Numerical Integration

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Outline

Introduction to Quadrature

We now approach the subject of numerical integration. The goal is to approximate the definite integral of $f(x)$ over the interval $[a, b]$ by evaluating $f(x)$ at a finite number of sample points.

Definition 7.1

Suppose that $a = x_0 < x_1 < \cdots < x_M = b$. A formula of the form.

$$Q[f] = \sum_{k=0}^{M} w_k f(x_k) = w_0 f(x_0) + w_1 f(x_1) + \cdots + w_M f(x_M) \tag{1}$$

with the property that

$$\int_a^b f(x)dx = Q[f] + E[f] \tag{2}$$

is called a numerical integration or quadrature formula. The term $E[f]$ is called the **truncation error** for integration. The values $\{x_k\}_{k=0}^{M}$ are called the **quadrature nodes**, and $\{w_k\}_{k=0}^{M}$ are called the **weights**.

Introduction to Quadrature

Depending on the application, the nodes $\{x_k\}$ are chosen in various ways. For the trapezoidal rule, Simpson's rule, and Boole's rule, the nodes are chosen to be equally spaced. For Gauss-Legendre quadrature, the nodes are chosen to be zeros of certain Legendre polynomials. When the integration formula is used to develop a predictor formula for differential equations, all the nodes are chosen less than b. For all applications, it is necessary to know something about the accuracy of the numerical solution.

Introduction to Quadrature

Definition 7.2

The **degree of precision** of a quadrature formula is the positive integer n such that $E[P_i] = 0$ for all polynomials $P_i(x)$ of degree $i \leq n$, but for which $E[P_{n+1}] \neq 0$ for some polynomial $P_{n+1}(x)$ of degree $n+1$.

The form of $E[P_i]$ can be anticipated by studying what happens when $f(x)$ is a polynomial. Consider the arbitrary polynomial

$$P_i(x) = a_i x^i + a_{i-1} x^{i-1} + \cdots + a_1 x + a_0$$

of degree i. If $i \leq n$, then $P_i^{(n+1)}(x) \equiv 0$ for all x, and $P_{n+1}^{(n+1)}(x) = (n+1)!\, a_{n-1}$ for all x. Thus it is not surprising that the general form for the truncation error term is

$$E[f] = K f^{(n+1)}(c), \tag{3}$$

where K is a suitably chosen constant and n is the degree of precision.

The derivation of quadrature formula is sometimes based on polynomial interpolation. Recall that there exists a unique polynomial $P_M(x)$ of degree $\leq M$ passing through the $M+1$ equally spaced points $\{(x_k, f(x_k))\}_{k=0}^{M}$. When this polynomial is used to approximate $f(x)$ over $[a, b]$,and then the integral of $f(x)$ is approximated by the integral of $P_M(x)$, the resulting formula is called a **Newton-Cotes quadrature formula** (see figure). When the sample points $x_0 = a$ and $x_M = b$ are used, it is called a **closed** Newton-Cotes formula.

Introduction to Quadrature

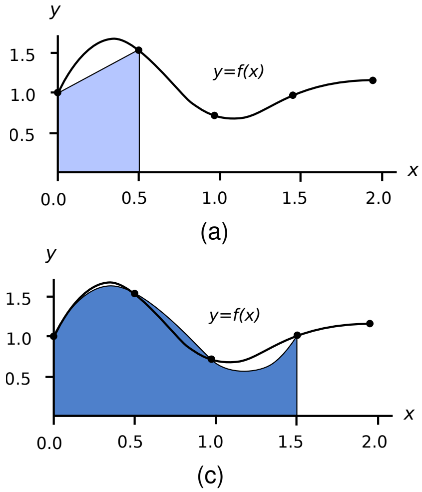

Figure 7.2: (a) The trapezoidal rule integrates $y = P_1(x)$ over $[x_0, x_1] = [0.0, 0.5]$. (b) Simpson's rule integrates $y = P_2(x)$ over $[x_0, x_1] = [0.0, 1.0]$. (c) Simpson's $\frac{3}{8}$ rule integrates $y = P_3(x)$ over $[x_0, x_3] = [0.0, 1.5]$. (d) Boole's rule integrates $y = P_4(x)$ over $[x_0, x_4] = [0.0, 2.0]$.

Theorem 7.1 (Closed Newton-Cotes Quadrature Formula).

