

Chapter 1

Numerical Analysis and Scientific Computing

Numerical analysis is a branch of applied mathematics that deals with methods for solving problems by purely numerical computations. To understand what this means and why such an approach is needed, let us look at a simple example familiar from calculus.

Example 1.1 A three-dimensional solid of revolution can be created by revolving the curve

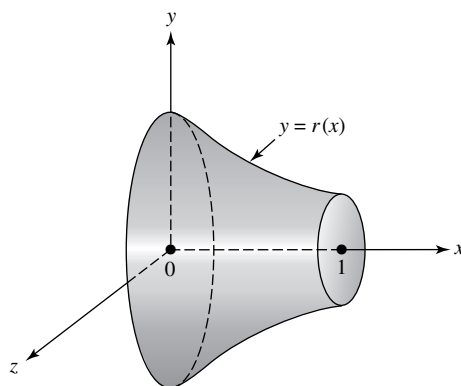
$$y = r(x)$$

about the x -axis (Figure 1.1).

As we know from calculus, the volume of such a solid is given by

$$V = \pi \int_0^1 r^2(x) dx. \quad (1.1)$$

Figure 1.1
A solid created by revolving a curve around the x -axis.



If $r(x)$ is simple, the definite integral can be computed by finding the anti-derivative of the integrand and then substituting the limits. Therefore, if $r(x) = e^x$, then

$$\begin{aligned} V &= \pi \int_0^1 e^{2x} dx \\ &= \frac{\pi}{2} e^{2x} \Big|_0^1 \\ &= \frac{\pi}{2} (e^2 - 1). \end{aligned}$$

We call the explicit formula for the integral in terms of elementary functions a *closed form* solution. When a closed form solution can be found, the value of the integral is easily obtained by putting in appropriate numerical values; in this case, $V = 10.0359$.

Unfortunately, closed form solutions are often impossible to get. If we complicate the problem just slightly by taking $r(x) = e^{x^2}$, the integral for the volume

$$V = \pi \int_0^1 e^{2x^2} dx \tag{1.2}$$

can no longer be found by elementary methods because no simple closed form solution exists. Here is where numerical analysis comes in.

The answer we are looking for is just a number, so we can try using numerical techniques to find it. To do so, we must reduce the problem to a sequence of steps that can be performed numerically, either on a pocket calculator for simple cases, or on a computer for more typical problems. Suppose we subdivide the interval $[0, 1]$ into n equal parts, using the partition points

$$x_i = \frac{i}{n}, \quad i = 0, 1, \dots, n - 1$$

Table 1.1
Approximating the
integral (1.2) by
the sum (1.3).

n	V_n
10	6.5016
100	7.3286
1000	7.4181
10000	7.4271

and form the sum

$$V_n = \frac{\pi}{n} \sum_{i=0}^{n-1} e^{2x_i^2}. \quad (1.3)$$

We know from calculus that a definite integral is the limit of such sums as $n \rightarrow \infty$, so we can claim that V_n approximates V . We write this as

$$\pi \int_0^1 e^{2x^2} dx \cong \frac{\pi}{n} \sum_{i=0}^{n-1} e^{2x_i^2}.$$

Table 1.1 shows how this works. We see that each n gives us a different value and that the sequence of values slowly tends to approximately 7.43. We might guess from the results that for $n = 10000$ we have at least three correct digits.¹

This specific example is easily generalized. For a given function $f(x)$, the integral

$$I = \int_a^b f(x) dx \quad (1.4)$$

can be approximated by

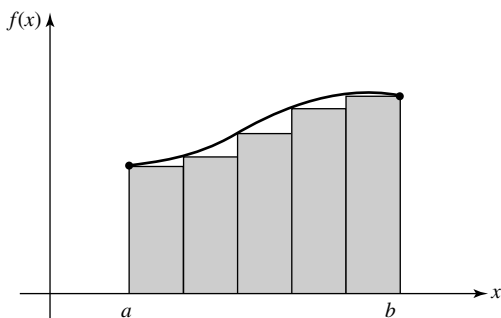
$$I_n = \frac{b-a}{n} \sum_{i=0}^{n-1} f(x_i), \quad (1.5)$$

with

$$x_i = a + i \frac{(b-a)}{n}.$$

¹All computations in this book were done on a computer that carries about 16 decimal digit accuracy. Normally we do not display all computed digits, but only those relevant to the specific discussion.

