Solution of Nonlinear Equations $f(x) = 0$

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Outline: Chapter 7

1. Introduction to Quadrature
2. Composite Trapezoidal and Simpson's Rule
3. Recursive Rules and Romberg Integration
4. Gauss-Legendre Integration

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.

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

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.

Introduction to Quadrature

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

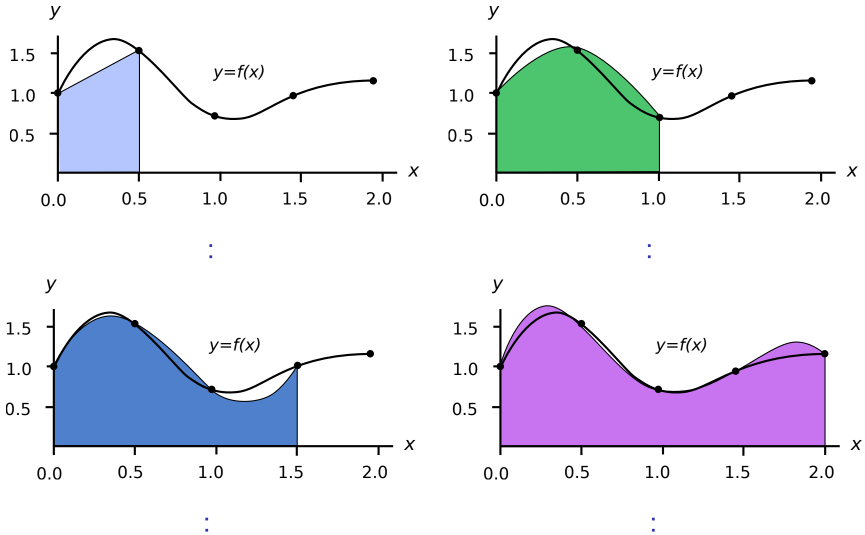

Figure 7.2: (a) The trapezoidal rule integrates $y = P_1(x)$ over

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

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

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

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

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 $f(x)$:

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

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

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

Introduction to Quadrature

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

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

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

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

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

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

and the proof is complete.

Introduction to Quadrature

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

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

Introduction to Quadrature

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

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

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

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

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.

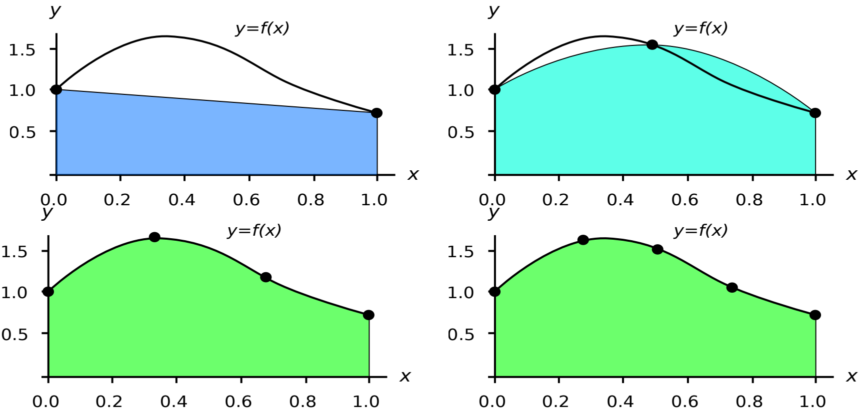

Figure 7.2: (a) The trapezoidal rule used over $[0, 1]$ yields the approximation 0.86079. (b) Simpson's rule used over $[0, 1]$ yields the approximation 1.32128. (c) Simpson's $\frac{3}{8}$ rule used over $[0, 1]$ yields the approximation 1.31440. (d) Boole's rule used over $[0, 1]$ yields the approximation 1.30859.

Introduction to Quadrature

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.

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

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

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.

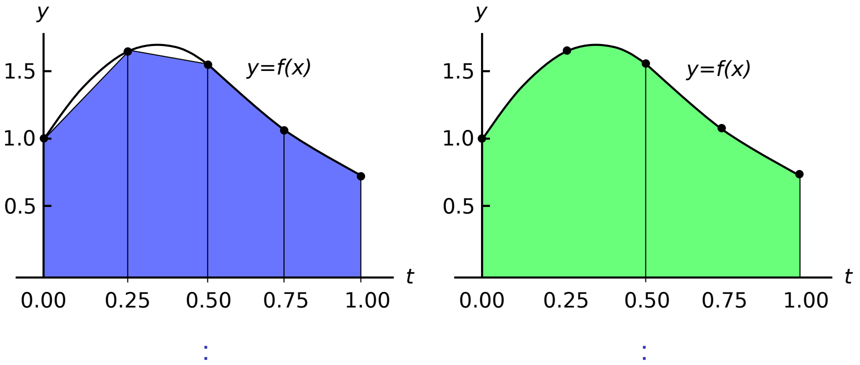

Figure 7.4: (a) The composite trapezoidal rule yields the approximation 1.28358. (b) The composite Simpson rule yields the approximation 1.30938.

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 $n = 3$.

Composite Trapezoidal and Simpson's Rule

An intuitive method of finding the area under the curve $y = f(x)$ over $[a, b]$ is by approximating that area with a series of trapezoids that lie above the intervals $\{[x_k, x_{k+1}]\}$.

