Numerical Integration

Numerical Integration

Calculating the definite integral of a given function $f(x)$ over an interval $[a, b]$,

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

is a classic problem.

By the fundamental theorem of Calculus, this problem is solved by

finding an anti-derivative F of f, that is, $F'(x) = f(x)$, and then

$$\int_a^b f(x)\,dx = F(b) - F(a).$$

But finding an anti-derivative is not an easy task in general.

Elements of Numerical Integration

$$\int_a^b f(x)\,dx = F(b) - F(a). \qquad (*)$$

The basic method involved in approximating the integration (*) is called numerical quadrature and uses a sum of the type

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i).$$

The method of quadrature in this section is based on the polynomial interpolation.

We first select a set of distinct nodes $\{x_0, x_1, \ldots, x_n\}$ from the interval $[a, b]$.

Then the Lagrange polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x) = \sum_{i=0}^{n} f(x_i) \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

is used to approximate $f(x)$.

With the error term we have

$$f(x) = P_n(x) + E_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x) + \frac{f^{(n+1)}(\zeta_x)}{(n+1)!} \prod_{i=0}^{n} (x - x_i),$$

where $\zeta_x \in [a, b]$ and depends on x, and

The quadrature formula is, therefore,

$$\int_a^b f(x)\,dx \approx \int_a^b P_n(x)\,dx = \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)\,dx \equiv \sum_{i=0}^{n} c_i f(x_i),$$

where

$$c_i = \int_a^b L_i(x)\,dx = \int_a^b \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx.$$

Moreover, the error in the quadrature formula is given by

$$E = \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\zeta_x)\prod_{i=0}^{n}(x-x_i)\,dx,$$

for some $\zeta_x \in [a,b]$. If $|f^{(n+1)}(x)| \le M$ on $[a,b]$, then

$$\left|\int_a^b f(x)\,dx - \sum_{i=0}^{n} c_i f(x_i)\right| \le \frac{M}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x-x_i)\,dx.$$

The choice of nodes that makes the right-hand side of this error bound as small as possible is know to be

$$x_i = \frac{a+b}{2} + \frac{b-a}{2}\cos\left[\frac{(i+1)\pi}{n+2}\right], \qquad i = 0,1,\ldots,n.$$

Of course, a polynomial interpolation to f can be obtained in other ways, for example, polynomial in Newton's form using divided-difference method,

$$P_n(x) = f(x_0) + \sum_{i=1}^{n} f[x_0,x_1,\ldots,x_i]\prod_{j=0}^{i-1}(x-x_j)$$

where $f[x_0,x_1,\ldots,x_i]$ are evaluated with the divided difference algorithm. Then

$$\int_a^b f(x)\,dx \approx f(x_0)(b-a) + \sum_{i=1}^{n} f[x_0,x_1,\ldots,x_i]\int_a^b \prod_{j=0}^{i-1}(x-x_j)\,dx.$$

The standard derivation of quadrature error formulas is based on determining the class of polynomials for which theses formulas produce exact results. The next definition is used to facilitate the discussion of this derivation.

Definition 7.1 *The degree of accuracy, or precision, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, when $k = 0, 1, \ldots, n$.*

The definition implies that the degree of accuracy of a quadrature formula is n if and only if the error $E = 0$ for all polynomials $P(x)$ of degree less than or equal to n, but $E \neq 0$ for some polynomials of degree greater than n.

Newton-Cotes Formulas

A quadrature formula of the form
$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i).$$
is called a Newton-Cotes formula if the nodes $\{x_0, x_1, \ldots, x_n\}$ are equally spaced.

Closed Newton-Cotes Formulas

Consider a uniform partition of the closed interval $[a, b]$ by

$$x_i = a + ih, \quad i = 0, 1, \ldots, n, \quad h = \frac{b-a}{n},$$

where n is a positive integer and h is called the step length.

By introduction a new variable t such that $x = a + ht$, the fundamental Lagrange polynomial becomes

$$L_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{a + ht - a - jh}{a + ih - a - jh} = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{t - j}{i - j} \equiv \varphi_i(t).$$

Therefore, the integration gives

$$c_i = \int_a^b L_i(x)\,dx = \int_0^n \varphi_i(t)h\,dt = h\int_0^n \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{t-j}{i-j}\,dt,$$

and the general Newton-Cotes formula has the form

$$\int_a^b f(x)\,dx = h\sum_{i=0}^{n} f(x_i)\int_0^n \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{t-j}{i-j}\,dt + \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\zeta_x)\prod_{i=0}^{n}(x-x_i)\,dx.$$

Trapezoidal Rule:

The simplest case is to choose $n = 1$, $x_0 = a$, $x_1 = b$, $h = b - a$, and use the linear Lagrange polynomial

$$P_1(x) = f(x_0)\frac{x-x_1}{x_0-x_1} + f(x_1)\frac{x-x_0}{x_1-x_0} = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a}.$$

to interpolate $f(x)$. Then

$$c_0 = h\int_0^1 \frac{t-1}{0-1}\,dt = \frac{h}{2}, \qquad c_1 = h\int_0^1 \frac{t-0}{1-0}\,dt = \frac{h}{2},$$

and

$$\int_a^b P_1(x)\,dx = c_0 f(x_0) + c_1 f(x_1) = \frac{h}{2}\left[f(a) + f(b)\right].$$