Figure 1.2
Approximating an integral by the rectangular rule. The area under the curve represents the true value of the integral. The shaded area is the approximation by the rectangular rule.



This method of approximating integrals is called the *rectangular rule*, since we approximate the area under a curve by a set of rectangles (Figure 1.2). The rectangular rule is one of the simplest numerical algorithms.

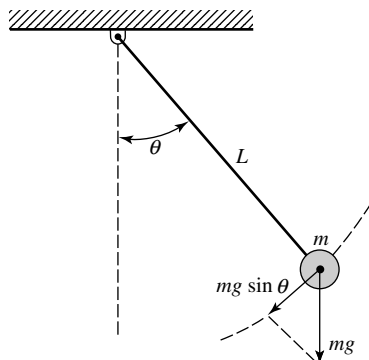
The problems we encounter in practice are usually much more complicated than computing definite integrals. To study physical phenomena, scientists and engineers construct *mathematical models* that embody the physical laws in order to describe the real situation. These models frequently involve differential equations, which are the mainstay of applied mathematics and engineering computations. The solutions of the modeling equations allow us to understand real-life systems and predict their behavior. Different areas of mathematics, from calculus to the theory of partial differential equations, were developed for studying and solving such mathematical models. Arriving at a successful solution often requires a great deal of insight and inventiveness.

Classical applied mathematics of the nineteenth and early twentieth centuries emphasized analytical methods for finding closed form solutions. Many methods, such as the separation of variables, were devised for this purpose and are still studied in courses on differential equations. Analytical techniques are often useful for getting insight into the general nature of a problem, and can give closed form solutions for simple cases. In most instances, though, they break down somewhere and have to be supplemented with numerical methods.

Example 1.2

The motion of a pendulum is a problem from elementary physics. An object of mass m is attached to a pivot by a string of length L , as shown in Figure 1.3. When the object is released from rest at an angle θ_0 the pendulum, following the laws of motion, will oscillate about the equilibrium position $\theta = 0$. A mathematical model allows us to predict the motion.

Figure 1.3
A simple
pendulum.



Using Newton’s second law and the force diagram in Figure 1.3, we are led to the modeling equation

$$mL \frac{d^2\theta}{dt^2} = -mg \sin \theta,$$

or

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L} \sin \theta. \tag{1.6}$$

If at time $t = 0$ the pendulum is at rest in position θ_0 , the conditions

$$\theta(0) = \theta_0 \tag{1.7}$$

and

$$\theta'(0) = 0 \tag{1.8}$$

must also be satisfied. The solution of (1.6), subject to (1.7) and (1.8), will give us the dependence of the angle θ in terms of the time t , the length of the pendulum L , and the constant of gravity g .

If θ is very small, then $\sin \theta$ is very close to θ and we can replace (1.6) by the small-angle approximation

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L} \theta. \tag{1.9}$$

Equation (1.9), with conditions (1.7) and (1.8), has the known closed form solution

$$\theta(t) = \theta_0 \cos \left(\sqrt{\frac{g}{L}} t \right).$$

Therefore the pendulum executes a periodic motion with period

$$T = 2\pi \sqrt{\frac{L}{g}}.$$

The small-angle approximation is inaccurate when θ_0 is more than a few degrees, so if high accuracy is required we may have to work with (1.6). In real-life situations there may be additional complications, such as the drag created by air resistance. If we can represent the effect of drag by a term proportional to some power of the velocity, an equation of the form

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L} \sin \theta + c \left(\frac{d\theta}{dt} \right)^\alpha$$

may represent the physical situation much better than (1.9). This equation has no known closed form solution so will have to be solved numerically.

