▶ EXAMPLE 5.9 Find the number of panels m necessary for the composite Simpson's Rule to approximate

$$\int_0^{\pi} \sin^2 x \, dx$$

within six correct decimal places.

We require the error to satisfy

$$\frac{(\pi - 0)h^4}{180} |f^{(iv)}(c)| < 0.5 \times 10^{-6}.$$

Since the fourth derivative of $\sin^2 x$ is $-8\cos 2x$, we need

$$\frac{\pi h^4}{180} 8 < 0.5 \times 10^{-6},$$

or $h < 0.0435$. Therefore, $m = \texttt{ceil}(\pi/(2h)) = 37$ panels will be sufficient. ◀

5.2.4 Open Newton–Cotes Methods

The so-called closed Newton–Cotes Methods like Trapezoid and Simpson's Rules require input values from the ends of the integration interval. Some integrands that have a removable singularity at an interval endpoint may be more easily handled with an open Newton–Cotes Method, which does not use values from the endpoints. The following rule is applicable to functions f whose second derivative f'' is continuous on $[a, b]$:

Midpoint Rule

$$\int_{x_0}^{x_1} f(x)\, dx = hf(w) + \frac{h^3}{24} f''(c), \tag{5.26}$$

where $h = (x_1 - x_0)$, w is the midpoint $x_0 + h/2$, and c is between x_0 and x_1.

The Midpoint Rule is also useful for cutting the number of function evaluations needed. Compared with the Trapezoid Rule, the closed Newton–Cotes Method of the same order, it requires one function evaluation rather than two. Moreover, the error term is half the size of the Trapezoid Rule error term.

The proof of (5.26) follows the same lines as the derivation of the Trapezoid Rule. Set $h = x_1 - x_0$. The degree 1 Taylor expansion of $f(x)$ about the midpoint $w = x_0 + h/2$ of the interval is

$$f(x) = f(w) + (x - w)f'(w) + \frac{1}{2}(x - w)^2 f''(c_x),$$

where c_x depends on x and lies between x_0 and x_1. Integrating both sides yields

$$\begin{aligned}\int_{x_0}^{x_1} f(x)\, dx &= (x_1 - x_0) f(w) + f'(w) \int_{x_0}^{x_1} (x - w)\, dx + \frac{1}{2}\int_{x_0}^{x_1} f''(c_x)(x - w)^2\, dx \\ &= hf(w) + 0 + \frac{f''(c)}{2} \int_{x_0}^{x_1} (x - w)^2\, dx \\ &= hf(w) + \frac{h^3}{24} f''(c),\end{aligned}$$

where $x_0 < c < x_1$. Again, we have used the Mean Value Theorem for Integrals to pull the second derivative outside of the integral. This completes the derivation of (5.26).

The proof of the composite version is left to the reader (Exercise 12).

Composite Midpoint Rule

$$\int_a^b f(x)\, dx = h \sum_{i=1}^{m} f(w_i) + \frac{(b - a)h^2}{24} f''(c), \tag{5.27}$$

where $h = (b - a)/m$ and c is between a and b. The w_i are the midpoints of the m equal subintervals of $[a, b]$.

▶ EXAMPLE 5.10 Approximate $\int_0^1 \sin x/x \, dx$ by using the Composite Midpoint Rule with $m = 10$ panels.

First note that we cannot apply a closed method directly to the problem, without special handling at $x = 0$. The midpoint method can be applied directly. The midpoints are $0.05, 0.15, \ldots, 0.95$, so the Composite Midpoint Rule delivers

$$\int_0^1 f(x)\, dx \approx 0.1 \sum_1^{10} f(m_i) = 0.94620858.$$

The correct answer to eight places is 0.94608307. ◀

Another useful open Newton–Cotes Rule is

$$\int_{x_0}^{x_4} f(x)\, dx = \frac{4h}{3}[2f(x_1) - f(x_2) + 2f(x_3)] + \frac{14h^5}{45} f^{(iv)}(c), \tag{5.28}$$

where $h = (x_4 - x_0)/4, x_1 = x_0 + h, x_2 = x_0 + 2h, x_3 = x_0 + 3h,$ and where $x_0 < c < x_4$. The rule has degree of precision three. Exercise 11 asks you to extend it to a composite rule.

