6 Additional Topics on Numerical Integration

Some interesting test integrals (for which numerical values are known) are

$$\int_0^1 \frac{dx}{\sqrt{\sin x}} \qquad \int_0^\infty e^{-x^3}\,dx \qquad \int_0^1 x\left|\sin(1/x)\right|\,dx$$

An important feature that is desirable in a numerical integration scheme is the capability of dealing with functions that have peculiarities, such as becoming infinite at some point or being highly oscillatory on certain subintervals. Another special case arises when the interval of integration is infinite. In this chapter, additional methods for numerical integration are introduced: the Gaussian quadrature formulas and an adaptive scheme based on Simpson's Rule. Gaussian formulas can often be used when the integrand has a singularity at an endpoint of the interval. The adaptive Simpson code is *robust* in the sense that it can concentrate the calculations on troublesome parts of the interval, where the integrand may have some unexpected behavior. Robust quadrature procedures automatically detect singularities or rapid fluctuations in the integrand and deal with them appropriately.

6.1 Simpson's Rule and Adaptive Simpson's Rule

Basic Simpson's Rule

The basic trapezoid rule for approximating $\int_a^b f(x)\,dx$ is based on an estimation of the area beneath the curve over the interval $[a, b]$ using a trapezoid. The function of integration $f(x)$ is taken to be a straight line between $f(a)$ and $f(b)$. The numerical integration formula is of the form

$$\int_a^b f(x)\,dx \approx Af(a) + Bf(b)$$

where the values of A and B are selected so that the resulting approximate formula will correctly integrate any linear function. It suffices to integrate exactly the two functions 1 and x because a polynomial of degree at most one is a linear combination of these two monomials. To simplify the calculations, let $a = 0$ and $b = 1$ and find a formula of the following type:

$$\int_0^1 f(x)\,dx \approx Af(0) + Bf(1)$$

Thus, these equations should be fulfilled:

$$\begin{aligned} f(x) = 1: &\quad \int_0^1 dx = A + B \\ f(x) = x: &\quad \int_0^1 x\,dx = \frac{1}{2} = B \end{aligned}$$

The solution is $A = B = \frac{1}{2}$, and the integration formula is

$$\int_0^1 f(x)\,dx \approx \frac{1}{2}[f(0) + f(1)]$$

By a linear mapping $y = (b-a)x + a$ from $[0, 1]$ to $[a, b]$, the **basic Trapezoid Rule** for the interval $[a, b]$ is obtained:

$$\int_a^b f(x)\,dx \approx \frac{1}{2}(b-a)[f(a) + f(b)]$$

See Figure 6.1 for a graphical illustration.

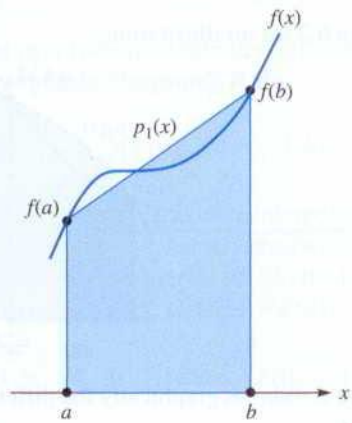

FIGURE 6.1
Basic Trapezoid Rule

The next obvious generalization is to take two subintervals $\left[a, \frac{a+b}{2}\right]$ and $\left[\frac{a+b}{2}, b\right]$ and to approximate $\int_a^b f(x)\,dx$ by taking the function of integration $f(x)$ to be a quadratic polynomial passing through the three points $f(a)$, $f\left(\frac{a+b}{2}\right)$, and $f(b)$. Let us seek a numerical integration formula of the following type:

$$\int_a^b f(x)\,dx \approx Af(a) + Bf\left(\frac{a+b}{2}\right) + Cf(b)$$

The function f is assumed to be continuous on the interval $[a, b]$. The coefficients A, B, and C will be chosen such that the formula above will give correct values for the integral whenever f is a quadratic polynomial. It suffices to integrate correctly the three functions 1, x, and x^2 because a polynomial of degree at most 2 is a linear combination of those

3 monomials. To simplify the calculations, let $a = -1$ and $b = 1$ and consider the equation

$$\int_{-1}^{1} f(x)\,dx \approx Af(-1) + Bf(0) + Cf(1)$$

Thus, these equations should be fulfilled:

$$\begin{aligned} f(x) = 1: &\quad \int_{-1}^{1} dx = 2 = A + B + C \\ f(x) = x: &\quad \int_{-1}^{1} x\,dx = 0 = -A + C \\ f(x) = x^2: &\quad \int_{-1}^{1} x^2\,dx = \frac{2}{3} = A + C \end{aligned}$$