Assume that $x_k = x_0 + kh$ are equally spaced nodes and $f_k = f(x_k)$. The first four closed Newton-Cotes quadrature formulas are

$$\int_{x_0}^{x_1} f(x)\,dx \approx \frac{h}{2}(f_0 + f_1) \quad \text{(trapezoidal rule)}, \tag{4}$$

$$\int_{x_0}^{x_2} f(x)\,dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2) \quad \text{(Simpson's rule)}, \tag{5}$$

$$\int_{x_0}^{x_3} f(x)\,dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) \quad \text{(Simpson's } \tfrac{3}{8} \text{ rule)}, \tag{6}$$

$$\int_{x_0}^{x_4} f(x)\,dx \approx \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) \quad \text{(Boole's rule)} \tag{7}$$

Corollary 7.1 (Newton-Cotes Precision).

Assume that $f(x)$ is sufficiently differentiable; then $E[f]$ for Newton-Cotes quadrature involves an appropriate higher derivative. The trapezoidal rule has degree of precision $n = 1$. If $f \in C^2[a, b]$, then

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12} f^{(2)}(c). \tag{8}$$

Simpson's rule has degree of precision $n = 3$. If $f \in C^4[a, b]$, then

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90} f^{(4)}(c). \tag{9}$$

Corollary 7.1 (Newton-Cotes Precision).

Simpson's $\frac{3}{8}$ rule has degree of precision $n = 3$. If $f \in C^4[a, b]$, then

$$\int_{x_0}^{x_3} f(x)\, dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80} f^{(4)}(c). \quad (10)$$

Boole's rule has degree of precision $n = 5$. If $f \in C^6[a, b]$, then

$$\int_{x_0}^{x_4} f(x)\, dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) - \frac{8h^7}{945} f^{(6)}(c). \quad (11)$$

proof of theorem 7.1

Start with the Lagrange polynomial $P_M(x)$ based on $x_0, x_1, ..., x_M$ that can be used to approximate $f(x)$:

$$f(x) \approx P_M(x) = \sum_{k=0}^{M} f_k L_{M,k}(x), \tag{12}$$

where $f_k = f(x_k)$ for $k = 0, 1, ..., M$. An approximation for the integral is obtained by replacing the integrand $f(x)$ with the polynomial $P_M(x)$. This is the general method for obtaining a Newton-Cotes integration formula:

$$\begin{aligned} \int_{x_0}^{x_M} f(x)\,dx &\approx \int_{x_0}^{x_M} P_M(x)\,dx \\ &= \int_{x_0}^{x_M} \left(\sum_{k=0}^{M} f_k L_{M,k}(x)\right) dx = \sum_{k=0}^{M} \left(\int_{x_0}^{x_M} f_k L_{M,k}(x)\,dx\right) \\ &= \sum_{k=0}^{M} \left(\int_{x_0}^{x_M} L_{M,k}(x)\,dx\right) f_k = \sum_{k=0}^{M} w_k f_k. \end{aligned} \tag{13}$$

The details for the general computations of the coefficients of w_k in (13) are tedious. We shall give a sample proof of Simpson's rule, which is the case $M = 2$. This case involves the approximating polynomial

$$P_2(x) = f_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}. \quad (14)$$

Since f_0, f_1, and f_2 are constants with respect to integration, the relations in (13) lead to

$$\begin{aligned} \int_{x_0}^{x_2} f(x)\,dx \quad &\approx \quad f_0 \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} dx + f_1 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} dx \\ &+ f_2 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} dx. \end{aligned} \quad (15)$$

We introduce the change of variable $x = x_0 + ht$ with $dx = h\,dt$ to assist with the evaluation of the integrals in (15). The new limits of integration are from $t = 0$ to $t = 2$. The equal spacing of the nodes $x_k = x_0 + kh$ leads to $x_k - x_j = (k - j)h$ and $x - x_k = h(t - k)$, which are used to simplify (15) and get

$$
\begin{aligned}
\int_{x_0}^{x_2} f(x)\,dx &\approx f_0 \int_0^2 \frac{h(t-1)h(t-2)}{(-h)(-2h)} h\,dt + f_1 \int_0^2 \frac{h(t-0)h(t-2)}{(h)(-h)} h\,dt \qquad (16)\\
&\quad + f_2 \int_0^2 \frac{h(t-0)h(t-1)}{(2h)(h)} h\,dt \\
&= f_0 \frac{h}{2} \int_0^2 (t^2 - 3t + 2)\,dt - f_1 h \int_0^2 (t^2 - 2t)dt + f_2 \frac{h}{2} \int_0^2 (t^2 - t)\,dt \\
&= f_0 \frac{h}{2} \left(\frac{t^3}{3} - \frac{3t^2}{2} + 2t \right) \Bigg|_{t=0}^{t=2} - f_1 h \left(\frac{t^3}{3} - t^2 \right) \Bigg|_{t=0}^{t=2} \\
&\quad + f_2 \frac{h}{2} \left(\frac{t^3}{3} - \frac{t^2}{2} \right) \Bigg|_{t=0}^{t=2} \\
&= f_0 \frac{h}{2} \left(\frac{2}{3} \right) - f_1 h \left(\frac{-4}{3} \right) + f_2 \frac{h}{2} \left(\frac{2}{3} \right) \\
&= \frac{h}{3} (f_0 + 4f_1 + f_2)
\end{aligned}
$$

and the proof is complete.