Theorem 7.2 (Composite trapezoidal rule

Suppose that the interval $[a, b]$ is subdivided into M subintervals $[x_k, x_{k+1}]$ of width $h = (b - a)/M$ by using the equally spaced nodes $x_k = a + kh$, for $k = 0, 1, ..., M$. The composite trapezoidal rule for M subintervals can be expressed in any of three equivalent ways

$$(1a) \quad T(f, h) = \frac{h}{2} \sum_{k=1}^{M} (f(x_{k-1}) + f(x_k))$$

$$(1b) \quad T(f, h) = \frac{h}{2} (f_0 + 2f_1 + 2f_2 + 2f_3 + ... + 2f_{M-2} + 2f_{M-1} + f_M)$$

$$(1c) \quad T(f, h) = \frac{h}{2} (f(a) + f(b)) + h \sum_{k=1}^{M-1} (f(x_k))$$

Composite Trapezoidal and Simpson's Rule

This is an approximation to the integral of $f(x)$ over $[a,b]$ and we write

$$(2) \quad \int_a^b f(x)dx \approx T(f,h)$$

Proof. Apply the trapezoidal rule over each subinterval $[x_{k-1}, x_k]$. Use the additive property of integral for subintervals

$$(3) \quad \int_a^b f(x)dx = \sum_{k=1}^{M} \int_{x_{k-1}}^{x_k} f(x)dx \approx \frac{h}{2} \sum_{k=1}^{M} (f(x_{k-1}) + f(x_k))$$

Since $h/2$ is a constant, the distributive law of addition can be applied to obtain (1a). Formula (1b) is the expanded version of (1a). Formula (1c) shows how to group all the intermediate terms in (1b) that are multiplied by 2.

Composite Trapezoidal and Simpson's Rule

Example. Consider $f(x) = 2 + sin(2\sqrt{x})$. Use the composite trapezoidal rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1, 6]$. To generate 11 sample points we use $M = 10$ and $h = (6-1)/10 = 1/2$. Using formula (1c), the computation is

$$T(f, \tfrac{1}{2}) =$$
$$\frac{1/2}{2}(f(1)+f(6))+\frac{1}{2}(f(\tfrac{3}{2})+f(2)+f(\tfrac{5}{2})+f(3)+f(\tfrac{7}{2})+f(4)+f(\tfrac{9}{2})+f(5)+f(\tfrac{11}{2}))$$

$$= \frac{1}{4}(2.90929743 + 1.01735756) + \frac{1}{2}(2.63815764 + 2.30807174 + 1.97931647$$

$$+1.68305284+1.43530410+1.24319750+1.10831775+1.02872220+1.00024140)$$

$$= \frac{1}{4}(3.92665499) + \frac{1}{2}(14.42438165) = 0.98166375 + 7.21219083 = 8.19385457$$

Composite Trapezoidal and Simpson's Rule

Theorem 7.3 (Composite Simpson Rule)

Suppose that $[a, b]$ is subdivided into $2M$ subintervals $[x_k, x_{k+1}]$ of equal width $h = (b-a)/2M$ by using $x_k = a + kh$ for $k = 0, 1, ..., 2M$. The composite Simpson rule for $2M$ subintervals can be expressed in any of three equivalent ways:

$$(4a) \quad S(f,h) = \frac{h}{3}\sum_{k=1}^{M}(f(x_{2k-2}) + 4f(x_{2k-1}) + f(x_{2k}))$$

$$(4b) \quad S(f,h) = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + ... + 2f_{M-2} + 4f_{M-1} + f_M)$$

$$(4c) \quad S(f,h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3}\sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3}\sum_{k=1}^{M} f(x_{2k-1})$$

This is an approximation to the integral of $f(x)$ over $[a, b]$, and we write

$$(5) \quad \int_a^b f(x)dx \approx S(f,h)$$

Composite Trapezoidal and Simpson's Rule

Proof. Apply Simpson's rule over each subinterval $[x_{k-1}, x_k]$. Use the additive property of the integral for subintervals:

$$(3) \quad \int_a^b f(x)dx = \sum_{k=1}^{M} \int_{x_{2k-2}}^{2x_k} f(x)dx \approx \frac{h}{3} \sum_{k=1}^{M} (f(x_{2k-2}) + 4f(x_{2k-1} + f(x_{2k}))$$

Since $h/3$ is a constant, the distributive law of addition can be applied to obtain (4a). Formula (4b) is the expanded version of (4a). Formula (4c) shows how to group all the intermediate terms in (4b) that are multiplied by 2 and those that are multiplied by 4.

Example Consider $f(x) = 2 + sin(2\sqrt{x})$. Use the composite Simpson rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1, 6]$. To generate 11 sample points, we must use $M = 5$ and $h = (6-1)/10 = 1/2$. Using formula (4c), the computation is

