CHAPTER

11 Numerical and Monte Carlo Methods

Simple classical and Monte Carlo methods including importance sampling are illustrated in the context of the numerical evaluation of definite integrals.

11.1 ■ NUMERICAL INTEGRATION METHODS IN ONE DIMENSION

In this chapter we will learn that we can use sequences of random numbers to estimate definite integrals, a problem that seemingly has nothing to do with randomness. To place the Monte Carlo numerical integration methods in perspective, we will first discuss several common classical methods for numerically evaluating definite integrals. We will find that these methods, although usually preferable in low dimensions, are impractical for multidimensional integrals and that Monte Carlo methods are essential for the evaluation of the latter if the number of dimensions is sufficiently high.

Consider the one-dimensional definite integral of the form

$$F = \int_a^b f(x)\,dx. \tag{11.1}$$

For some choices of the integrand $f(x)$, the integration in (11.1) can be done analytically, found in tables of integrals, or evaluated as a series. However, there are relatively few functions that can be evaluated analytically, and most functions must be integrated numerically.

Most classical methods of numerical integration are based on the geometrical interpretation of the integral (11.1) as the area under the curve of the function $f(x)$ from $x = a$ to $x = b$ (see Figure 11.1). In these methods the x-axis is divided into n equal intervals of width Δx, where Δx is given by

$$\Delta x = \frac{b-a}{n}, \tag{11.2a}$$

and

$$x_n = x_0 + n\,\Delta x. \tag{11.2b}$$

In the above, $x_0 = a$ and $x_n = b$.

The simplest approximation of the area under the curve $f(x)$ is the sum of the area of the rectangles shown in Figure 11.2. In the *rectangular* approximation, $f(x)$ is evaluated at the *beginning* of the interval, and the approximate of the integral F_n is given by

$$F_n = \sum_{i=0}^{n-1} f(x_i)\Delta x \quad \text{(rectangular approximation)}. \tag{11.3}$$

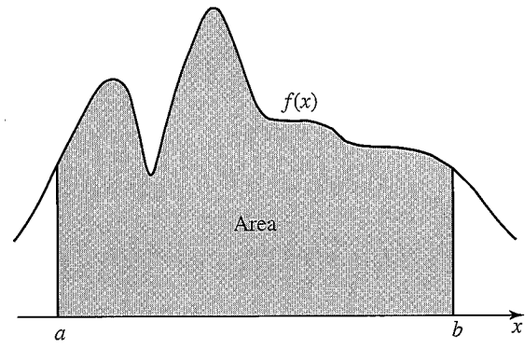

Figure 11.1 The integral F equals the area under the curve $f(x)$.

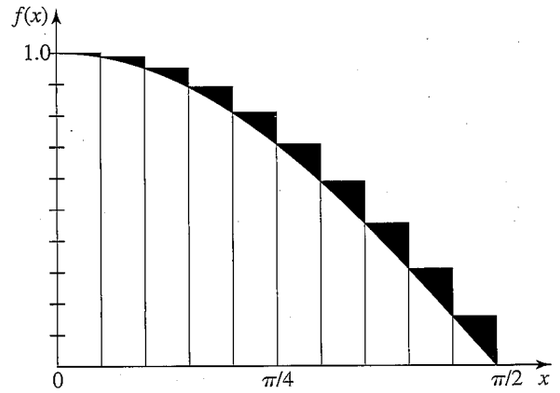

Figure 11.2 The rectangular approximation for $f(x) = \cos x$ for $0 \le x \le \pi/2$. The error is shaded. The error for various values of the number of intervals n is given in Table 11.1.

In the *trapezoidal* approximation, the integral is approximated by a sum of trapezoids. The area is computed by choosing one side equal to $f(x)$ at the beginning of the interval and the other side equal to $f(x)$ at the end of the interval. This approximation is equivalent to replacing the function by a straight line connecting the values of $f(x)$ at the beginning and the end of each interval. Because the area of the trapezoid from x_i to x_{i+1} is given by $\frac{1}{2}[f(x_{i+1}) + f(x_i)]\Delta x$, the total area F_n of the trapezoids is given by

$$F_n = \left[\frac{1}{2}f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2}f(x_n)\right]\Delta x \quad \text{(trapezoidal approximation)}. \tag{11.4}$$

A generally more accurate method is to use a quadratic or parabolic interpolation procedure through adjacent triplets of points. (The general problem of interpolation between data points using polynomials is discussed in Appendix 11D.) For example, the equation of the second-order polynomial that passes through the points (x_0, y_0), (x_1, y_1), and (x_2, y_2)