7.4 Adaptive Quadrature

The composite quadrature rules necessitate the use of equally spaced points. Typically, a small step size h was used uniformly across the entire interval of integration to ensure the overall accuracy. This does not take into account that some portions of the curve may have large functional variations that require more attention than other portions of the curve. It is useful to introduce a method that adjusts the step size to be smaller over portions of the curve where a larger functional variation occurs. This technique is called ***adaptive quadrature***. The method is based on Simpson's rule.

Simpson's rule uses two subintervals over $[a_k, b_k]$:

$$S(a_k, b_k) = \frac{h}{3}(f(a_k) + 4f(c_k) + f(b_k)), \tag{1}$$

where $c_k = \frac{1}{2}(a_k + b_k)$ is the center of $[a_k, b_k]$ and $h = (b_k - a_k)/2$. Furthermore, if $f \in C^4[a_k, b_k]$, then there exists a value $d_1 \in [a_k, b_k]$ so that

$$\int_{a_k}^{b_k} f(x)\,dx = S(a_k, b_k) - h^5 \frac{f^{(4)}(d_1)}{90}. \tag{2}$$

Refinement

A composite Simpson rule using four subintervals of $[a_k, b_k]$ can be performed by bisecting this interval into two equal subintervals $[a_{k1}, b_{k1}]$ and $[a_{k2}, b_{k2}]$ and applying formula (1) recursively over each piece. Only two additional evaluations of $f(x)$ are needed, and the result is

$$\begin{aligned} S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) &= \frac{h}{6}(f(a_{k1}) + 4f(c_{k1}) + f(b_{k1})) \\ &\quad + \frac{h}{6}(f(a_{k2}) + 4f(c_{k2}) + f(b_{k2})), \end{aligned} \tag{3}$$

where $a_{k1} = a_k$, $b_{k1} = a_{k2} = c_k$, $b_{k2} = b_k$, c_{k1} is the midpoint of $[a_{k1}, b_{k1}]$, and c_{k2} is the midpoint of $[a_{k2}, b_{k2}]$. In formula (3) the step size is $h/2$, which accounts for the factors $h/6$ on the right side of the equation. Furthermore, if $f \in C^4[a, b]$, there exists a value $d_2 \in [a_k, b_k]$ so that

$$\int_{a_k}^{b_k} f(x)\,dx = S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) - \frac{h^5}{16}\frac{f^{(4)}(d_2)}{90}. \tag{4}$$

Assume that $f^{(4)}(d_1) \approx f^{(4)}(d_2)$; then the right sides of equations (2) and (4) are used to obtain the relation

$$S(a_k, b_k) - h^5\frac{f^{(4)}(d_2)}{90} \approx S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) - \frac{h^5}{16}\frac{f^{(4)}(d_2)}{90}, \tag{5}$$

which can be written as

$$-h^5\frac{f^{(4)}(d_2)}{90} \approx \frac{16}{15}(S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) - S(a_k, b_k)). \tag{6}$$

Then (6) is substituted in (4) to obtain the error estimate:

$$\begin{aligned} &\left| \int_{a_k}^{b_k} f(x)\,dx - S(a_{k1}, b_{k1}) - S(a_{k2}, b_{k2}) \right| \\ &\qquad \approx \frac{1}{15}\left|S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) - S(a_k, b_k)\right|. \end{aligned} \tag{7}$$

Because of the assumption $f^{(4)}(d_1) \approx f^{(4)}(d_2)$, the fraction $\frac{1}{15}$ is replaced with $\frac{1}{10}$ on the right side of (7) when implementing the method. This justifies the following test.

Accuracy Test

Assume that the tolerance $\epsilon_k > 0$ is specified for the interval $[a_k, b_k]$. If

$$\frac{1}{10}\left|S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}) - S(a_k, b_k)\right| < \epsilon_k, \tag{8}$$

we infer that

(9) $$\left| \int_{a_k}^{b_k} f(x)\,dx - S(a_{k1}, b_{k1}) - S(a_{k2}, b_{k2}) \right| < \epsilon_k.$$

Thus the composite Simpson rule (3) is used to approximate the integral

(10) $$\int_{a_k}^{b_k} f(x)\,dx \approx S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2}),$$

and the error bound for this approximation over $[a_k, b_k]$ is ϵ_k.