$S(f, \frac{1}{2}) = \frac{1}{6}(f(1) + f(6)) + \frac{1}{3}(f(2) + f(3) + f(4) + f(5)) + \frac{2}{3}(f(\frac{3}{2}) + f(\frac{5}{2}) + f(\frac{7}{2}) + f(\frac{9}{2}) + f(\frac{11}{2}))$

$$= \frac{1}{6}(2.90929743+1.01735756)+\frac{1}{3}(2.30807174+1.6835284+1.24319750+1.0287222$$

$$= \frac{2}{3}(2.63815764 + 1.97931647 + 1.43530410 + 1.10831775 + 1.00024140)$$

$$= \frac{1}{6}(3.926654499) + \frac{1}{3}(6.26304429) + \frac{2}{3}(8.16133735)$$

$$= 0.65444250 + 2.0876814 + 5.44089157 = 8.18301550.$$

Error Analysis

The significance of the next two results is to understand that the error terms $E_T(f,h)$ and $E_S(f,h)$ for the composite trapezoidal rule and composite Simpson rule are of the order $O(h^2)$ and $O(h^4)$, respectively. This shows that the error for Simpson's rule converges to zero faster than the error for the trapezoidal rule as the step size h decreases to zero. In cases where the derivatives of $f(x)$ are known, the formulas

$$E_T(f,h) = \frac{-(b-a)f^{(2)}(c)h^2}{12} \quad and \quad E_S(f,h) = \frac{-(b-a)f^{(4)}(c)h^4}{180}$$

Can be used to eliminate the number of subintervals required to achieve a specified accuracy

Composite Trapezoidal and Simpson's Rule

Corollary 7.2. (Trapezoidal rule error analysis)

Suppose that $[a, b]$ is subdivided into M subintervals $[x_k, x_{k+1}]$ of width $h = (b-a)/M$. The composite trapezoidal rule

$$(7) \quad T(f,h) = \frac{h}{2}(f(a)+f(b)) + h\sum_{k=1}^{M-1} f(x_k)$$

is an approximation to the integral

$$(8) \quad \int_a^b f(x)dx = T(f,h) + E_T(f,h).$$

Furthermore, if $f \in C^2[a,b]$, there exists a value c with $a < c < b$ so that the error term $E_T(f,h)$ has the form

$$(9) \quad E_T(f,h) = \frac{-(b-a)f^{(2)}(c)h^2}{12} = O(h^2).$$

Proof. We first determine the error term when the rule is applied over $[x_0, x_1]$. Integrating the Lagrange polynomial $P_1(x)$ and its reminder yields

$$(10) \quad \int_{x_0}^{x_1} f(x)dx = \int_{x_0}^{x_1} P_1(x)dx + \int_{x_0}^{x_1} \frac{(x-x_0)(x-x_1)f^{(2)}(c(x))}{21}dx.$$

The term $(x-x_0)(x-x_1)$ does not change sign on $[x_0, x_1]$, and $f^{(2)}(c(x))$ is continuous Hence the second mean value theorem for integrals implies that there exist a value c_1 so that

$$(11) \quad \int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) + f^{(2)}(c_1)\int_{x_0}^{x_1} \frac{(x-x_0)(x-x_1)}{2!}dx.$$

Composite Trapezoidal and Simpson's Rule

Use the change of variable $x = x_0 + ht$ in the integral on the right side of (11):

$$(12) \quad \int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) + \frac{f^{(2)}(c_1)}{2}\int_0^1 h(t-0)h(t-1)hdt.$$

$$= \frac{h}{2}(f_0 + f_1) + \frac{f^{(2)}(c_1)h^3}{2}\int_0^1 (t^2 - t)dt.$$

$$= \frac{h}{2}(f_0 + f_1) - \frac{f^{(2)}(c_1)h^3}{12}.$$

Now we are ready to add up the error terms for all of the intervals $[x_k, x_{k-1}]$:

$$(13) \quad \int_a^b f(x)dx = \sum_{k=1}^{M}\int_{x_{k-1}}^{x_k} f(x)dx$$

$$= \sum_{k=1}^{M}\frac{h}{2}(f(x_{k-1}) + f(x_k)) - \frac{h^3}{12}\sum_{k=1}^{M} f^{(2)}(c_k).$$

Composite Trapezoidal and Simpson's Rule

The first sum is the composite trapezoidal rule $T(f,h)$. In the second term, one factor of h replaced with its equivalent $h = (b-a)/M$, and the result is

$$\int_a^b f(x)dx = T(f,h) - \frac{(b-a)h^2}{12}\left(\frac{1}{M}\sum_{k=1}^{M} f^{(2)}(c_k)\right)$$

The term in parentheses can be recognized as an average of values for the second derivative and hence is replaced by $f^{(2)}(c)$. Therefore we have established that

$$\int_a^b f(x)dx = T(f,h) - \frac{(b-a)f^{(2)}(c)}{12},$$

and the proof of corollary is complete.

Composite Trapezoidal and Simpson's Rule

Corollary 7.3. (Simpson's rule: error analysis)

Suppose that $[a, b]$ is subdivided into $2M$ subintervals $[x_k, x_{k+1}]$ of equal width $h = (b-a)/2M$. The composite Simpson rule

$$(14) \quad S(f,h) = \frac{h}{3}(f(a)+f(b)) + \frac{2h}{3}\sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3}\sum_{k=1}^{M} f(x_{2k-1})$$

is an approximation to the integral

$$(15) \quad \int_a^b f(x)dx = S(f,h) + E_S(f,h).$$

Furthermore, if $f \in C^4[a,b]$, there exists a value c with $a < c < b$ so that the error term $E_S(f,h)$ has the form

$$(16) \quad E_S(f,h) = \frac{-(b-a)f^{(4)}(c)h^4}{180} = O(h^4).$$

Composite Trapezoidal and Simpson's Rule

Example7.8 Consider $f(x) = 2 + sin(2\sqrt{x})$. Investigate the error when the composite trapezoidal rule is over $[1, 6]$ and the number of subintervals is 10, 20, 40, 80 and 160.

