |x - x_0| < \delta$ implies that $|f(x) - L| < \epsilon$. When the h-increment notation $x = x_0 + h$ is used, equation (1) becomes

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

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 $C^n(S)$ stands for the set of all functions f such that f and its first n derivatives are continuous on S. When S is an interval, say $[a, b]$, then the notation $C^n[a, b]$ is used. As an example, consider the function $f(x) = x^{4/3}$ on the interval $[-1, 1]$. Clearly, $f(x)$ and $f'(x) = (4/3)x^{1/3}$ are continuous on $[-1, 1]$, while $f''(x) = (4/9)x^{-2/3}$ is not continuous at $x = 0$. ▲

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

$$\lim_{n \to \infty} x_n = L, \tag{4}$$

if, given any $\epsilon > 0$, there exists a positive integer $N = N(\epsilon)$ such that $n > N$ implies that $|x_n - L| < \epsilon$. ▲

When a sequence has a limit, we say that it is a ***convergent sequence***. Another commonly used notation is "$x_n \to L$ as $n \to \infty$." Equation (4) is equivalent to

$$\lim_{n \to \infty} (x_n - L) = 0. \tag{5}$$

Thus we can view the sequence $\{\epsilon_n\}_{n=1}^{\infty} = \{x_n - L\}_{n=1}^{\infty}$ as an ***error sequence***. The following theorem relates the concepts of continuity and convergent sequence.

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

(6)

(a) The function f is continuous at x_0.

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

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 number c, with $c \in (a, b)$, such that $f(c) = L$.

Example 1.1. The function $f(x) = \cos(x - 1)$ is continuous over $[0, 1]$, and the constant $L = 0.8 \in (\cos(0), \cos(1))$. The solution to $f(x) = 0.8$ over $[0, 1]$ is $c_1 = 0.356499$. Similarly, $f(x)$ is continuous over $[1, 2.5]$, and $L = 0.8 \in (\cos(2.5), \cos(1))$. The solution to $f(x) = 0.8$ over $[1, 2.5]$ is $c_2 = 1.643502$. These two cases are shown in Figure 1.2. ■

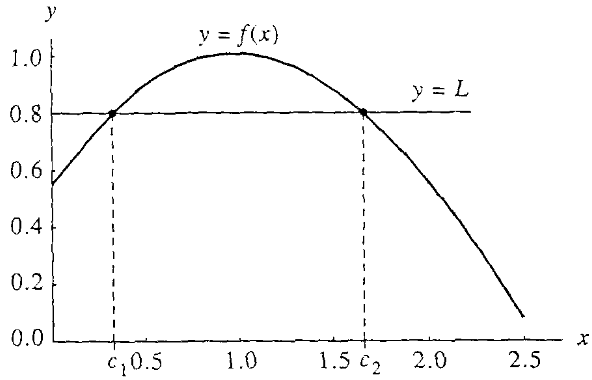

Figure 1.2 The intermediate value theorem applied to the function $f(x) = \cos(x - 1)$ over $[0, 1]$ and over the interval $[1, 2.5]$.

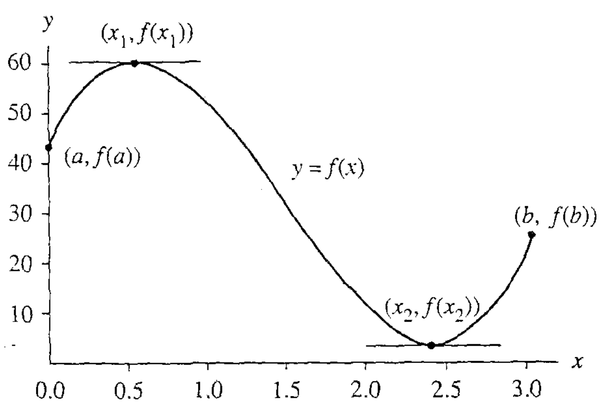

Figure 1.3 The extreme value theorem applied to the function $f(x) = 35 + 59.5x - 66.5x^2 + 15x^3$ over the interval $[0, 3]$.