Example 7.1 Consider the function $f(x) = 1 + e^{-x}sin(4x)$, the equally spaced quadrature nodes $x_0 = 0.0, x_1 = 0.5, x_2 = 1.0, x_3 = 1.5$, and $x_4 = 2.0$, and the corresponding function values $f_0 = 1.00000, f_1 = 1.55152, f_2 = 0.72159, f_3 = 0.93765$, and $f_4 = 1.13390$. Apply the various quadrature formulas (4) through (7).

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The step size is $h = 0.5$, and the computations are

$$\begin{aligned}
\int_0^{0.5} f(x)\,dx &\approx \frac{0.5}{2}(1.00000 + 1.55152) = 0.63788 \\
\int_0^{1.0} f(x)\,dx &\approx \frac{0.5}{3}(1.00000 + 4(1.55152) + 0.72159) = 1.32128 \\
\int_0^{1.5} f(x)\,dx &\approx \frac{3(0.5)}{8}(1.00000 + 3(1.55152) + 3(0.72159) + 0.93765) \\
&= 1.64193 \\
\int_0^{2.0} f(x)\,dx &\approx \frac{2(0.5)}{45}(7(1.00000) + 32(1.55152) + 12(0.72159) \\
&\quad +32(0.93765) + 7(1.13390)) = 2.29444.
\end{aligned}$$

It is important to realize that the quadrature formulas (4) through (7) applied in the illustration above give approximations for definite integrals over different intervals. The graph of the curve $y = f(x)$ and the areas under the Lagrange polynomials $y = P_1(x), y = P_2(x), y = P_3(x)$, and $y = P_4(x)$ are shown in Figure 7.2(a) through (d), respectively.

In Example 7.1 we applied the quadrature rules with $h = 0.5$. If the endpoints of the interval $[a, b]$ are held fixed, the step size must be adjusted for each rule. The step sizes are $h = b - a, h = (b - a)/2, h = (b - a)/3$, and $h = (b - a)/4$ for the trapezoidal rule, Simpson's rule, Simpson's $\frac{3}{8}$ rule, and Boole's rule, respectively.The next example illustrates this point.

Example 7.2 Consider the integration of the function $f(x) = 1 + e^{-x}sin(4x)$ over the fixed interval $[a, b] = [0, 1]$. Apply the various formulas (4) through (7).

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For the trapezoidal rule, h=1 and

$$\begin{aligned} \int_0^1 f(x)\, dx &\approx \frac{1}{2}(f(0) + f(1)) \\ &= \frac{1}{2}(1.00000 + 0.72159) = 0.86079. \end{aligned}$$

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For Simpson's rule, $h = 1/2$, and we get

$$\begin{aligned} \int_0^1 f(x)\,dx &\approx \frac{1/2}{3}(f(0) + 4f(\frac{1}{2}) + f(1)) \\ &= \frac{1}{6}(1.00000 + 4(1.55152) + 0.72159) = 1.32128. \end{aligned}$$

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For Simpson's $\frac{3}{8}$ rule, $h = 1/3$, and we obtain

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{3(1/3)}{8}(f(0) + 3f(\frac{1}{3}) + 3f(\frac{2}{3}) + f(1)) \\ &= \frac{1}{8}(1.00000 + 3(1.69642) + 3(1.23447) + 0.72159) = 1.31440\end{aligned}$$

Introduction to Quadrature

For Simpson's $\frac{3}{8}$ rule, $h = 1/3$, and we obtain

$$\begin{aligned}
\int_0^1 f(x)\,dx &\approx \frac{3(1/3)}{8}(f(0) + 3f(\frac{1}{3}) + 3f(\frac{2}{3}) + f(1)) \\
&= \frac{1}{8}(1.00000 + 3(1.69642) + 3(1.23447) + 0.72159) = 1.31440
\end{aligned}$$

For Boole's rule, $h = 1/4$, and the result is

$$\begin{aligned}
\int_0^1 f(x)\,dx &\approx \frac{2(1/4)}{45}(7f(0) + 32f(\frac{1}{4}) + 12f(\frac{1}{2}) + 32f(\frac{3}{4}) + 7f(1)) \\
&= \frac{1}{90}(7(1.00000) + 32(1.65534) + 12(1.55152) \\
&\quad +32(1.06666) + 7(0.72159)) = 1.30859.
\end{aligned}$$

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The true value of the definite integral is

$$\int_0^1 f(x)\,dx = \frac{21e - 4cos(4) - sin(4)}{17e} = 1.3082506046426...,$$

and the approximation 1.30859 from Boole's rule is best. The area under each of the Lagrange polynomials $P_1(x), P_2(x), P_3(x)$, and $P_4(x)$ is shown in Figure 7.3(a) through (d), respectively.