Intuitive methods for the numerical solution of such differential equations are not hard to invent, but the subject is complicated and we defer any discussion to later chapters. For the moment, we just want to understand the need for numerical methods that can solve various kinds of differential equations.

Let us return briefly to the numerical integration in Example 1.1. Even though numerical integration is a very simple problem, it has all the major characteristics of more complicated numerical methods.

- ◆ A continuous and infinitesimal operation, in this case integration, is replaced by a finite sequence of arithmetic operations. This process is called *discretization*. In a sense, discretization reverses the limit process that is the basis of calculus.
- ◆ The result of a numerical calculation is not exact. The error that it has comes from discretization, and is called the *discretization error*. The statement that I_n approximates I is intuitively clear, but we can make it a little more precise by saying that I_n becomes closer and closer to I as n increases or, as we normally state it, that I_n *converges* to I . The approximation will never give us an exact answer, but we can get increasingly better accuracy by simply taking more terms in the sum in (1.5).²
- ◆ If the result is to be useful, we need to have some idea of how large the discretization error is. From Table 1.1 we guessed that the final result had about a three digit accuracy, but we did not give a rigorous justification for this claim.
- ◆ Numerical methods may involve thousands, perhaps millions, of simple individual operations. This raises the question of *efficiency* and the relative merits of different algorithms. Example 1.1 shows that the

²Shortly we will see that there is a practical limit to the accuracy we can get, but this is not important at the moment.

rectangular rule requires a great deal of work to get even moderate accuracy, so we should look for better ways. As we will see, there are methods that give the same accuracy with just a few computations.

These issues need to be addressed in every numerical computation, and they represent the focus of our discussion in this book. To solve a problem numerically, we first have to be able to discretize it so that it can be put on a computer. Conceptually, discretization itself may not be a major difficulty. Even for partial differential equations there are fairly obvious and intuitive discretization methods. The more demanding task comes when we try to put the concepts into practice. The production of a computer program for a complicated mathematical model is a lengthy and tedious matter. Another challenge is to construct methods that are effective and efficient, and whose performance can be predicted using convincing arguments. If possible, we also want to have ways for assessing the errors so that we can have some faith in the numbers that are produced. The analysis of numerical methods is not always easy and often requires a blend of mathematical sophistication, insight, and experience.

Although some simple numerical methods date back to the eighteenth and nineteenth centuries, the development of numerical analysis is closely tied to the history of digital computers. The first digital computers of the 1940s and early 1950s were created specifically to aid in the complex calculations connected with the design of nuclear weapons, and their use was limited to a few universities and government institutions. By current standards, these early machines were primitive and their use required much tedious work by experts writing programs in machine language. Nevertheless, some fairly significant problems were attacked and solved by these early computers. The next phase, starting around 1950, saw a huge increase in the power of computers and a proliferation of these machines into the industrial and academic world. The advent of the so-called higher-level programming languages, Fortran, Algol, and Cobol, coupled with the increased capacity of the new computers, made numerical computation a powerful tool for scientists and engineers. Numerical analysis became a standard topic of applied mathematics and computer science, and the ensuing activity led to the invention of many new numerical algorithms. Libraries of commonly used numerical methods were created that saved users much effort. However, doing numerical work, while certainly less tedious, continued to call for detailed programming and much routine work. Since the most important numerical techniques were developed during this period, numerical analysis is often still viewed in this light.

In the last decade or so another transformation has taken place. The large, centrally-located computer systems have given way to networks of powerful desktop systems. At the same time, the old style procedure-oriented languages are being replaced by high level object-oriented languages. Instead of submitting decks of punched cards, we now type our