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, an upper bound M_2, and two numbers $x_1, x_2 \in [a, b]$ such that

$$(7) \qquad M_1 = f(x_1) \le f(x) \le f(x_2) = M_2 \quad \text{whenever } x \in [a, b].$$

We sometimes express this by writing

$$(8) \qquad M_1 = f(x_1) = \min_{a \le x \le b} \{f(x)\} \quad \text{and} \quad M_2 = f(x_2) = \max_{a \le x \le b} \{f(x)\}.$$

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

$$(9) \qquad \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

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:

$$\lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0). \tag{10}$$

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

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

It follows from Theorem 1.3 that, if a function f is differentiable on a closed interval $[a, b]$, then its extreme values occur at the end points of the interval or at the critical points (solutions of $f'(x) = 0$) in the open interval (a, b).

Example 1.2. The function $f(x) = 15x^3 - 66.5x^2 + 59.5x + 35$ is differentiable on $[0, 3]$. The solutions to $f'(x) = 45x^2 - 123x + 59.5 = 0$ are $x_1 = 0.54955$ and $x_2 = 2.40601$. The maximum and minimum values of f on $[0, 3]$ are:

$$\min\{f(0), f(3), f(x_1), f(x_2)\} = \min\{35, 20, 50.10438, 2.11850\} = 2.11850$$

and

$$\max\{f(0), f(3), f(x_1), f(x_2)\} = \max\{35, 20, 50.10438, 2.11850\} = 50.10438.$$ ■

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

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

$$f'(c) = \frac{f(b) - f(a)}{b - a}. \tag{11}$$

Geometrically, the Mean Value Theorem says that there is at least one number $c \in (a, b)$ such that the slope of the tangent line to the graph of $y = f(x)$ at the point $(c, f(c))$ equals the slope of the secant line through the points $(a, f(a))$ and $(b, f(b))$.

Example 1.3. The function $f(x) = \sin(x)$ is continuous on the closed interval $[0.1, 2.1]$ and differentiable on the open interval $(0.1, 2.1)$. Thus, by the Mean Value Theorem, there is a number c such that

$$f'(c) = \frac{f(2.1) - f(0.1)}{2.1 - 0.1} = \frac{0.863209 - 0.099833}{2.1 - 0.1} = 0.381688.$$

The solution to $f'(c) = \cos(c) = 0.381688$ in the interval $(0.1, 2.1)$ is $c = 1.179174$. The graphs of $f(x)$, the secant line $y = 0.381688x + 0.099833$, and the tangent line $y = 0.381688x + 0.474215$ are shown in Figure 1.4. ■

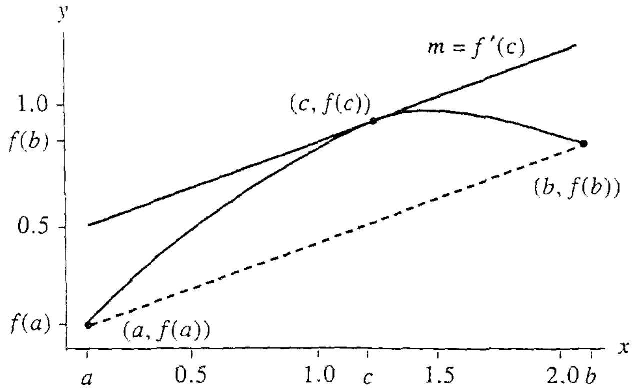

Figure 1.4 The mean value theorem applied to $f(x) = \sin(x)$ over the interval $[0.1, 2.1]$.

Theorem 1.7 (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 number c, with $c \in (a, b)$, such that $f^{(n)}(c) = 0$.