Introduction to Quadrature

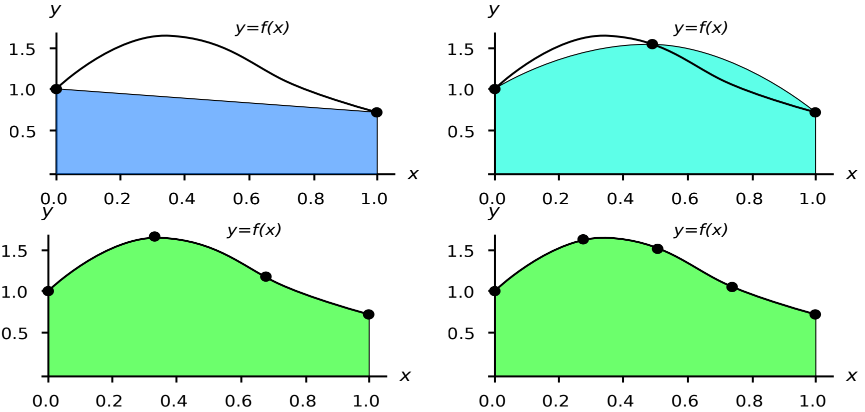

Figure 7.3: (a) The trapezoidal rule used over $[0, 1]$ yields the approximation 0.86079. (b) Simpson's rule used over $[0, 1]$ yields the approximation 1.32128. (c) Simpson's $\frac{3}{8}$ rule used over $[0, 1]$ yields the approximation 1.31440. (d) Boole's rule used over $[0, 1]$ yields the approximation 1.30859.

To make a fair comparison of quadrature methods, we must use the same number of function evaluations in each method. Our final example is concerned with comparing integration over a fixed interval $[a, b]$ using exactly five function evaluations $f_k = f(x_k)$,for $k = 0, 1, ..., 4$ for each method. when the trapezoidal rule is applied on the four subintervals $[x_0, x_1], [x_1, x_2], [x_2, x_3]$, and $[x_3, x_4]$, it is called a **composite trapezoidal rule**:

$$\begin{aligned}\int_{x_0}^{x_4} f(x)\,dx &= \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \int_{x_2}^{x_3} f(x)\,dx + \int_{x_3}^{x_4} f(x)\,dx \\ &\approx \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \frac{h}{2}(f_2 + f_3) + \frac{h}{2}(f_3 + f_4) \\ &= \frac{h}{2}(f_0 + 2f_1 + 2f_2 + 2f_3 + f_4).\end{aligned} \tag{17}$$

Simpson's rule can also be used in this manner. When Simpson's rule is applied on the two subintervals $[x_0, x_2]$ and $[x_2, x_4]$, it is called a **composite Simpson's rule**:

$$\begin{aligned}\int_{x_0}^{x_4} f(x)\,dx &= \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx \\ &\approx \frac{h}{3}(f_0 + 4f_1 + f_2) + \frac{h}{3}(f_2 + 4f_3 + f_4) \\ &= \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4).\end{aligned} \tag{18}$$

The next example compares the values obtained with (17), (18), and (7).

Example 7.3 Consider the integration of the function $f(x) = 1 + e^{-x}sin(4x)$ over $[a, b] = [0, 1]$. Use exactly five function evaluations and compare the results from the composite trapezoidal rule, composite Simpson rule, and Boole's rule.

Example 7.3 Consider the integration of the function $f(x) = 1 + e^{-x} sin(4x)$ over $[a, b] = [0, 1]$. Use exactly five function evaluations and compare the results from the composite trapezoidal rule, composite Simpson rule, and Boole's rule.

The uniform step size is $h = 1/4$. The composite trapezoidal rule (17) produces

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{1/4}{2}\left(f(0) + 2f(\frac{1}{4}) + 2f(\frac{1}{2}) + 2f(\frac{3}{4}) + f(1)\right) \\ &= \frac{1}{8}(1.00000 + 2(1.65534) + 2(1.55152) + 2(1.06666) + 0.72159) \\ &= 1.28358.\end{aligned}$$

Example 7.3 Consider the integration of the function $f(x) = 1 + e^{-x} sin(4x)$ over $[a,b] = [0,1]$. Use exactly five function evaluations and compare the results from the composite trapezoidal rule, composite Simpson rule, and Boole's rule.