5.2 Exercises

1. Apply the composite Trapezoid Rule with $m = 1, 2$, and 4 panels to approximate the integral. Compute the error by comparing with the exact value from calculus.

   (a) $\int_0^1 x^2\, dx$ (b) $\int_0^{\pi/2} \cos x\, dx$ (c) $\int_0^1 e^x\, dx$

2. Apply the Composite Midpoint Rule with $m = 1, 2$, and 4 panels to approximate the integrals in Exercise 1, and report the errors.

3. Apply the composite Simpson's Rule with $m = 1, 2$, and 4 panels to the integrals in Exercise 1, and report the errors.

4. Apply the composite Simpson's Rule with $m = 1, 2$, and 4 panels to the integrals, and report the errors.

   (a) $\int_0^1 xe^x\, dx$ (b) $\int_0^1 \frac{dx}{1 + x^2}\, dx$ (c) $\int_0^{\pi} x \cos x\, dx$

5. Apply the Composite Midpoint Rule with $m = 1, 2$, and 4 panels to approximate the integrals. Compute the error by comparing with the exact value from calculus.

   (a) $\int_0^1 \frac{dx}{\sqrt{x}}$ (b) $\int_0^1 x^{-1/3}\, dx$ (c) $\int_0^2 \frac{dx}{\sqrt{2 - x}}$

6. Apply the Composite Midpoint Rule with $m = 1, 2,$ and 4 panels to approximate the integrals.

$$\text{(a)} \int_0^{\pi/2} \frac{1-\cos x}{x^2}\,dx \quad \text{(b)} \int_0^1 \frac{e^x-1}{x}\,dx \quad \text{(c)} \int_0^{\pi/2} \frac{\cos x}{\frac{\pi}{2}-x}\,dx$$

7. Apply the open Newton-Cotes rule (5.28) to approximate the integrals of Exercise 5, and report the errors.
8. Apply the open Newton-Cotes rule (5.28) to approximate the integrals of Exercise 6.
9. Apply Simpson's Rule approximation to $\int_0^1 x^4\,dx$, and show that the approximation error matches the error term from (5.22).
10. Integrate Newton's divided-difference interpolating polynomial to prove the formula (a) (5.18) (b) (5.19).
11. Find the degree of precision of the following approximation for $\int_{-1}^1 f(x)\,dx$: (a) $f(1) + f(-1)$ (b) $2/3[f(-1) + f(0) + f(1)]$ (c) $f(-1/\sqrt{3}) + f(1/\sqrt{3})$.
12. Find $c_1, c_2,$ and c_3 such that the rule

$$\int_0^1 f(x)\,dx \approx c_1 f(0) + c_2 f(0.5) + c_3 f(1)$$

has degree of precision greater than one. (Hint: Substitute $f(x) = 1, x,$ and x^2.) Do you recognize the method that results?

13. Develop a composite version of the rule (5.28), with error term.
14. Prove the Composite Midpoint Rule (5.27).
15. Find the degree of precision of the degree four Newton–Cotes Rule (often called Boole's Rule)

$$\int_{x_0}^{x_4} f(x)\,dx \approx \frac{2h}{45}(7y_0 + 32y_1 + 12y_2 + 32y_3 + 7y_4).$$

16. Use the fact that the error term of Boole's Rule is proportional to $f^{(6)}(c)$ to find the exact error term, by the following strategy: Compute Boole's approximation for $\int_0^{4h} x^6\,dx$, find the approximation error, and write it in terms of h and $f^{(6)}(c)$.
17. Let $P_3(x)$ be a degree 3 polynomial, and let $P_2(x)$ be its interpolating polynomial at the three points $x = -h, 0,$ and h. Prove directly that $\int_{-h}^h P_3(x)\,dx = \int_{-h}^h P_2(x)\,dx$. What does this fact say about Simpson's Rule?