Table7.2 Composite trapezoidal rule for $f(x) = 2 + sin(2\sqrt{x})$ over $[1, 6]$

M	h	$T(f, h)$	$E_T(f, h) = O(h^2)$
10	0.5	8.19385457	-0.01037540
20	0.25	8.18604926	-0.00257006
40	0.125	8.18412019	-0.00064098
80	0.0625	8.18363936	-0.00016015
160	0.03125	8.18351924	-0.00004003

Table 7.2 shows the approximations $T(f, h)$. The antiderivative of $f(x)$ is

$$F(x) = 2x - \sqrt{x}cos(2\sqrt{x}) + \frac{sin(2\sqrt{x})}{2},$$

and the true value of definite integral is

$$\int_1^6 f(x)dx = F(x)|_{x=1}^{x=6} = 8.1834792077.$$

This value was used to compute the values $E_t(f,h) = 8.1834792077 - T(f,h)$ in table 7.2. It is important to observe that when h is reduced by a factor of 1/2 the successive errors $E_T(f,h)$ are diminished by approximately 1/4. This confirm that the order is of $O(h^2)$.

Example7.9 Find the number M and the step size h so that the error $E_T(f,h)$ for the composite trapezoidal rule is less than $5\text{x}10^{-9}$ for the approximation $\int_2^7 dx/x \approx T(f,h)$. The integral is $f(x) = 1/x$ and the first two derivatives are $f'(x) = -1/x^2$ and $f^{(2)}(x) = 2/x^3$. The maximum value of $|f^{(2)}(x)|$ taken over $[2,7]$ occurs at the endpoint $x = 2$, and those we have the bound $|f^{(2)}(c)| \leq |f^{(2)}(2)| = 1/4$, for $2 \leq c \leq 7$. This is used with formula (9) to obtain

$$(17) \quad |E_T(f,h)| = \frac{|-(b-a)f^{(2)}(c)h^2|}{12} \leq \frac{(7-2)\frac{1}{4}h^2}{12} = \frac{5h^2}{48}.$$

Composite Trapezoidal and Simpson's Rule

The step size h and number M satisfy the relation $h = 5/M$, and this is used in (17) to get the relation

$$|E_T(f,h)| \leq \frac{125}{48M^2} \leq 5 * 10^{-9} \tag{18}$$

Now rewrite (18) so that is easier to solve for M:

$$\frac{25}{48 * 10^9} \leq M^2. \tag{19}$$

Solving (19), we find that $22821.77 \leq M$. Since M must be an integer, we choose $M = 22822$ and the corresponding step size is $h = 5/22822 = 0.000219086846$. When the composite trapezoidal rule is implemented with this main function evaluations, there is a possibility that the rounded-off function evaluation will produce a significant amount of error. When the computation was perform, the result was

$$T\left(f, \frac{5}{10000}\right) = 1.252762973$$

The composite trapezoidal rule usually requires a large number of function evaluations to achieve and accurate answer. This is contrasted in the next example with Simpson's rule, which will require significantly fewer evaluations

Example7.10 Find the number M and the step size h so that the error $E_S(f,h)$ for the composite Simpson rule is less than $5 \text{x} 10^{-9}$ for the approximation $\int_2^7 dx/x \approx S(f,h)$. The integral is $f(x) = 1/x$ and $f^{(4)}(x) = 24/x^5$. The maximum value of $|f^{(4)}(x)|$ taken over $[2,7]$ occurs at the endpoint $x = 2$, and those we have the bound $|f^{(4)}(c)| \leq |f^{(4)}(2)| = 3/4$, for $2 \leq c \leq 7$. This is used with formula (16) to obtain

$$(20) \quad |E_S(f,h)| = \frac{|-(b-a)f^{(4)}(c)h^4|}{180} \leq \frac{(7-2)\frac{3}{4}h^4}{180} = \frac{h^4}{48}.$$

Composite Trapezoidal and Simpson's Rule

The step size h and number M satisfy the relation $h = 5/2M$, and this is used in (20) to get the relation

$$(21) \quad |E_S(f,h)| \leq \frac{625}{768M^4} \leq 5 * 10^{-9}$$

Now rewrite (21) so that is easier to solve for M:

$$(22) \quad \frac{125}{768} * 10^9 \leq M^4.$$

Solving (22), we find that $112.95 \leq M$. Since M must be an integer, we choose $M = 113$, and the corresponding step size is $h = 5/226 = 0.02212389381$. When the composite Simpson rule was perform, the result was

$$S\left(f, \frac{5}{226}\right) = 1.252762969,$$

which agrees with $\int_2^7 dx/x = ln(x)|_2^7 = 1.252762968$.

Composite Trapezoidal and Simpson's Rule

Experimentation shows that it takes about 129 function evaluations to achieve the desired accuracy of $5 * 10^{-9}$ and one the calculation is performed with $M = 64$ the result is

$$S\left(f, \frac{5}{128}\right) = 1.252762973.$$

So we see that the composite Simpson rule using 229 evaluations of $f(x)$ and the composite trapezoidal rule using 22823 evaluations of $f(x)$ achieve the same accuracy. In Example 7.10, Simpson's rule required about $\frac{1}{100}$ the number of function evaluations.