Adaptive quadrature is implemented by applying Simpson's rules (1) and (3). Start with $\{[a_0, b_0], \epsilon_0\}$, where ϵ_0 is the tolerance for numerical quadrature over $[a_0, b_0]$. The interval is refined into subintervals labeled $[a_{01}, b_{01}]$ and $[a_{02}, b_{02}]$. If the accuracy test (8) is passed, quadrature formula (3) is applied to $[a_0, b_0]$ and we are done. If the test in (8) fails, the two subintervals are relabeled $[a_1, b_1]$ and $[a_2, b_2]$, over which we use the tolerances $\epsilon_1 = \frac{1}{2}\epsilon_0$ and $\epsilon_2 = \frac{1}{2}\epsilon_0$, respectively. Thus we have two intervals with their associated tolerances to consider for further refinement and testing: $\{[a_1, b_1], \epsilon_1\}$ and $\{[a_2, b_2], \epsilon_2\}$, where $\epsilon_1 + \epsilon_2 = \epsilon_0$. If adaptive quadrature must be continued, the smaller intervals must be refined and tested, each with its own associated tolerance.

In the second step we first consider $\{[a_1, b_1], \epsilon_1\}$ and refine the interval $[a_1, b_1]$ into $[a_{11}, b_{11}]$ and $[a_{12}, b_{12}]$. If they pass the accuracy test (8) with the tolerance ϵ_1, quadrature formula (3) is applied to $[a_1, b_1]$ and accuracy has been achieved over this interval. If they fail the test in (8) with the tolerance ϵ_1, each subinterval $[a_{11}, b_{11}]$ and $[a_{12}, b_{12}]$ must be refined and tested in the third step with the reduced tolerance $\frac{1}{2}\epsilon_1$. Moreover, the second step involves looking at $\{[a_2, b_2], \epsilon_2\}$ and refining $[a_2, b_2]$ into $[a_{21}, b_{21}]$ and $[a_{22}, b_{22}]$. If they pass the accuracy test (8) with tolerance ϵ_2, quadrature formula (3) is applied to $[a_2, b_2]$ and accuracy is achieved over this interval. If they fail the test in (8) with the tolerance ϵ_2, each subinterval $[a_{21}, b_{21}]$ and $[a_{22}, b_{22}]$ must be refined and tested in the third step with the reduced tolerance $\frac{1}{2}\epsilon_2$. Therefore, the second step produces either three or four intervals, which we relabel consecutively. The three intervals would be relabeled to produce $\{\{[a_1, b_1], \epsilon_1\}, \{[a_2, b_2], \epsilon_2\}, \{[a_3, b_3], \epsilon_3\}\}$, where $\epsilon_1 + \epsilon_2 + \epsilon_3 = \epsilon_0$. In the case of four intervals, we would obtain $\{\{[a_1, b_1], \epsilon_1\}, \{[a_2, b_2], \epsilon_2\}, \{[a_3, b_3], \epsilon_3\}, \{[a_4, b_4], \epsilon_4\}\}$, where $\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4 = \epsilon_0$.

If adaptive quadrature must be continued, the smaller intervals must be tested, each with its own associated tolerance. The error term in (4) shows that each time a refinement is made over a smaller subinterval there is a reduction of error by about a factor of $\frac{1}{16}$. Thus the process will terminate after a finite number of steps. The bookkeeping for implementing the method includes a sentinel variable which indicates if a particular subinterval has passed its accuracy test. To avoid unnecessary additional evaluations of $f(x)$, the function values can be included in a data list corresponding to each subinterval. The details are shown in Program 7.6.