5.2 Computer Problems

1. Use the composite Trapezoid Rule with $m = 16$ and 32 panels to approximate the definite integral. Compare with the correct integral and report the two errors.

$$\text{(a)} \int_0^4 \frac{x\,dx}{\sqrt{x^2+9}} \quad \text{(b)} \int_0^1 \frac{x^3\,dx}{x^2+1} \quad \text{(c)} \int_0^1 xe^x\,dx \quad \text{(d)} \int_1^3 x^2 \ln x\,dx$$

$$\text{(e)} \int_0^{\pi} x^2 \sin x\,dx \quad \text{(f)} \int_2^3 \frac{x^3\,dx}{\sqrt{x^4-1}} \quad \text{(g)} \int_0^{2\sqrt{3}} \frac{dx}{\sqrt{x^2+4}}\,dx \quad \text{(h)} \int_0^1 \frac{x\,dx}{\sqrt{x^4+1}}$$

2. Apply the composite Simpson's Rule to the integrals in Computer Problem 1. Use $m = 16$ and 32, and report errors.
3. Use the composite Trapezoid Rule with $m = 16$ and 32 panels to approximate the definite integral.

$$\text{(a)} \int_0^1 e^{x^2}\,dx \quad \text{(b)} \int_0^{\sqrt{\pi}} \sin x^2\,dx \quad \text{(c)} \int_0^{\pi} e^{\cos x}\,dx \quad \text{(d)} \int_0^1 \ln(x^2+1)\,dx$$

$$\text{(e)} \int_0^1 \frac{x\,dx}{2e^x - e^{-x}} \quad \text{(f)} \int_0^{\pi} \cos e^x\,dx \quad \text{(g)} \int_0^1 x^x\,dx \quad \text{(h)} \int_0^{\pi/2} \ln(\cos x + \sin x)\,dx$$

4. Apply the composite Simpson's Rule to the integrals of Computer Problem 3, using $m = 16$ and 32.
5. Apply the Composite Midpoint Rule to the improper integrals of Exercise 5, using $m = 10, 100,$ and 1000. Compute the error by comparing with the exact value.
6. Apply the Composite Midpoint Rule to the improper integrals of Exercise 6, using $m = 16$ and 32.
7. Apply the Composite Midpoint Rule to the improper integrals

$$\text{(a)} \int_0^{\frac{\pi}{2}} \frac{x}{\sin x}\,dx \quad \text{(b)} \int_0^{\frac{\pi}{2}} \frac{e^x-1}{\sin x}\,dx \quad \text{(c)} \int_0^1 \frac{\arctan x}{x}\,dx,$$

using $m = 16$ and 32.

8. The arc length of the curve defined by $y = f(x)$ from $x = a$ to $x = b$ is given by the integral $\int_a^b \sqrt{1 + f'(x)^2}\,dx$. Use the composite Simpson's Rule with $m = 32$ panels to approximate the lengths of the curves

$$\text{(a)}\ y = x^3 \text{ on } [0,1] \quad \text{(b)}\ y = \tan x \text{ on } [0,\pi/4] \quad \text{(c)}\ y = \arctan x \text{ on } [0,1].$$

9. For the integrals in Computer Problem 1, calculate the approximation error of the composite Trapezoid Rule for $h = b - a, h/2, h/4, \ldots, h/2^8$, and plot. Make a log–log plot, using, for example, MATLAB's `loglog` command. What is the slope of the plot, and does it agree with theory?
10. Carry out Computer Problem 9, but use the composite Simpson's Rule instead of the composite Trapezoid Rule.

5.3 ROMBERG INTEGRATION

In this section, we begin discussing efficient methods for calculating definite integrals that can be extended by adding data until the required accuracy is attained. Romberg Integration is the result of applying extrapolation to the composite Trapezoid Rule. Recall from Section 5.1 that, given a rule $N(h)$ for approximating a quantity M, depending on a step size h, the rule can be extrapolated if the order of the rule is known. Equation (5.24) shows that the composite Trapezoid Rule is a second-order rule in h. Therefore, extrapolation can be applied to achieve a new rule of (at least) third order.