Recursive Rules and Romberg Integration

Theorem (Successive Trapezoidal Rules)

Suppose that $J \geq 1$ and the points$\{x_k = a + kh\}$ subdivide $[a, b]$ into $2^J = 2M$ subintervals of equal width $h = (b - a)/2^J$. The trapezoidal rules $T(f, h)$ and $T(f.2h)$ obey the relationship

$$T(f, h) = \frac{T(f, 2h)}{2} + h \sum_{k=1}^{M} f(x_{2k-1}). \tag{1}$$

Definition (Sequence of trapezoidal Rules)

Define $T(0) = (h/2)(f(a) + f(b))$, which is the trapezoidal rule with step size $h = b - a$. Then for each $J \geq 1$ define $T(J) = T(f, h)$, where $T(f, h)$ is the trapezoidal rule with step size $h = (b - a)/2^J$.

Recursive Rules and Romberg Integration

Corollary (Recursive Trapezoidal Rules)

Start with $t(0) = (h/2)(f(a) + f(b))$. Then a sequence of trapezoidal rules $\{T(J)\}$ is generated by the recursive formula

$$(2) \qquad T(J) = \frac{T(J-1)}{2} + h\sum_{k=1}^{M} f(x_{2k-1}). \quad forJ = 1, 2, ...,$$

where $h = (b-a)/2^J$ and $\{x_k = a + kh\}$

Recursive Rules and Romberg Integration

Corollary (Recursive Trapezoidal Rules)

Start with $t(0) = (h/2)(f(a) + f(b))$. Then a sequence of trapezoidal rules $\{T(J)\}$ is generated by the recursive formula

$$(2) \qquad T(J) = \frac{T(J-1)}{2} + h\sum_{k=1}^{M} f(x_{2k-1}). \quad forJ = 1, 2, ...,$$

where $h = (b-a)/2^J$ and $\{x_k = a + kh\}$

Proof. For the even nodes $x_0 < x_2 < ... < x_{2M-2} < x_{2M}$, we use the trapezoidal rule with step size $2h$:

$$(3) \qquad T(J-1) = \frac{2h}{2}(f_0 + 2f_2 + 2f_4 + ... + 2f_{2M-4} + 2f_{2M-2} + f_{2M})$$

For all the nodes $x_0 < x_2 < ... < x_{2M-2} < x_{2M}$, we use the trapezoidal rule with step size h

$$(4) \quad T(J) = \frac{h}{2}(f_0 + 2f_1 + 2f_2 + ... + 2f_{2M-2} + 2f_{2M-1} + f_{2M}).$$

Collecting the even and odd subscripts in (4) yields

$$(5) \quad T(J) = \frac{h}{2}(f_0 + 2f_1 + 2f_2 + ... + 2f_{2M-2} + 2f_{2M-1} + f_{2M}) + h\sum_{k=1}^{M} f_{2k-1}.$$

Substituting (3) into (5) results in $T(J)$

Example

Use the sequential trapezoidal rule to compute the approximations $T(0)$, $T(1)$, $T(2)$, and $T(3)$ for the integral $\int_a^b dx/x = ln(5) - ln(1) = 1.609437912$. The table shows the nine values required to compute $T(3)$ and the mid-points required to compute $T(1)$, $T(2)$, and $T(3)$. Details for obtaining the results are as follows:

$$When \quad h = 4: \quad T(0) = \frac{4}{2}(1.000000 + 0.200000)$$

$$When \quad h = 2: \quad T(1) = \frac{T(0)}{2} + 2(0.333333) = 1.200000 + 0.666666 = 1.866666.$$

Recursive rules

$$When\ h = 1 : T(2) = \frac{T(1)}{2} + 1(0.500000 + 0.250000) = 0.933333 + 0.750000 = 1.6833$$

$$When\ h = \frac{1}{2} : \quad T(3) = \frac{T(2)}{2} + \frac{1}{2}(0.666667 + 0.400000 + 0.285714 + 0.222222)$$
$$= 0.841667 + 0.787302 = 1.628968.$$

The nine points used to computed $T(3)$ and the midpoints required to compute $T(1)$, $T(2)$ and $T(3)$

x	$f(x) = \frac{1}{x}$	Endpoints for computing $T(0)$	Midpoints for computing $T(1)$	Midpoints for computing $T(2)$	Midpoints for, computing $T(3)$
1.0	1.000000	1.000000			
1.5	0.666667				0.666667
2.0	0.500000			0.500000	
2.5	0.400000				0.400000
3.0	0.333333		0.333333		
3.5	0.285714				0.285714
4.0	0.250000			0.250000	
4.5	0.222222				0.222222
5.0	0.200000	0.200000			

Recursive rules

Our next result shows an important relationships between the trapezoidal rule and the Simpson's rule. When the trapezoidal rule is computed using step sizes $2h$ and h, the result is $T(f, 2h)$ and $T(f, h)$, respectively. This values are combined to obtain Simpson‘s rule:

$$(6) \qquad S(f,h) = \frac{4T(f,h) - T(f,2h)}{3}.$$

Theorem (Recursive Simpson rules)