Integrals

Theorem 1.8 (First Fundamental Theorem). If f is continuous over $[a, b]$ and F is any antiderivative of f on $[a, b]$, then

$$\int_a^b f(x)\,dx = F(b) - F(a) \quad \text{where } F'(x) = f(x). \tag{12}$$

Theorem 1.9 (Second Fundamental Theorem). If f is continuous over $[a, b]$ and $x \in (a, b)$, then

$$\frac{d}{dx}\int_a^x f(t)\,dt = f(x). \tag{13}$$

Example 1.4. The function $f(x) = \cos(x)$ satisfies the hypotheses of Theorem 1.9 over the interval $[0, \pi/2]$, thus by the chain rule

$$\frac{d}{dx}\int_0^{x^2} \cos(t)\,dt = \cos(x^2)(x^2)' = 2x\cos(x^2).$$ ■

Theorem 1.10 (Mean Value Theorem for Integrals). Assume that $f \in C[a, b]$. Then there exists a number c, with $c \in (a, b)$, such that

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

The value $f(c)$ is the average value of f over the interval $[a, b]$.

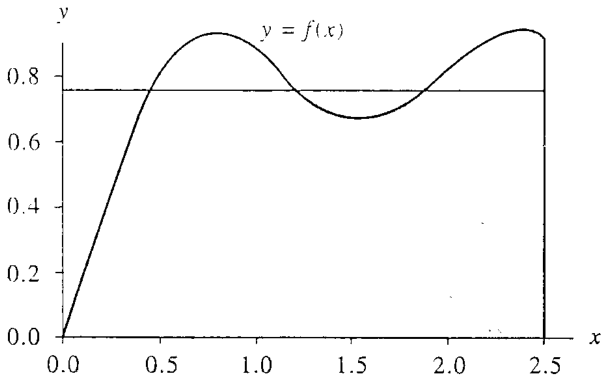

Figure 1.5 The mean value theorem for integrals applied to $f(x) = \sin(x) + \frac{1}{3}\sin(3x)$ over the interval $[0, 2.5]$.

Example 1.5. The function $f(x) = \sin(x) + \frac{1}{3}\sin(3x)$ satisfies the hypotheses of Theorem 1.10 over the interval $[0, 2.5]$. An antiderivative of $f(x)$ is $F(x) = -\cos(x) - \frac{1}{9}\cos(3x)$. The average value of the function $f(x)$ over the interval $[0, 2.5]$ is:

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

There are three solutions to the equation $f(c) = 0.749496$ over the interval $[0, 2.5]$: $c_1 = 0.440566$, $c_2 = 1.268010$, and $c_3 = 1.873583$. The area of the rectangle with base $b - a = 2.5$ and height $f(c_j) = 0.749496$ is $f(c_j)(b-a) = 1.873740$. The area of the rectangle has the same numerical value as the integral of $f(x)$ taken over the interval $[0, 2.5]$. A comparison of the area under the curve $y = f(x)$ and that of the rectangle can be seen in Figure 1.5. ■

Theorem 1.11 (Weighted Integral Mean Value Theorem). Assume that $f, g \in C[a, b]$ and $g(x) \geq 0$ for $x \in [a, b]$. Then there exists a number c, with $c \in (a, b)$, such that

$$\int_a^b f(x)g(x)\,dx = f(c)\int_a^b g(x)\,dx. \tag{14}$$

Example 1.6. The functions $f(x) = \sin(x)$ and $g(x) = x^2$ satisfy the hypotheses of Theorem 1.11 over the interval $[0, \pi/2]$. Thus there exists a number c such that

$$\sin(c) = \frac{\int_0^{\pi/2} x^2 \sin(x)\,dx}{\int_0^{\pi/2} x^2\,dx} = \frac{1.14159}{1.29193} = 0.883631$$

or $c = \sin^{-1}(0.883631) = 1.08356$. ■

Series

Definition 1.5. Let $\{a_n\}_{n=1}^{\infty}$ be a sequence. Then $\sum_{n=1}^{\infty} a_n$ is an infinite series. The nth partial sum is $S_n = \sum_{k=1}^{n} a_k$. The infinite series ***converges*** if and only if the sequence $\{S_n\}_{n=1}^{\infty}$ converges to a limit S, that is,