Examining the error of the Trapezoid Rule (5.24) more carefully, it can be shown that, for an infinitely differentiable function f, where we have applied Theorem 5.1 to consolidate the error terms. Subtracting (5.40) from (5.39) yields

$$S_{[a,b]} - (S_{[a,c]} + S_{[c,b]}) = h^5 \frac{f^{(iv)}(c_0)}{90} - \frac{h^5}{16}\frac{f^{(iv)}(c_3)}{90}$$
$$\approx \frac{15}{16} h^3 \frac{f^{(iv)}(c_3)}{90}, \tag{5.41}$$

where we make the approximation $f^{(iv)}(c_3) \approx f^{(iv)}(c_0)$.

Since $S_{[a,b]} - (S_{[a,c]} + S_{[c,b]})$ is now 15 times the error of the approximation $S_{[a,c]} + S_{[c,b]}$ for the integral, we can make our new criterion

$$|S_{[a,b]} - (S_{[a,c]} + S_{[c,b]})| < 15 * \text{TOL} \tag{5.42}$$

and proceed as before. It is traditional to replace the 15 by 10 in the criterion to make the algorithm more conservative. Figure 5.5(b) shows an application of Adaptive Simpson's Quadrature to the same integral. The approximate integral is 2.500 when a tolerance of 0.005 is used, using 20 subintervals, a considerable savings over adaptive Trapezoid Rule Quadrature. Decreasing the tolerance to 0.5×10^{-4} yields 2.5008, using just 58 subintervals.

5.4 Exercises

1. Apply Adaptive Quadrature by hand, using the Trapezoid Rule with tolerance TOL = 0.05 to approximate the integrals. Find the approximation error.

$$\text{(a)} \int_0^1 x^2\,dx \quad \text{(b)} \int_0^{\pi/2} \cos x\,dx \quad \text{(c)} \int_0^1 e^x\,dx$$

2. Apply Adaptive Quadrature by hand, using Simpson's Rule with tolerance TOL = 0.01 to approximate the integrals. Find the approximation error.

$$\text{(a)} \int_0^1 xe^x\,dx \quad \text{(b)} \int_0^1 \frac{dx}{1+x^2}\,dx \quad \text{(c)} \int_0^\pi x\cos x\,dx$$

3. Develop an Adaptive Quadrature method for the Midpoint Rule (5.26). Begin by finding a criterion for meeting the tolerance on subintervals.

4. Develop an Adaptive Quadrature method for rule (5.28).

5.4 Computer Problems

1. Use Adaptive Trapezoid Quadrature to approximate the definite integral within 0.5×10^{-8}. Report the answer with eight correct decimal places and the number of subintervals required.

$$\text{(a)} \int_0^4 \frac{x\,dx}{\sqrt{x^2+9}} \quad \text{(b)} \int_0^1 \frac{x^3\,dx}{x^2+1} \quad \text{(c)} \int_0^1 xe^x\,dx \quad \text{(d)} \int_1^3 x^2 \ln x\,dx$$

$$\text{(e)} \int_0^\pi x^2 \sin x\,dx \quad \text{(f)} \int_2^3 \frac{x^3\,dx}{\sqrt{x^4-1}} \quad \text{(g)} \int_0^{2\sqrt{3}} \frac{dx}{\sqrt{x^2+4}}\,dx \quad \text{(h)} \int_0^1 \frac{x\,dx}{\sqrt{x^4+1}}\,dx$$

2. Modify the MATLAB code for Adaptive Trapezoid Rule Quadrature to use Simpson's Rule instead, applying the criterion (5.42) with the 15 replaced by 10. Approximate the integral in Example 5.12 within 0.005, and compare with Figure 5.5(b). How many subintervals were required?

3. Carry out the steps of Computer Problem 1 for adaptive Simpson's Rule, developed in Computer Problem 2.

4. Carry out the steps of Computer Problem 1 for the adaptive Midpoint Rule, developed in Exercise 3.

5. Carry out the steps of Computer Problem 1 for the adaptive open Newton–Cotes Rule developed in Exercise 4. Use criterion (5.42) with the 15 replaced by 10.