Suppose that $\{T(J)\}$ is the sequence of trapezoidal rules generated by Corollary. If $J \geq 1$ and $S(J)$ is Simpson's rule for 2^J subintervals of $[a, b]$, then $S(J)$ and the trapezoidal rules $T(J-1)$ and $\{T(J)\}$ obey the relationship

$$(7) \qquad S(J) = \frac{4T(J) - T(J-1)}{3} \quad for \quad J = 1, 2, \ldots$$

Recursive rules

Proof. The trapezoidal rule $T(J)$ with step size h yields the approximation

$$(8) \qquad \int_a^b f(x)dx \approx \frac{h}{2}(f_0+2f_1+2f_2+\ldots+2f_{2M-2}+2f_{2M-1}+f_{2M}) = T(J).$$

The trapezoidal rule $T(J-1)$ with step size $2h$ produces

$$(9) \qquad \int_a^b f(x)dx \approx h(f_0+2f_1+2f_2+\ldots+2f_{2M-2}+f_{2M}) = T(J-1).$$

Multiplying relation (8) by 4 yields

$$(10) \quad 4\int_a^b f(x)dx \approx h(2f_0+4f_1+4f_2+\ldots+4f_{2M-2}+4f_{2M-1}+2f_{2M}) = 4T(J).$$

Recursive rules

Now subtract (9) from (10) and the result is

$$(11)\quad 3\int_a^b f(x)dx \approx h(f_0 + 4f_1 + 2f_2 + ... + 2f_{2M-2} + 4f_{2M-1} + f_{2M})$$

$$= 4T(J) - T(J-1).$$

This can be rearranged to obtain

$$(12)\quad \int_a^b f(x)dx \approx \frac{h}{3}(f_0 + 4f_1 + 2f_2 + ... + 2f_{2M-2} + 4f_{2M-1} + f_{2M})$$

$$= \frac{4T(J) - T(J-1)}{3}.$$

The middle term in (12) is Simpson's rule $S(J) = S(f,h)$ and hence the theorem is proved.

Example

Use the sequential Simpson rule to compute the approximations $S(1)$, $S(2)$ and $S(3)$ for the integral $\int_a^b dx/x = ln(5) - ln(1) = 1.609437912$. Using the results of the example above and formula (7) with $J = 1, 2$ and 3, we compute

$$S(1) = \frac{4T(1) - T(0)}{3} = \frac{4(1.866666) - 2.400000}{3} = 1.688888,$$

$$S(2) = \frac{4T(2) - T(1)}{3} = \frac{4(1.683333) - 1.866666}{3} = 1.622222,$$

$$S(3) = \frac{4T(3) - T(2)}{3} = \frac{4(1.628968) - 1.683333}{3} = 1.610846.$$

We will now show that formulas (7) and (14) are special cases of the process of Romberg integration. Let us announce that the next level of approximation for the integral of the example is

$$S(1) = \frac{64B(3) - B(2)}{63} = \frac{64(1.610088) - 1.617778}{63} = 1.609490,$$

Romberg Integration

We saw that the error terms $E_T(f,h)$ and $E_S(f,h)$ for the composite trapezoidal rule and composite Simpson rule are of order $O(h^2)$ and $O(h^4)$, respectively. It is not difficult to show that the error term $E_B(f,h)$ for the composite Boole rule is of the order $O(h^6)$. Thus we have the pattern

$$(15) \quad \int_a^b f(x)dx = T(f,h) + O(h^2),$$

$$(16) \quad \int_a^b f(x)dx = S(f,h) + O(h^4),$$

$$(17) \quad \int_a^b f(x)dx = B(f,h) + O(h^6),$$

The pattern for the remainders in (15) through (17) is extended in the following sense. Suppose that an approximation rule is used with step sizes h and $2h$; then an algebraic manipulation of the two answers is used to produces an improved answer.

Romberg integration

Each successive level of improvement increases the order of the error term from $O(h^{2N})$ to $O(h^{2N+2})$. This process, called *Romberg integration*, has its strengths and weaknesses.

The Newton-Cotes rules are seldom used past Boole's rule. This is because the nine-point Newton-Cotes quadrature rule involves negative weights, and all the rules past the 10-point rule involve negative weights. This could introduce loss of significance error due to round off. The Romberg method has the advantages that all the weights are positive and the equally spaced abscissas are easy to compute.

A computational weakness of romberg integration is that twice as many function evaluations are needed to decrease the error from $O(h^{2N})$ to $O(h^{2N+2})$. The use of the sequential rules will help keep the number of computations down.

Romberg integration

The development of Romberg integration relies on the theoretical assumption that, if $f \in C^N[a,b]$ for all N, then the error term for the trapezoidal rule can be represented in a series involving only even powers of h; that is,

$$(18) \quad \int_a^b f(x)dx = T(f,h) + E_T(f,h),$$

where

$$(19) \quad E_T(f,h) = a_1h^2 + a_2h^4 + a_3h^6 + \ldots$$

Since only even powers of h can occur in (19), the Richardson improvement process is used successively first to eliminate a_1, next to eliminate a_2, then to eliminate a_3, and so on. This process generates quadrature formulas whose error terms have even orders $O(h^4)$, $O(h^6)$, $O(h^8)$, and so on. We shall show that the first improvement is Simpson's rule for $2M$ intervals. Start with $T(f,2h)$ and $T(f,h)$ and the equations

$$(20) \quad \int_a^b f(x)dx = T(f,2h) + a_1 4h^2 + a_2 16h^4 + a_3 64h^6 + \ldots$$