commands directly into the computer, interacting with computer programs to guide the solution process and explore options. Digital scanners and direct links to measuring devices are used to get data into the system, and powerful graphical communication interfaces have replaced the reams of computer printout. Several existing systems, including MATLAB, now give engineers the ability to solve complex problems in a few minutes. As users of modern numerical methods we are faced by very different challenges from our counterparts forty years ago. We are no longer entirely pre-occupied with the minutiae of algorithm design or the incidentals of programming language syntax. Instead, we are concerned with how to use available resources to solve problems quickly and reliably. We have to learn how to select the appropriate programs from a large body of available software. Sometimes we find existing software that solves our problem, but most of the time we need to integrate existing routines into a larger program. This means that we have to be able to evaluate software and learn how to select that which is appropriate for our purpose. We also have to be concerned with the best way of getting voluminous data into the computer, and how to display the results most effectively. The term *scientific computing* is used to denote the use of numerical methods in a complex hardware and software environment to solve models from various scientific disciplines. The tools of scientific computing give engineers and scientists the ability to deal effectively with very complicated and realistic mathematical models of real-world situations.

EXERCISES

1. Based on the results of Table 1.1, estimate what value of n would be required to evaluate the integral (1.2) to an accuracy of eight decimal digits.
2. Write a computer program that evaluates integrals by the rectangular rule (1.5). Use this program to find an approximate value of the volume for the solid of revolution given by (1.1) in Example 1.1 with $r(x) = \frac{1}{1 + \sqrt{x^5}}$.
3. Use the program from Exercise 2 to correctly compute

$$\int_0^{\pi/2} \frac{x \cos^2(x)}{\sqrt{1+x}} dx$$

to three decimal digits. Provide arguments that lead you to believe that your answer meets the accuracy requirement.

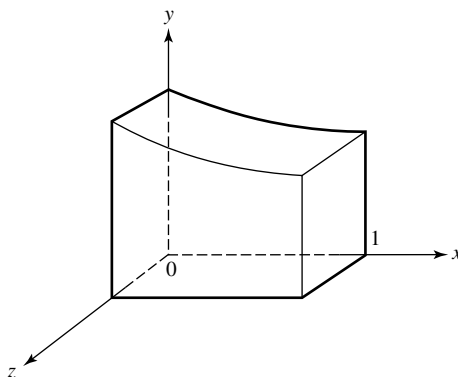
4. Use the rectangular method to approximate the area of the ellipse with boundary

$$x^2 + 2y^2 = 1$$

to four correct decimal digits.

5. Use the rectangular method to approximate the circumference of the ellipse in Exercise 4 to three correct decimal digits.
6. The taper of a beam with the rectangular cross-section shown below is given by the function

$$y = \frac{e^{-\sqrt{x}}}{1+x}.$$



Find the x -coordinate of the center of gravity of the beam to three correct decimal digits.

7. The differential equation

$$\frac{dy}{dt} = \frac{t\sqrt{t+1}}{ye^t},$$

with initial condition $y(0) = 0$, has a particular solution

$$y(x) = \sqrt{2 \int_0^x \frac{t\sqrt{t+1}}{e^t} dt}$$

for $x > 0$. Use the rectangular method to approximate $y(1)$ to four decimal digits.

8. Intelligence Quotient (IQ) scores are distributed normally with mean 100 and standard deviation 15 by the probability density function

$$f(x) = \frac{1}{15\sqrt{2\pi}} e^{-(x-100)^2/450}.$$

Use the program from Exercise 2 to compute the percentage of the probability that has an IQ score between 80 and 120 by taking the integral

$$p(80 \leq x \leq 120) = \int_{80}^{120} f(x) dx.$$

Justify that your answer is correct to three decimal digits.

9. Write a computer program to approximate

$$S = \sum_{i=0}^{\infty} \frac{1}{1+i^4}$$

to six decimal digit accuracy. Defend your claim that the desired accuracy is achieved.

10. In another version of the rectangular rule, the integral I in (1.4) is approximated by

$$\bar{I}_n = \frac{b-a}{n} \sum_{i=1}^n f(x_i).$$

- (a) Give a graphical interpretation for this formula.
- (b) In general, would you expect this modification to give better results than (1.5)?
- (c) What could you expect if you averaged these two approximations and used

$$\tilde{I}_n = \frac{1}{2}(I_n + \bar{I}_n)$$

as an approximation to the integral? Explore this suggestion numerically.