$$\lim_{n\to\infty} S_n = \lim_{n\to\infty} \sum_{k=1}^{n} a_k = S. \tag{15}$$

If a series does not converge, we say that it ***diverges***. ▲

Example 1.7. Consider the infinite sequence $\{a_n\}_{n=1}^{\infty} = \left\{\frac{1}{n(n+1)}\right\}_{n=1}^{\infty}$. Then the nth partial sum is

$$S_n = \sum_{k=1}^{n} \frac{1}{k(k+1)} = \sum_{k=1}^{n} \left(\frac{1}{k} - \frac{1}{k+1}\right) = 1 - \frac{1}{n+1}.$$

Therefore, the *sum* of the infinite series is

$$S = \lim_{n\to\infty} Sn = \lim_{n\to\infty} \left(1 - \frac{1}{n+1}\right) = 1.$$

■

Theorem 1.12 (Taylor's Theorem). Assume that $f \in C^{n+1}[a,b]$ and let $x_0 \in [a,b]$. Then, for every $x \in (a,b)$, there exists a number $c = c(x)$ (the value of c depends on the value of x) that lies between x_0 and x such that

$$f(x) = P_n(x) + R_n(x), \tag{16}$$

where

$$P_n(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k \tag{17}$$

and

$$R_n(x) = \frac{f^{(n+1)}(c)}{(n+1)!}(x - x_0)^{n+1}. \tag{18}$$

Example 1.8. The function $f(x) = \sin(x)$ satisfies the hypotheses of Theorem 1.12. The Taylor polynomial $P_n(x)$ of degree $n = 9$ expanded about $x_0 = 0$ is obtained by evaluating

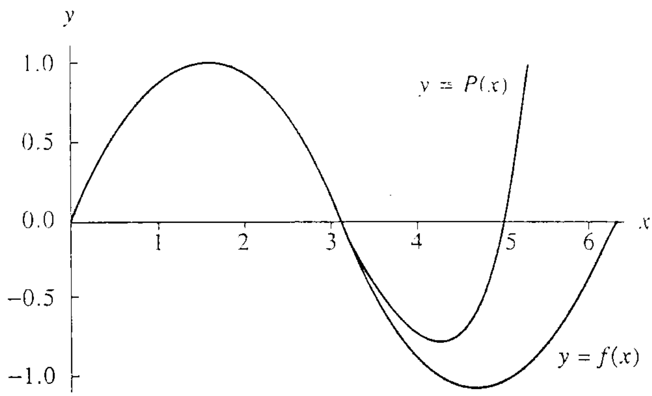

Figure 1.6 The graph of $f(x) = \sin(x)$ and the Taylor polynomial $P(x) = x - x^3/3! + x^5/5! - x^7/7! + x^9/9!$.

the following derivatives at $x = 0$ and substituting the numerical values into formula (17).

$$\begin{aligned} f(x) &= \sin(x), & f(0) &= 0, \\ f'(x) &= \cos(x), & f'(0) &= 1, \\ f''(x) &= -\sin(x), & f''(0) &= 0, \\ f^{(3)}(x) &= -\cos(x), & f^{(3)}(0) &= -1, \\ &\vdots & &\vdots \\ f^{(9)}(x) &= \cos(x), & f^{(9)}(0) &= 1, \end{aligned}$$

$$P_9(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!}.$$

A graph of both f and P_9 over the interval $[0, 2\pi]$ is shown in Figure 1.6. ■

Corollary 1.1. If $P_n(x)$ is the Taylor polynomial of degree n given in Theorem 1.12, then

(19) $$P_n^{(k)}(x_0) = f^{(k)}(x_0) \quad \text{for } k = 0, 1, \ldots, n.$$

Evaluation of a Polynomial

Let the polynomial $P(x)$ of degree n have the form

(20) $$P(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_2 x^2 + a_1 x + a_0.$$