Romberg integration

And

$$(21)\quad \int_a^b f(x)dx = T(f,h) + a_1h^2 + a_2h^4 + a_3h^6 + \ldots$$

Multiply equation (21) by 4 and obtain

$$(22)\quad 4\int_a^b f(x)dx = 4T(f,h) + a_1 4h^2 + a_2 4h^4 + a_3 4h^6 + \ldots$$

Eliminate a_1 by subtracting (20) from (22). The result is

$$(23)\quad 3\int_a^b f(x)dx = 4T(f,h) - T(f,2h) - a_2 12h^4 - a_3 60h^6 + \ldots$$

Now divide equation (23) by 3 and renamed the coefficients in the series:

$$(24)\quad \int_a^b f(x)dx = \frac{4T(f,h) - T(f,2h)}{3} + a_1h^4 + b_2h^6 + \ldots$$

Romberg integration

As noted in (6), the first quantity on the right side of (24) is Simpson's rule $S(f,h)$. This shows that $E_s(f,h)$ involves only even powers of h:

$$(25) \quad \int_a^b f(x)dx = S(f,h) + b_1h^4 + b_2h^6 + b_3h^8 + \ldots$$

To show that the second improvement is Boole's rule, start with (25) and write down the formula involving $S(f,2h)$

$$(26) \quad \int_a^b f(x)dx = S(f,2h) + b_1 16h^4 + b_2 64h^6 + b_3 256h^8 + \ldots$$

When b_1 is eliminated from (25) and (26), the results involves Boole's rule

$$(27) \quad \int_a^b f(x)dx = \frac{16S(f,h) - S(f,2h)}{15} - \frac{b_2 48h^6}{15} - \frac{b_3 240h^8}{15} - \ldots$$

$$= B(f,h) - \frac{b_2 48h^6}{15} - \frac{b_3 240h^8}{15} - \ldots$$

Romberg integration

Lemma(Richardson's improvement for Romberg integration

Given two approximations $R(2h, K-1)$ and $R(h, K-1)$ for the quantity Q satisfy

$$Q = R(h, K-1) + c_1 h^{2K} + c_2 h^{2K+2} + \ldots \tag{28}$$

And

$$Q = R(2h, K-1) + c_1 4^K h^{2k} + c_2 4^{K+1} h^{K+2} + \ldots \tag{29}$$

An improved approximation has the form

$$Q = \frac{4^K R(h, K-1) - R(2h, K-1)}{4^K - 1} + O(h^{2K+2}). \tag{30}$$

Definition

Define the sequence $\{R(J,K) : J \geq K\}_{J=0}^{\infty}$ of quadrature formulas for $f(x)$ over $[a,b]$ as follows:

$$\begin{aligned} R(J,0) &= T(J) \quad \textit{for} \quad J \geq 0, \text{ is the sequential trapezoidal rule.} \\ R(J,1) &= S(J) \quad \textit{for} \quad J \geq 1, \text{ is the sequential Smpson rule.} \\ R(J,2) &= B(J) \quad \textit{for} \quad J \geq 2, \text{ is the sequential Boole's rule.} \end{aligned} \tag{31}$$

The starting rules $\{R(J,0)\}$ are used to generate the first improvement, $\{R(J,1)\}$, which in turn is to generate the second improvement, $\{R(J,2)\}$. We have already seen the patterns

$$(32) \quad R(J,1) = \frac{4^1 R(J,0) - R(J-1,0)}{4^1 - 1} \quad \textit{for } J \geq 1.$$

$$(32) \quad R(J,2) = \frac{4^2 R(J,1) - R(J-1,1)}{4^2 - 1} \quad \textit{for } J \geq 2.$$

which are the rules in (24) and (27) stated using the notation in (31). The general rule for constructing improvements is

$$(33) \quad R(J,3) = \frac{4^K R(J,K-1) - R(J-1,K-1)}{4^K - 1} \quad \textit{for } J \geq K.$$

Table 7.5. Romberg integration tableau

J	$R(J,0)$ Trapezoidal rule	$R(J,1)$ Simpson's rule	$R(J,2)$ Boole's rule	$R(J,3)$ Third improvement	$R(J,4)$ Fourth improvement
0	$R(0,0)$				
1	$R(1,0)$	$R(1,1)$			
2	$R(2,0)$	$R(2,1)$	$R(2,2)$		
3	$R(3,0)$	$R(3,1)$	$R(3,2)$	$R(3,3)$	
4	$R(4,0)$	$R(4,1)$	$R(4,2)$	$R(4,3)$	$R(4,4)$

Example Use Romberg integration to find approximation for the definite integral

$$\int_0^{\pi/2} (x^2 + x + 1) cos(x) dx = -2 + \frac{\pi}{2} + \frac{\pi}{4} = 2.038197427067\ldots$$

The computation are given in Table 7.6. In each column the numbers are converging to the value 2.038197427067... The values in the Simpson's rule column converge faster than the values in the trapezoidal rule column. For this example, convergence in columns to the right is faster than the adjacent column to the left.