6. Use Adaptive Trapezoid Quadrature to approximate the definite integral within 0.5×10^{-8}.

$$\text{(a)} \int_0^1 e^{x^2}\,dx \quad \text{(b)} \int_0^{\sqrt{\pi}} \sin x^2\,dx \quad \text{(c)} \int_0^\pi e^{\cos x}\,dx \quad \text{(d)} \int_0^1 \ln(x^2+1)\,dx$$

$$\text{(e)} \int_0^1 \frac{x\,dx}{2e^x - e^{-x}} \quad \text{(f)} \int_0^\pi \cos e^x\,dx \quad \text{(g)} \int_0^1 x^x\,dx \quad \text{(h)} \int_0^{\pi/2} \ln(\cos x + \sin x)\,dx$$

7. Carry out the steps of Problem 6, using Adaptive Simpson's Quadrature.

8. The probability within σ standard deviations of the mean of the normal distribution is

$$\frac{1}{\sqrt{2\pi}} \int_{-\sigma}^{\sigma} e^{-x^2/2}\,dx.$$

Use Adaptive Simpson's Quadrature to find, within eight correct decimal places, the probability within (a) 1 (b) 2 (c) 3 standard deviations.

9. Write a MATLAB function called `myerf.m` that uses Adaptive Simpson's Rule to calculate the value of

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-s^2}\,ds$$

within eight correct decimal places for arbitrary input x. Test your program for $x = 1$ and $x = 3$ by comparing with MATLAB's function `erf`.

5.5 GAUSSIAN QUADRATURE

The degree of precision of a quadrature method is the degree for which all polynomial functions are integrated by the method with no error. Newton–Cotes Methods of degree n have degree of precision n (for n odd) and $n+1$ (for n even). The Trapezoid Rule (Newton–Cotes for $n=1$) has degree of precision one. Simpson's Rule ($n=2$) is correct up to and including third degree polynomials.

To achieve this degree of precision, the Newton–Cotes formulas use $n+1$ function evaluations, done at evenly spaced points. The question we ask is reminiscent of our discussion in Chapter 3 about Chebyshev polynomials. Are the Newton–Cotes formulas optimal for their degree of precision, or can more powerful formulas be developed? In particular, if the requirement that evaluation points be evenly spaced is relaxed, are there better methods?

At least from the point of view of degree of precision, there are more powerful and sophisticated methods. We pick out the most famous one to discuss in this section. Gaussian Quadrature has degree of precision $2n+1$ when $n+1$ points are used, double that of Newton–Cotes. The evaluation points are not evenly spaced. Explaining how Gaussian

5.5 Exercises

1. Approximate the integrals, using $n = 2$ Gaussian Quadrature. Compare with the correct value, and give the approximation error.

   (a) $\int_{-1}^{1} (x^3 + 2x)\,dx$ (b) $\int_{-1}^{1} x^4\,dx$ (c) $\int_{-1}^{1} e^x\,dx$ (d) $\int_{-1}^{1} \cos\pi x\,dx$

2. Approximate the integrals in Exercise 1, using $n = 3$ Gaussian Quadrature, and give the error.

3. Approximate the integrals in Exercise 1, using $n = 4$ Gaussian Quadrature, and give the error.

4. Change variables, using the substitution (5.46) to rewrite as an integral over $[-1, 1]$.

   (a) $\int_0^4 \frac{x\,dx}{\sqrt{x^2+9}}$ (b) $\int_0^1 \frac{x^3\,dx}{x^2+1}$ (c) $\int_0^1 xe^x\,dx$ (d) $\int_1^3 x^2 \ln x\,dx$

5. Approximate the integrals in Exercise 4, using $n = 3$ Gaussian Quadrature.

6. Approximate the integrals, using $n = 4$ Gaussian Quadrature.

   (a) $\int_0^1 (x^3 + 2x)\,dx$ (b) $\int_1^4 \ln x\,dx$ (c) $\int_{-1}^{2} x^5\,dx$ (d) $\int_{-3}^{3} e^{-\frac{x^2}{2}}\,dx$

7. Show that the Legendre polynomials $p_1(x) = x$ and $p_2(x) = x^2 - 1/3$ are orthogonal on $[-1, 1]$.

8. Find the Legendre polynomials up to degree 3 and compare with Example 5.13.

9. Verify the coefficients c_i and x_i in Table 5.1 for degree $n = 3$.

10. Verify the coefficients c_i and x_i in Table 5.1 for degree $n = 4$.

Reality Check 5 Motion Control in Computer-Aided Modeling

Computer-aided modeling and manufacturing requires precise control of spatial position along a prescribed motion path. We will illustrate the use of Adaptive Quadrature to solve a fundamental piece of the problem: equipartition, or the division of an arbitrary path into equal-length subpaths.