The solution is $A = \frac{1}{3}$, $C = \frac{1}{3}$, and $B = \frac{4}{3}$. The resulting formula is

$$\int_{-1}^{1} f(x)\,dx \approx \frac{1}{3}[f(-1) + 4f(0) + f(1)]$$

Using a linear mapping $y = \frac{1}{2}(b-a) + \frac{1}{2}(a+b)$ from $[-1, 1]$ to $[a, b]$, we obtain the **basic Simpson's Rule** over the interval $[a, b]$:

$$\int_{a}^{b} f(x)\,dx \approx \frac{1}{6}(b-a)\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

See Figure 6.2 for an illustration.

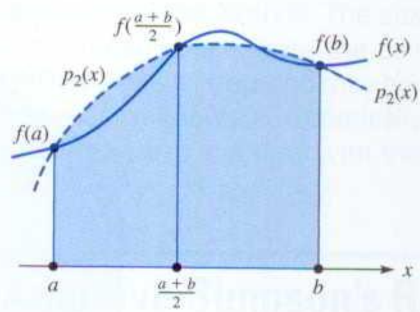

FIGURE 6.2 Basic Simpson's Rule

Figure 6.3 shows graphically the difference between the Trapezoid Rule and the Simpson's Rule.

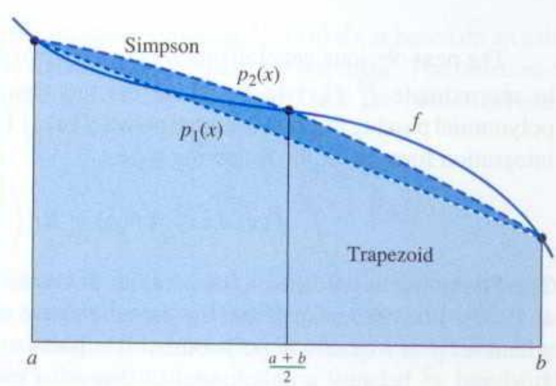

FIGURE 6.3 Example of Trapezoid Rule vs. Simpson's Rule

EXAMPLE 1 Find approximate values for the integral

$$\int_{-1}^{1} e^{-x^2}\,ds$$

using the basic Trapezoid Rule and the basic Simpson's Rule. Carry five significant digits.

Solution Let $a = 0$ and $b = 1$. For the basic Trapezoid Rule (1), we obtain

$$\int_0^1 e^{-x^2}\,ds \approx \frac{1}{2}\left[e^0 + e^{-1}\right] \approx 0.5[1 + 0.36788] = 0.68394$$

which is correct to only one significant decimal place (rounded). For the basic Simpson's Rule (2), we find

$$\int_0^1 e^{-x^2}\,ds \approx \frac{1}{6}\left[e^0 + 4e^{-0.25} + e^{-1}\right]$$

$$\approx 0.16667[1 + 4(0.77880) + 0.36788] = 0.7472$$

which is correct to three significant decimal places (rounded). Recall that $\int_0^1 e^{-x^2}\,dx = \frac{1}{2}\sqrt{\pi}\,\mathrm{erf}(1) \approx 0.74682.$ ■

Simpson's Rule

A numerical integration rule over two equal subintervals with partition points a, $a + h$, and $a + 2h = b$ is the widely used **basic Simpson's Rule**:

$$\int_a^{a+2h} f(x)\,dx \approx \frac{h}{3}[f(a) + 4f(a+h) + f(a+2h)] \tag{1}$$

Simpson's Rule computes exactly the integral of an interpolating quadratic polynomial over an interval of length $2h$ using three points; namely, the two endpoints and the middle point. It can be derived by integrating over the interval $[0, 2h]$ the Lagrange quadratic polynomial p through the points $(0, f(0))$, $(h, f(h))$, and $(2h, f(2h))$:

$$\int_0^{2h} f(x)\,dx \approx \int_0^{2h} p(x)\,dx = \frac{h}{3}[f(0) + 4f(h) + f(2h)]$$

where

$$p(x) = \frac{1}{2h^2}(x-h)(x-2h)f(0) - \frac{1}{h^2}x(x-2h)f(h) + \frac{1}{2h^2}x(x-h)f(2h)$$