Table 7.8 Adaptive Quadrature Computations for $f(x) = 13(x - x^2)e^{-3x/2}$

a_k	b_k	$S(a_{k1}, b_{k1}) + S(a_{k2}, b_{k2})$	Error bound on the left side of (8)	Tolerance ϵ_k for $[a_k, b_k]$
0.0	0.0625	0.02287184840	0.00000001522	0.00000015625
0.0625	0.125	0.05948686456	0.00000001316	0.00000015625
0.125	0.1875	0.08434213630	0.00000001137	0.00000015625
0.1875	0.25	0.09969871532	0.00000000981	0.00000015625
0.25	0.375	0.21672136781	0.00000025055	0.0000003125
0.375	0.5	0.20646391592	0.00000018402	0.0000003125
0.5	0.625	0.17150617231	0.00000013381	0.0000003125
0.625	0.75	0.12433363793	0.00000009611	0.0000003125
0.75	0.875	0.07324515141	0.00000006799	0.0000003125
0.875	1.0	0.02352883215	0.00000004718	0.0000003125
1.0	1.125	−0.02166038952	0.00000003192	0.0000003125
1.125	1.25	−0.06065079384	0.00000002084	0.0000003125
1.25	1.5	−0.21080823822	0.00000031714	0.000000625
1.5	2.0	−0.60550965007	0.00000003195	0.00000125
2.0	2.25	−0.31985720175	0.00000008106	0.000000625
2.25	2.5	−0.30061749228	0.00000008301	0.000000625
2.5	2.75	−0.27009962412	0.00000007071	0.000000625
2.75	3.0	−0.23474721177	0.00000005447	0.000000625
3.0	3.5	−0.36389799695	0.00000103699	0.00000125
3.5	4.0	−0.24313827772	0.00000041708	0.00000125
	Totals	−1.54878823413	0.00000296809	0.00001

Example 7.16. Use adaptive quadrature to numerically approximate the value of the definite integral $\int_0^4 13(x - x^2)e^{-3x/2}\,dx$ with the starting tolerance $\epsilon_0 = 0.00001$.

Implementation of the method revealed that 20 subintervals are needed. Table 7.8 lists each interval $[a_k, b_k]$, composite Simpson rule $S(a_{k1}, b_{k1})+S(a_{k2}, b_{k2})$, the error bound for this approximation, and the associated tolerance ϵ_k. The approximate value of the integral is obtained by summing the Simpson rule approximations to get

$$\int_0^4 13(x - x^2)e^{-3x/2}\,dx \approx -1.54878823413. \tag{11}$$

The true value of the integral is

$$\int_0^4 13(x - x^2)e^{-3x/2}\,dx = \frac{4108e^{-6} - 52}{27} = -1.5487883725279481333. \tag{12}$$

Therefore, the error for adaptive quadrature is

$$|-1.54878837253 - (-1.54878823413)| = 0.00000013840, \tag{13}$$

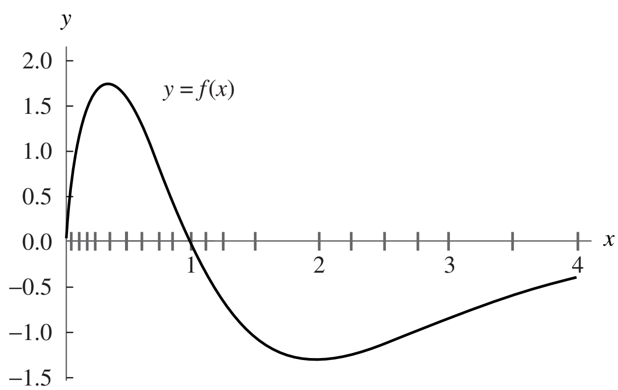

Figure 7.9 The subintervals of [0, 4] used in adaptive quadrature.

which is smaller than the specified tolerance $\epsilon_0 = 0.00001$. The adaptive method involves 20 subintervals of [0, 4], and 81 function evaluations were used. Figure 7.9 shows the graph of $y = f(x)$ and these 20 subintervals. The intervals are smaller where a larger functional variation occurs near the origin.

In the refinement and testing process in the adaptive method, the first four intervals of width 0.25 were bisected into eight subintervals of width 0.03125. If this uniform spacing is continued throughout the interval [0, 4], $M = 128$ subintervals are required for the composite Simpson rule, which yields the approximation -1.54878844029, which is in error by the amount 0.00000006776. Although the composite Simpson method contains half the error of the adaptive quadrature method, 176 more function evaluations are required. This gain of accuracy is negligible; hence there is a considerable saving of computing effort with the adaptive method. ∎

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