In numerical machining problems, it is preferable to maintain constant speed along the path. During each second, progress should be made along an equal length of the machine–material interface. In other motion planning applications, including computer animation, more complicated progress curves may be required: A hand reaching for a doorknob might begin and end with low velocity and have higher velocity in between. Robotics and virtual reality applications require the construction of parametrized curves and surfaces to be navigated. Building a table of small equal increments in path distance is often a necessary first step.

Assume that a parametric path $P = \{x(t), y(t) | 0 \le t \le 1\}$ is given. Figure 5.6 shows the example path

$$P = \begin{cases} x(t) = 0.5 + 0.3t + 3.9t^2 - 4.7t^3 \\ y(t) = 1.5 + 0.3t + 0.9t^2 - 2.7t^3 \end{cases},$$

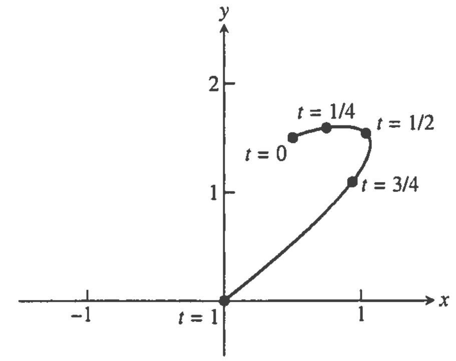

Figure 5.6 Parametrized curve given by Bézier spline. Typically, equal intervals of the parameter t do not divide the path into segments of equal length.

which is the Bézier curve defined by the four points $(0.5, 1.5), (0.6, 1.6), (2, 2), (0, 0)$. (See Section 3.5.) Points defined by evenly spaced parameter values $t = 0, 1/4, 1/2, 3/4, 1$ are shown. Note that even spacing in parameter does not imply even spacing in arc length. Your goal is to apply quadrature methods to divide this path into n equal lengths.

Recall from calculus that the arc length of the path from t_1 to t_2 is

$$\int_{t_1}^{t_2} \sqrt{x'(t)^2 + y'(t)^2}\,dt.$$

Only rarely does the integral yield a closed-form expression, and normally an Adaptive Quadrature technique is used to control the parametrization of the path.

Suggested activities:

1. Write a MATLAB function that uses Adaptive Quadrature to compute the arc length from $t = 0$ to $t = T$ for a given $T \le 1$.

2. Write a program that, for any input s between 0 and 1, finds the parameter $t^*(s)$ that is s of the way along the curve. In other words, the arc length from $t = 0$ to $t = t^*(s)$ divided by the arc length from $t = 0$ to $t = 1$ should be equal to s. Use the Bisection Method to locate the point $t^*(s)$ to three correct decimal places. What function is being set to zero? What bracketing interval should be used to start the Bisection Method?

3. Equipartition the path of Figure 5.6 into n subpaths of equal length, for $n = 4$ and $n = 20$. Plot analogues of Figure 5.6, showing the equipartitions. If your computations are too slow, consider speeding up the Adaptive Quadrature with Simpson's Rule, as suggested in Computer Problem 5.4.2.

4. Replace the Bisection Method in Step 2 with Newton's Method, and repeat Steps 2 and 3. What is the derivative needed? What is a good choice for the initial guess? Is computation time decreased by this replacement?

5. Appendix A demonstrates animation commands available in MATLAB. For example, the commands

```
set(gca,'XLim',[-2 2],'YLim',[-2 2],'Drawmode','fast',...
   'Visible','on');
cla
axis square
```