Convergence of the Romberg values in Table 7.6 is easier to see if we look at the error terms $E(J,K) = -2 + \pi/2 + \pi/4 - R(J,K)$. Suppose that the interval width is $h = b - a$ and that the higher derivatives of the Romberg table diminishes by about a factor of $1/2^{2K+2} = 1/4^{k+1}$ as one progresses down its rows. The errors $E(J,0)$ diminish by a factor of $1/4$, the errors $E(J,1)$ diminish by a factor of $1/16$, and so on. This can be observed by inspecting the entries $\{E(J,K)\}$ in Table 7.7

Table 7.6. Romberg integration tableau for the example

J	$R(J,0)$ Trapezoidal rule	$R(J,1)$ Simpson's rule	$R(J,2)$ Boole's rule	$R(J,3)$, Third improvement
0	0.785398163397			
1	1.726812656758	2.040617487878		
2	1.960534166564	2.038441336499	2.038296259740	
3	2.018793948078	2.038213875249	2.038198711166	2.038197162776
4	2.033347341805	2.038198473047	2.038197446234	2.038197426156
5	2.036984954990	2.038197492719	2.038197427363	2.038197427064

Table 7.7. Romberg error tableau for the example

J	h	$E(J,0) = O(h^2)$	$E(J,1) = O(h^4)$	$E(J,2) = O(h^6)$	$E(J,3) = O(h^8)$
0	$b-a$	-1.252799263670			
1	$b-a/2$	-0.311384770309	0.002420060811		
2	$b-a/4$	-0.077663260503	0.000243909432	0.000098832673	
3	$b-a/8$	-0.019403478989	0.000016448182	0.000001284099	-0.000000264291
4	$b-a/16$	-0.004850085262	0.000001045980	0.000000019167	-0.000000000912
5	$b-a/32$	-0.001212472077	0.000000065651	0.000000000296	- 0.000000000003

Theorem 7.7 (Precision of Romberg Integration

Assume that $f \in C^{2K+2}[a,b]$. Then the truncation error term for the Romberg approximation is given in the formula

$$\int_a^b f(x)dx = R(J,K) + b_K h^{(2k+2)} f^{2k+2}(c_{J,K}) = R(J,K) + O(h^{2k+2}) \tag{34}$$

Where $h = (b-a)/2^J$, b_K is a constant that depends on K, and $c_{J,K} \in [a,b]$.

Example. Apply Theorem and show that

$$\int_0^2 10x^9 dx = 1024 \equiv R(4,4).$$

The integral is $f(x) = 10x^9$, and $f^{(10)}(x) \equiv 0$. Thus the value $K = 4$ will make the error term identically zero. A numerical computation will produce $R(4,4) = 1024$.

Gauss-Legendre Integration

We wish to find the area under the curve

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

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

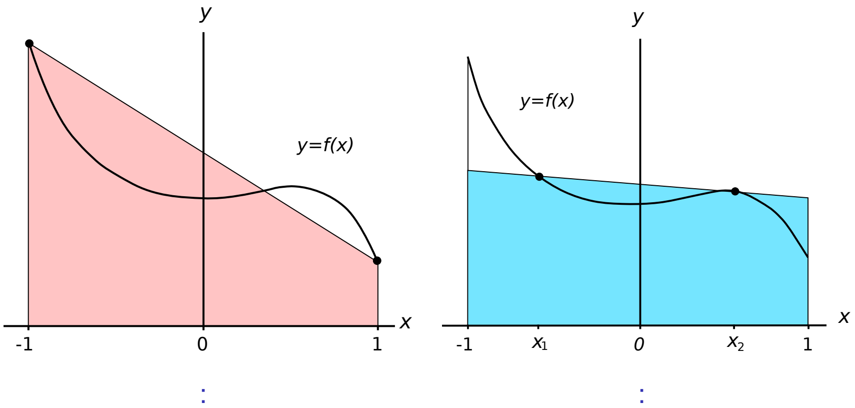

Figure 7.10: (a) Trapezoidal approximation using the abscissas -1 and 1. (b) Trapezoidal approximation using the abscissas x_1 and x_2.

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, $f(x) = a_3x^3 + a_2x^2 + a_1x + a_0$).

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

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

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.

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

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

Gauss-Legendre Integration

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 $h = 1$.

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

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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

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

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 0.5773502692	1.0000000000 1.0000000000	$\dfrac{f^{(4)}(c)}{135}$
3	± 0.7745966692 0.0000000000	0.5555555556 0.8888888888	$\dfrac{f^{(6)}(c)}{15{,}750}$
4	± 0.8611363116 ± 0.3399810436	0.3478548451 0.6521451549	$\dfrac{f^{(8)}(c)}{3{,}472{,}875}$
5	± 0.9061798459 ± 0.5384693101 0.0000000000	0.2369268851 0.4786286705 0.5688888888	$\dfrac{f^{(10)}(c)}{1{,}237{,}732{,}650}$

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	$\dfrac{f^{(12)}(c)2^{13}(6!)^4}{(12!)^3 13!}$
	± 0.6612093865	0.3607615730	
	± 0.2386191861	0.4679139346	
7	± 0.9491079123	0.1294849662	$\dfrac{f^{(14)}(c)2^{15}(7!)^4}{(14!)^3 15!}$
	± 0.7415311856	0.2797053915	
	± 0.4058451514	0.3818300505	
	0.0000000000	0.4179591837	
8	± 0.9602898565	0.1012285363	$\dfrac{f^{(16)}(c)2^{17}(8!)^4}{(16!)^3 17!}$
	± 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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$$\int_{-1}^{1} 5x^4\, dx = 2 = G_3(f).$$

Since the integral 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

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

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

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

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

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

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

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

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 behavior 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.