The uniform step size is $h = 1/4$. The composite trapezoidal rule (17) produces

$$\begin{aligned}
\int_0^1 f(x)\,dx &\approx \frac{1/4}{2}(f(0) + 2f(\frac{1}{4}) + 2f(\frac{1}{2}) + 2f(\frac{3}{4}) + f(1)) \\
&= \frac{1}{8}(1.00000 + 2(1.65534) + 2(1.55152) + 2(1.06666) + 0.72159) \\
&= 1.28358.
\end{aligned}$$

Using the composite Simpson's rule (18), we get

$$\begin{aligned}
\int_0^1 f(x)\,dx &\approx \frac{1/4}{3}(f(0) + 4f(\frac{1}{4}) + 2f(\frac{1}{2}) + 4f(\frac{3}{4}) + f(1)) \\
&= \frac{1}{12}(1.00000 + 4(1.65534) + 2(1.55152) + 4(1.06666) + 0.72159) \\
&= 1.30938.
\end{aligned}$$

Introduction to Quadrature

We have already seen the result of Boole's rule in Example 7.2:

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{2(1/4)}{45}\left(7f(0) + 32f(\frac{1}{4}) + 12f(\frac{1}{2}) + 32f(\frac{3}{4}) + 7f(1)\right) \\ &= 1.30859.\end{aligned}$$

We have already seen the result of Boole's rule in Example 7.2:

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{2(1/4)}{45}(7f(0) + 32f(\frac{1}{4}) + 12f(\frac{1}{2}) + 32f(\frac{3}{4}) + 7f(1)) \\ &= 1.30859.\end{aligned}$$

The true value of the integral is

$$\int_0^1 f(x)\,dx = \frac{21e - 4cos(4) - sin(4)}{17e} = 1.3082506046426...,$$

and the approximation 1.30938 from Simpson's rule is much better than the value 1.28358 obtained from the trapezoidal rule. Again, the approximation 1.30859 from Boole's rule is closest. Graphs for the areas under the trapezoids and parabolas are shown in Figure 7.4(a) and (b), respectively.

Introduction to Quadrature

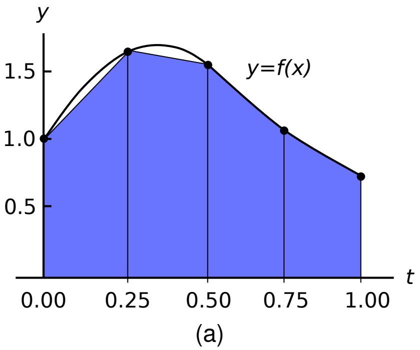

Figure 7.4: (a) The composite trapezoidal rule yields the approximation 1.28358. (b) The composite Simpson rule yields the approximation 1.30938.

Example 7.4 Determine the degree of precision of Simpson's $\frac{3}{8}$ rule.

It will suffice to apply Simpson's $\frac{3}{8}$ rule over the interval $[0,3]$ with the five test functions $f(x) = 1, x, x^2, x^3$,and x^4. For the first four functions, Simpson's $\frac{3}{8}$ rule is exact.

$$
\begin{aligned}
\int_0^3 1\,dx &= 3 = \frac{3}{8}(1 + 3(1) + 3(1) + 1) \\
\int_0^3 x\,dx &= \frac{9}{2} = \frac{3}{8}(0 + 3(1) + 3(2) + 3) \\
\int_0^3 x^2\,dx &= 9 = \frac{3}{8}(0 + 3(1) + 3(4) + 9) \\
\int_0^3 x^3\,dx &= \frac{81}{4} = \frac{3}{8}(0 + 3(1) + 3(8) + 27).
\end{aligned}
$$

The function $f(x) = x^4$ is the lowest power of x for which the rule is not exact.

$$\int_0^3 x^4\,dx = \frac{243}{5} \approx \frac{99}{2} = \frac{3}{8}(0 + 3(1) + 3(16) + 81).$$

Therefore, the degree of precision of Simpson's $3/8$ rule is $n = 3$.

Gauss-Legendre Integration

We wish to find the area under the curve

$$y = f(x) \qquad -1 \leq x \leq 1.$$

What method gives the best answer if only two function evaluations are to be made? We have already seen that the trapezoidal rule is a method for finding the area under the curve and that it uses two function evaluations at the endpoints $(-1, f(-1))$, and $(1, f(1))$. But if the graph of $y = f(x)$ is concave down, the error in approximation is the entire region that lies between the curve and the line segment joining the points; another instance is shown in Figure 7.10(a).
If we can use nodes x_1 and x_2 that lie inside the interval $[-1, 1]$, the line through the two points $(x_1, f(x_1))$ and $(x_2, f(x_2))$ crosses the curve, and the area under the line more closely approximates the area under the curve (see Figure 7.10(b)).