The error term in Simpson's rule can be established by using the Taylor series from Section 1.2:

$$f(a+h) = f + hf' + \frac{1}{2!}h^2 f'' + \frac{1}{3!}h^3 f''' + \frac{1}{4!}h^4 f^{(4)} + \cdots$$

where the functions $f, f', f'', \ldots$ on the right-hand side are evaluated at a. Now replacing h by $2h$, we have

$$f(a+2h) = f + 2hf' + 2h^2 f'' + \frac{4}{3}h^3 f''' + \frac{2^4}{4!}h^4 f^{(4)} + \cdots$$

Using these two series, we obtain

$$f(a) + 4f(a+h) + f(a+2h) = 6f + 6hf' + 4h^2 f'' + 2h^3 f''' + \frac{20}{4!}h^4 f^{(4)} + \cdots$$

and, thereby, we have

$$\frac{h}{3}[f(a) + 4f(a+h) + f(a+2h)] = 2hf + 2h^2 f' + \frac{4}{3}h^3 f'' + \frac{2}{3}h^4 f''' + \frac{20}{3 \cdot 4!}h^5 f^{(4)} + \cdots \tag{2}$$

Hence, we have a series for the right-hand side of Equation (1). Now let's find one for the left-hand side. The Taylor series for $F(a+2h)$ is

$$F(a+2h) = F(a) + 2hF'(a) + 2h^2 F''(a) + \frac{4}{3}h^3 F'''(a) + \frac{2}{3}h^4 F^{(4)}(a) + \frac{2^5}{5!}h^5 F^{(5)}(a) + \cdots$$

Let

$$F(x) = \int_a^x f(t)\,dt$$

By the Fundamental Theorem of Calculus, $F' = f$. We observe that $F(a) = 0$ and $F(a+2h)$ is the integral on the left-hand side of Equation (1). Since $F'' = f'$, $F''' = f''$, and so on, we have

$$\int_a^{a+2h} f(x)\,dx = 2hf + 2h^2 f' + \frac{4}{3}h^3 f'' + \frac{2}{3}h^4 f''' + \frac{2^5}{5 \cdot 4!}h^5 f^{(4)} + \cdots \tag{3}$$

Subtracting Equation (2) from Equation (3), we obtain

$$\int_a^{a+2h} f(x)\,dx = \frac{h}{3}[f(a) + 4f(a+h) + f(a+2h)] - \frac{h^5}{90}f^{(4)} - \cdots$$

A more detailed analysis will show that the error term for the basic Simpson's Rule (1) is $-(h^5/90)f^{(4)}(\xi) = \mathcal{O}(h^5)$ as $h \to 0$, for some ξ between a and $a+2h$. We can rewrite the **basic Simpson's Rule** over the interval $[a, b]$ as

$$\int_a^b f(x)\,dx \approx \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

with error term

$$-\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\xi)$$

for some ξ in (a, b).

Composite Simpson's Rule

Suppose that the interval $[a, b]$ is subdivided into an even number of subintervals, say n, each of width $h = (b-a)/n$. Then the partition points are $x_i = a + ih$ for $0 \leqq i \leqq n$, where

n is divisible by 2. Now from basic calculus, we have

$$\int_a^b f(x)\,dx = \sum_{i=1}^{n/2} \int_{a+2(i-1)h}^{a+2ih} f(x)\,dx$$

Using the basic Simpson's Rule, we have, for the right-hand side,

$$\begin{aligned}
&\approx \sum_{i=1}^{n/2} \frac{h}{3}\{f(a+2(i-1)h) + 4f(a+(2i-1)h) + f(a+2ih)\} \\
&= \frac{h}{3}\left\{ f(a) + \sum_{i=1}^{(n/2)-1} f(a+2ih) + 4\sum_{i=1}^{n/2} f(a+(2i-1)h) \right. \\
&\qquad\qquad \left. + \sum_{i=1}^{(n/2)-1} f(a+2ih) + f(b) \right\}
\end{aligned}$$

Thus, we obtain

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left\{ [f(a)+f(b)] + 4\sum_{i=1}^{n/2} f[a+(2i-1)h] + 2\sum_{i=1}^{(n-2)/2} f(a+2ih) \right\}$$

where $h = (b-a)/n$. The error term is

$$-\frac{1}{180}(b-a)h^4 f^{(4)}(\xi)$$

Many formulas for numerical integration have error estimates that involve derivatives of the function being integrated. An important point that is frequently overlooked is that such error estimates depend on the function having derivatives. So if a piecewise function is being integrated, the numerical integration should be broken up over the region to coincide with the regions of smoothness of the function. Another important point is that no polynomial ever becomes infinite in the finite plane, so any integration technique that uses polynomials to approximate the integrand will fail to give good results without extra work at integrable singularities.