Gauss-Legendre Integration

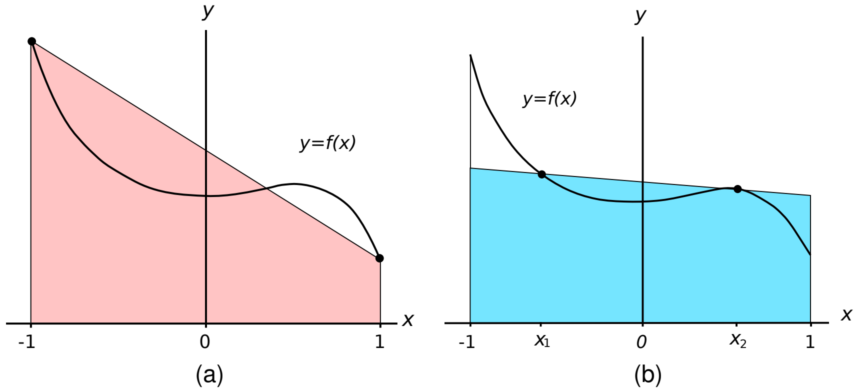

Figure 7.10: (a) Trapezoidal approximation using the abscissas -1 and 1. (b) Trapezoidal approximation using the abscissas x_1 and x_2.

Gauss-Legendre Integration

The equation of the line is

$$y = f(x_1) + \frac{(x - x_1)(f(x_2) - f(x_1))}{x_2 - x_1} \tag{1}$$

and the area of the trapezoid under the line is

$$A_{trap} = \frac{2x_2}{x_2 - x_1} f(x_1) - \frac{2x_1}{x_2 - x_1} f(x_2). \tag{2}$$

Notice that the trapezoidal rule is a special case of (2). When we choose $x_1 = -1$, $x_2 = 1$, and $h = 2$, then

$$T(f,h) = \frac{2}{2} f(x_1) - \frac{-2}{2} f(x_2) = f(x_1) + f(x_2).$$

We shall use the method of undetermined coefficients to find the abscissas x_1, x_2 and weights w_1, w_2 so that the formula

$$\int_{-1}^{1} f(x)\, dx \approx w_1 f(x_1) + w_2 f(x_2) \tag{3}$$

is the exact for cubic polynomials (i.e, $f(x) = a_3x^3 + a_2x^2 + a_1x + a_0$).

Gauss-Legendre Integration

Since four coefficients w_1, w_2, x_1, and x_2 need to be determined in equation (3), we can select four conditions to be satisfied. Using the fact that integration is additive, it will suffice to require that (3) be exact for the four functions $f(x) = 1, x, x^2, x^3$. The four integral conditions are

$$
\begin{aligned}
f(x) = 1: &\qquad \int_{-1}^{1} 1\,dx = 2 = w_1 + w_2 \\
f(x) = x: &\qquad \int_{-1}^{1} x\,dx = 0 = w_1 x_1 + w_2 x_2 \\
f(x) = x^2: &\qquad \int_{-1}^{1} x^2\,dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2 \\
f(x) = x^3: &\qquad \int_{-1}^{1} x^3\,dx = 0 = w_1 x_1^3 + w_2 x_2^3.
\end{aligned} \tag{4}
$$

Gauss-Legendre Integration

Now solve the system of nonlinear equations

$$\begin{aligned} w_1 + w_2 &= 2 && (5)\\ w_1 x_1 &= -w_2 x_2 && (6)\\ w_1 x_1^2 + w_2 x_2^2 &= \frac{2}{3} && (7)\\ w_1 x_1^3 &= -w_2 x_2^3 && (8) \end{aligned}$$

We can divide (8) by (6) and the result is

$$x_1^2 = x_2^2 \quad or \quad x_1 = -x_2. \tag{9}$$

Use (9) and divide (6) by x_1 on the left and $-x_2$ on the right to get

$$w_1 = w_2. \tag{10}$$

Substituting (10) into (5) results in $w_1 + w_2 = 2$. Hence

$$w_1 = w_2 = 1 \tag{11}$$

Gauss-Legendre Integration

Now using (11) and (9) in (7), we write

$$w_1 x_1^2 + w_2 x_2^2 = x_2^2 + x_2^2 = \frac{2}{3} \quad or \quad x_2^2 = \frac{1}{3}. \tag{12}$$

Finally, from(12) and (9) we see that the nodes are

$$-x_1 = x_2 = 1/3^{1/2} \approx 0.5773502692.$$

We have found the nodes and weights that make up the two-point Gauss-Legendre rule. Since the formula is exact for cubic equations, the error term will involve the fourth derivative.