An Adaptive Simpson's Scheme

Now we develop an adaptive scheme based on Simpson's Rule for obtaining a numerical approximation to the integral

$$\int_a^b f(x)\,dx$$

In this adaptive algorithm, the partitioning of the interval $[a, b]$ is not selected beforehand but is automatically determined. The partition is generated adaptively so that more and smaller subintervals are used in some parts of the interval and fewer and larger subintervals are used in other parts.

(*) In the adaptive process, we divide the interval $[a, b]$ into two subintervals and then decide whether each of them is to be divided into more subintervals. This procedure is continued until some specified accuracy is obtained throughout the entire interval $[a, b]$. Since the integrand f may vary in its behavior on the interval $[a, b]$, we do not expect the final partitioning to be uniform but to vary in the density of the partition points.

It is necessary to develop the test for deciding whether subintervals should continue to be divided. One application of Simpson's Rule over the interval $[a, b]$ can be written as

$$I \equiv \int_a^b f(x)\,dx = S(a,b) + E(a,b)$$

where

$$S(a,b) = \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

and

$$E(a,b) = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(a) + \cdots$$

Letting $h = b - a$, we have

$$I = S^{(1)} + E^{(1)} \tag{4}$$

where

$$S^{(1)} = S(a,b)$$

and

$$\begin{aligned} E^{(1)} &= -\frac{1}{90}\left(\frac{h}{2}\right)^5 f^{(4)}(a) + \cdots \\ &= -\frac{1}{90}\left(\frac{h}{2}\right)^5 C \end{aligned}$$

Here we assume that $f^{(4)}$ remains a constant value C throughout the interval $[a, b]$. Now two applications of Simpson's Rule over the interval $[a, b]$ give

$$I = S^{(2)} + E^{(2)} \tag{5}$$

where

$$S^{(2)} = S(a,c) + S(c,b)$$

where $c = (a+b)/2$, as in Figure 6.4, and

$$\begin{aligned} E^{(2)} &= -\frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)}(a) + \cdots - \frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)}(c) + \cdots \\ &= -\frac{1}{90}\left(\frac{h/2}{2}\right)^5 \left[f^{(4)}(a) + f^{(4)}(c)\right] + \cdots \\ &= -\frac{1}{90}\left(\frac{1}{2^5}\right)\left(\frac{h}{2}\right)^5 (2C) = \frac{1}{16}\left[-\frac{1}{90}\left(\frac{h}{2}\right)^5 C\right] \end{aligned}$$

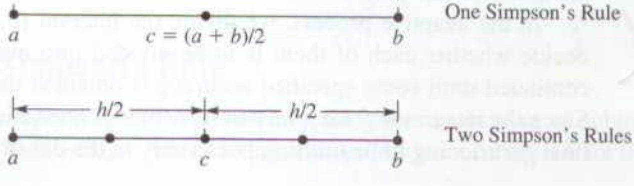

FIGURE 6.4
Simpson's rule

Again, we use the assumption that $f^{(4)}$ remains a constant value C throughout the interval $[a, b]$. We find that

$$16E^{(2)} = E^{(1)}$$

Subtracting Equation (5) from (4), we have

$$S^{(2)} - S^{(1)} = E^{(1)} - E^{(2)} = 15E^{(2)}$$

From this equation and Equation (4), we have

$$I = S^{(2)} + E^{(2)} = S^{(2)} + \tfrac{1}{15}\left(S^{(2)} - S^{(1)}\right)$$

This value of I is the best we have at this step, and we use the inequality

$$\tfrac{1}{15}\left|S^{(2)} - S^{(1)}\right| < \varepsilon \tag{6}$$

to guide the adaptive process.

If Test (6) is not satisfied, the interval $[a, b]$ is split into two subintervals, $[a, c]$ and $[c, b]$, where c is the midpoint $c = (a + b)/2$. On each of these subintervals, we again use Test (6) with ε replaced by $\varepsilon/2$ so that the resulting tolerance will be ε over the entire interval $[a, b]$. A recursive procedure handles this quite nicely.