Gauss-Legendre Integration

Theorem 7.8 (Gauss-Legendre Two-Point Rule).

If f is continuous on $[-1, 1]$, then

$$\int_{-1}^{1} f(x)\, dx \approx G_2(f) = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right). \tag{13}$$

The Gauss-Legendre rule $G_2(f)$ has degree of precision $n = 3$. If $f \in C^4[-1, 1]$, then

$$\int_{-1}^{1} f(x)\, dx = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) + E_2(f), \tag{14}$$

where

$$E_2(f) = \frac{f^{(4)}(c)}{135}. \tag{15}$$

Example 7.17 Use the two-point Gauss-Legendre rule to approximate

$$\int_{-1}^{1} \frac{dx}{x+2} = ln(3) - ln(1) \approx 1.09861$$

and compare the result with the trapezoidal rule $T(f,h)$ with $h=2$ and Simpson's rule $S(f,h)$ with $h=1$.

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Let $G_2(f)$ denote the two-point Gauss-Legendre rule; then

$$\begin{aligned} G_2(f) &= f(-0.57735) + f(0.57735) \\ &= 0.70291 + 0.38800 = 1.09091, \end{aligned}$$

$$\begin{aligned} T(f,2) &= f(-1.00000) + f(1.00000) \\ &= 1.00000 + 0.33333 = 1.33333, \end{aligned}$$

$$S(f,1) = \frac{f(-1) + 4f(0) + f(1)}{3} = \frac{1 + 2 + \frac{1}{3}}{3} = 1.11111.$$

Gauss-Legendre Integration

The errors are 0.00770, -0.23472, and -0.01250, respectively, so the Gauss-Legendre rule is seen to be best. Notice that the Gauss-Legendre rule required only two function evaluations and Simpson's rule required three. In this example the size of the error for $G_2(f)$ is about 61% of the size of the error for $S(f, 1)$.

Gauss-Legendre Integration

The general N-point Gauss-Legendre rule is exact for polynomial functions of degree $\leq 2N-1$, and the numerical integration formula is

$$G_N(f) = w_{N,1} f(x_{N,1}) + w_{N,2} f(x_{N,2}) + \cdots + w_{N,N} f(x_{N,N}). \qquad (16)$$

The abscissas $x_{N,k}$ and weights $w_{N,k}$ to be used have been tabulated and are easily available; Table 7.9 gives the value up to eight points. Also include in the table is the form of the error term $E_N(f)$ that corresponds to $G_N(f)$, and it can be used to determine the accuracy of the Gauss-Legendre integration formula.
The nodes are actually roots of the Legendre polynomials, and the corresponding weights must be obtained by solving a system of equations. For the three-point Gauss-Legendre rule the nodes are $-(0.6)^{1/2}, 0$, and $(0.6)^{1/2}$, and the corresponding weights are $5/9$, $8/9$, and $5/9$.

Gauss-Legendre Integration

Table 7.9 Gauss-Legendre Abscissas and Weights (1)

$$\int_{-1}^{1} f(x)\,dx = \sum_{k=1}^{N} w_{N,k} f(x_{N,k}) + E_N(f)$$

N	Abscissas, $x_{N,k}$	Weights, $w_{N,k}$	Truncation error $E_N(f)$
2	-0.5773502692	1.0000000000	$\frac{f^{(4)}(c)}{135}$
	0.5773502692	1.0000000000	
3	± 0.7745966692	0.5555555556	$\frac{f^{(6)}(c)}{15{,}750}$
	0.0000000000	0.8888888888	
4	± 0.8611363116	0.3478548451	$\frac{f^{(8)}(c)}{3{,}472{,}875}$
	± 0.3399810436	0.6521451549	
5	± 0.9061798459	0.2369268851	$\frac{f^{(10)}(c)}{1{,}237{,}732{,}650}$
	± 0.5384693101	0.4786286705	
	0.0000000000	0.5688888888	

Gauss-Legendre Integration

Table 7.9 Gauss-Legendre Abscissas and Weights (2)

$$\int_{-1}^{1} f(x)\,dx = \sum_{k=1}^{N} w_{N,k} f(x_{N,k}) + E_N(f)$$

N	Abscissas, $x_{N,k}$	Weights, $w_{N,k}$	Truncation error $E_N(f)$
6	± 0.9324695142	0.1713244924	$\frac{f^{(12)}(c)2^{13}(6!)^4}{(12!)^3 13!}$
	± 0.6612093865	0.3607615730	
	± 0.2386191861	0.4679139346	
7	± 0.9491079123	0.1294849662	$\frac{f^{(14)}(c)2^{15}(7!)^4}{(14!)^3 15!}$
	± 0.7415311856	0.2797053915	
	± 0.4058451514	0.3818300505	
	0.0000000000	0.4179591837	
8	± 0.9602898565	0.1012285363	$\frac{f^{(16)}(c)2^{17}(8!)^4}{(16!)^3 17!}$
	± 0.7966664774	0.2223810345	
	± 0.5255324099	0.3137066459	
	± 0.1834346425	0.3626837834	

Gauss-Legendre Integration

Theorem 7.9 (Gauss-Legendre Three-Point Rule).