To see why we take $\varepsilon/2$ on each subinterval, recall that

$$I = \int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx = I_{\text{left}} + I_{\text{right}}$$

If S is the sum of approximations $S^{(2)}_{\text{left}}$ over $[a, c]$ and $S^{(2)}_{\text{right}}$ over $[c, b]$, we have

$$\begin{aligned}
|I - S| &= \left|I_{\text{left}} + I_{\text{right}} - S^{(2)}_{\text{left}} - S^{(2)}_{\text{right}}\right| \\
&\leqq \left|I_{\text{left}} - S^{(2)}_{\text{left}}\right| + \left|I_{\text{right}} - S^{(2)}_{\text{right}}\right| \\
&= \tfrac{1}{15}\left|S^{(2)}_{\text{left}} - S^{(1)}_{\text{left}}\right| + \tfrac{1}{15}\left|S^{(2)}_{\text{right}} - S^{(1)}_{\text{right}}\right|
\end{aligned}$$

using Equation (6). Hence, if we require

$$\frac{1}{15}\left|S^{(2)}_{\text{left}} - S^{(1)}_{\text{left}}\right| \leqq \frac{\varepsilon}{2} \quad \text{and} \quad \frac{1}{15}\left|S^{(2)}_{\text{right}} - S^{(1)}_{\text{right}}\right| \leqq \frac{\varepsilon}{2}$$

then $|I - S| \leqq \varepsilon$ over the entire interval $[a, b]$.

We now describe an adaptive Simpson recursive procedure. The interval $[a, b]$ is partitioned into four subintervals of width $(b - a)/4$. Two Simpson approximations are computed by using two double-width subintervals and four single-width subintervals; that is,

$$\textit{one\_simpson} \leftarrow \frac{h}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

$$\textit{two\_simpson} \leftarrow \frac{h}{12}\left[f(a) + 4f\left(\frac{a+c}{2}\right) + 2f(c) + 4f\left(\frac{c+b}{2}\right) + f(b)\right]$$

where $h = b - a$ and $c = (a + b)/2$.

According to Inequality (6), if *one_simpson* and *two_simpson* agree to within 15ε, then the interval $[a, b]$ does not need to be subdivided further to obtain an accurate approximation to the integral $\int_a^b f(x)\,dx$. In this case, the value of $[16\,(\textit{two\_simpson}) - (\textit{one\_simpson})]/15$ is used as the approximate value of the integral over the interval $[a, b]$. If the desired accuracy for the integral has not been obtained, then the interval $[a, b]$ is divided in half. The with error term $-\frac{1}{90}[\frac{1}{2}(b-a)]^5 f^{(4)}(\xi)$ for some ξ in (a, b). Letting $h = (b-a)/2$, another form for the **basic Simpson's Rule** is

$$\int_a^{a+2h} f(x)\,dx \approx \frac{h}{3}[f(a) + 4f(a+h) + f(a+2h)]$$

with error term $-\frac{1}{90}h^5 f^{(4)}(\xi)$.

(2) The **composite Simpson's $\frac{1}{3}$ Rule** over n (even) subintervals

$$\int_a^b f(x)\,dx \approx \frac{h}{3}[f(a) + f(b)] + \frac{4h}{3}\sum_{i=1}^{n/2} f[a + (2i-1)h] + \frac{2h}{3}\sum_{i=1}^{(n-2)/2} f(a + 2ih)$$

where $h = (b-a)/n$ and the general error term is $-\frac{1}{180}(b-a)h^4 f^{(4)}(\xi)$.

(3) On the interval $[a, b]$ with $c = \frac{1}{2}(a+b)$, the test

$$\tfrac{1}{15}|S(a, c) + S(c, b) - S(a, b)| < \varepsilon$$

can be used in an **adaptive Simpson's algorithm**.

(4) Newton-Cotes quadrature rules encompass many common quadrature rules, such as the Trapezoid Rule, Simpson's Rule, and the Midpoint Rule.

Problems 6.1

[a]**1.** Compute $\int_0^1 (1+x^2)^{-1}\,dx$ by the basic Simpson's Rule, using the three partition points $x = 0, 0.5$, and 1. Compare with the true solution.

2. Consider the integral $\int_0^1 \sin(\pi x^2/2)\,dx$. Suppose that we wish to integrate numerically, with an error of magnitude less than 10^{-3}.

[a]**a.** What width h is needed if we wish to use the composite Trapezoid Rule?

[a]**b.** Composite Simpson's Rule? **c.** Composite Simpson's $\frac{3}{8}$ Rule?

3. A function f has the values shown.

x	1	1.25	1.5	1.75	2
$f(x)$	10	8	7	6	5

[a]**a.** Use Simpson's Rule and the function values at $x = 1, 1.5$, and 2 to approximate $\int_1^2 f(x)\,dx$.

[a]**b.** Repeat the preceding part, using $x = 1, 1.25, 1.5, 1.75$, and 2.

[a]**c.** Use the results from parts **a** and **b** along with the error terms to establish an improved approximation. *Hint:* Assume constant error term Ch^4.