If f is continuous on $[-1, 1]$, then

$$\int_{-1}^{1} f(x)\,dx \approx G_3(f) = \frac{5f(-\sqrt{3/5}) + 8f(0) + 5f(\sqrt{3/5})}{9}. \tag{17}$$

The Gauss-Legendre rule $G_3(f)$ has degree of precision $n = 5$. If $f \in C^6[-1, 1]$, then

$$\int_{-1}^{1} f(x)\,dx = \frac{5f(-\sqrt{3/5}) + 8f(0) + 5f(\sqrt{3/5})}{9} + E_3(f), \tag{18}$$

where

$$E_3(f) = \frac{f^{(6)}(c)}{15,750}. \tag{19}$$

Example 7.18 Show that the three-point Gauss-Legendre rule is exact for

$$\int_{-1}^{1} 5x^4 \, dx = 2 = G_3(f).$$

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Since the integrand is $f(x) = 5x^4$ and $f^{(6)}(x) = 0$, we can use (19) to see that $E_3(f) = 0$. But it is instructive to use (17) and do the calculations in this case.

$$G_3(f) = \frac{5(5)(0.6)^2 + 0 + 5(5)(0.6)^2}{9} = \frac{18}{9} = 2.$$

The next result shows how to change the variable of integration so that the Gauss-Legendre rules can be used on the interval $[a, b]$.

Gauss-Legendre Integration

Theorem 7.10 (Gauss-Legendre Translation).

Suppose that the abscissas $\{x_{N,k}\}_{k=1}^{N}$ and weights $\{w_{N,k}\}_{k=1}^{N}$ are given for the N-point Gauss-Legendre rule over $[-1, 1]$. To apply the rule over the interval $[a, b]$, use the change of variable

$$t = \frac{a+b}{2} + \frac{b-a}{2}x \quad and \quad dt = \frac{b-a}{2}dx \tag{20}$$

Then the relationship

$$\int_a^b f(t)\,dt = \int_{-1}^{1} f\left(\frac{a+b}{2} + \frac{b-a}{2}x\right)\frac{b-a}{2}dx \tag{21}$$

is used to obtain the quadrature formula

$$\int_a^b f(t)\,dt = \frac{b-a}{2}\sum_{k=1}^{N} w_{N,k} f\left(\frac{a+b}{2} + \frac{b-a}{2}x_{N,k}\right). \tag{22}$$

Example 7.19 Use the three-point Gauss-Legendre rule to approximate

$$\int_1^5 \frac{dt}{t} = ln(5) - ln(1) \approx 1.609438$$

and compare the result with Boole's rule $B(2)$ with $h = 1$.

Gauss-Legendre Integration

Example 7.19 Use the three-point Gauss-Legendre rule to approximate

$$\int_1^5 \frac{dt}{t} = ln(5) - ln(1) \approx 1.609438$$

and compare the result with Boole's rule $B(2)$ with $h = 1$.

Here $a = 1$ and $b = 5$, so the rule in (22) yields

$$G_3(f) = (2)\frac{5f(3-2(0.6)^{1/2}) + 8f(3+0) + 5f(3+2(0.6)^{1/2})}{9} \tag{23}$$

$$= (2)\frac{3.446359 + 2.666667 + 1.099096}{9} = 1.602694. \tag{24}$$

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$$G_3(f) = (2)\frac{5f(3 - 2(0.6)^{1/2}) + 8f(3 + 0) + 5f(3 + 2(0.6)^{1/2})}{9} \quad (23)$$

$$= (2)\frac{3.446359 + 2.666667 + 1.099096}{9} = 1.602694. \quad (24)$$

In Example 7.13 we saw that Boole's rule gave $B(2) = 1.617778$. The errors are 0.006744 and -0.008340, respectively, so that the Gauss-Legendre rule is slightly better in this case. Notice that the Gauss-Legendre rule requires three function evaluations and Boole's rule requires five. In this example the size of the two errors is about the same.

Gauss-Legendre integration formulas are extremely accurate, and the should be considered seriously when many integrals of a similar nature are to be evaluated. In this case, proceed as follows. Pick a few representative integrals, including some with the worst behaviour that is likely to occur. Determine the number of sample points N that is needed to obtain the required accuracy. Then fix the value N, and use the Gauss-Legendre rule with N sample points for all the integrals.