Weighted Mean Value Theorem for Integrals: Let f, g: $[a, b] \rightarrow \mathbb{R}$ be such that f is continuous and g is integrable and does not change the sign on $[a, b]$. Then, there exists a number $c \in (a, b)$ such that

$$\int_a^b f(x)g(x)dx = f(c)\int_a^b g(x)dx$$

Thus, if $x \in (a, b)$, it is possible to choose a number $a < c_x < x$ as a function of x on (a, b) such that

$$\int_a^x f(t)g(t)dt = f(c_x)\int_a^x g(t)dt$$

Since $(x-x_0)(x-x_1) = (x-a)(x-b)$ does not change sign on $[a, b]$, by the Weighted Mean-Value Theorem for integrals, there exists some $\xi \in (a, b)$ such that

$$\begin{aligned}
\int_a^b f''(\zeta_x)(x-x_0)(x-x_1)\,dx &= f''(\xi)\int_a^b (x-x_0)(x-x_1)\,dx \\
&= f''(\xi)\int_a^b (x-a)(x-b)\,dx \\
&= f''(\xi)\left[\frac{1}{3}x^3 - \frac{1}{2}(a+b)x^2 + abx\right]\Bigg|_a^b \\
&= -\frac{1}{6}f''(\xi)(b-a)^3 = -\frac{1}{6}f''(\xi)h^3.
\end{aligned}$$

Consequently, $$\int_a^b f(x)\,dx = \frac{h}{2}[f(a)+f(b)] - \frac{h^3}{12}f''(\xi).$$

This gives the so-called Trapezoidal rule.

Trapezoidal Rule:

$$\int_a^b f(x)\,dx = \frac{1}{2}(b-a)\left[f(a)+f(b)\right] - \frac{h^3}{12}f''(\xi),$$

where $h = b - a$ and $\xi \in (a, b)$.

It is evident that the error term of the Trapezoidal rule is $O(h^3)$. Since the rule involves f'', it gives the exact result when applied to any function whose second derivative is identically zero, e.g., any polynomial of degree 1 or less. Hence the degree of accuracy of Trapezoidal rule is one.

Simpson's Rule:

Simpson's Rule:

$$\int_a^b f(x)\,dx = \left(\frac{b-a}{2}\right)\left[\frac{1}{3}f(a) + \frac{4}{3}f(\frac{a+b}{2}) + \frac{1}{3}f(b)\right] + \frac{f^{(4)}(\xi)}{90}h^5,$$

for some $\xi \in (a, b)$. The Simpson's rule is an $O(h^5)$ scheme and the degree of accuracy is three.

we choose $n = 2$, $x_0 = a$, $x_1 = \frac{1}{2}(a+b)$, $x_2 = b$, $h = (b-a)/2$,

expanding f in the third Taylor's formula about x_1

Then for each $x \in [a, b]$, there exists $\zeta_x \in (a, b)$ such that

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(4)}(\zeta_x)}{24}(x-x_1)^4.$$

Then

$$\int_a^b f(x)\,dx = \left[f(x_1)(x-x_1) + \frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 + \frac{f'''(x_1)}{24}(x-x_1)^4\right]\Bigg|_a^b$$
$$+ \frac{1}{24}\int_a^b f^{(4)}(\zeta_x)(x-x_1)^4\,dx.$$

Note that $(b-x_1) = h$, $(a-x_1) = -h$, and since $(x-x_1)^4$ does not change sign in $[a,b]$, by the Weighted Mean-Value Theorem for Integral, there exists $\xi_1 \in (a,b)$ such that

$$\int_a^b f^{(4)}(\zeta_x)(x-x_1)^4\,dx = f^{(4)}(\xi_1)\int_a^b (x-x_1)^4\,dx = \frac{2f^{(4)}(\xi_1)}{5}h^5.$$

Consequently,

$$\int_a^b f(x)\,dx = 2f(x_1)h + \frac{f''(x_1)}{3}h^3 + \frac{f^{(4)}(\xi_1)}{60}h^5.$$

Finally we replace $f''(x_1)$ by the central finite difference formulation

$$f''(x_1) = \frac{f(x_0) - 2f(x_1) + f(x_2)}{h^2} - \frac{f^{(4)}(\xi_2)}{12}h^2,$$

for some $\xi_2 \in (a,b)$, to obtain

$$\begin{aligned}\int_a^b f(x)\,dx &= 2hf(x_1) + \frac{h}{3}\left(f(x_0) - 2f(x_1) + f(x_2)\right) - \frac{f^{(4)}(\xi_2)}{36}h^5 + \frac{f^{(4)}(\xi_1)}{60}h^5 \\ &= h\left[\frac{1}{3}f(x_0) + \frac{4}{3}f(x_1) + \frac{1}{3}f(x_2)\right] + \frac{1}{90}\left[\frac{3}{2}f^{(4)}(\xi_1) - \frac{5}{2}f^{(4)}(\xi_2)\right]h^5.\end{aligned}$$

By letting $f(x) = x^4$, one can show that there exists $\xi \in (a,b)$ such that

$$\int_a^b f(x)\,dx = h\left[\frac{1}{3}f(x_0) + \frac{4}{3}f(x_1) + \frac{1}{3}f(x_2)\right] + \frac{f^{(4)}(\xi)}{90}h^5.$$

This gives the Simpson's rule formulation.

Simpson's Rule:

$$\int_a^b f(x)\,dx = \left(\frac{b-a}{2}\right)\left[\frac{1}{3}f(a) + \frac{4}{3}f(\frac{a+b}{2}) + \frac{1}{3}f(b)\right] + \frac{f^{(4)}(\xi)}{90}h^5,$$

for some $\xi \in (a,b)$. The Simpson's rule is an $O(h^5)$ scheme and the degree of accuracy is three.

The Trapezoidal and Simpson's rules are examples of a class of methods known as closed Newton-Cotes formula. The $(n+1)$-point closed Newton-Cotes method uses nodes $x_i = a + ih$, for $i = 0, 1, \ldots, n$, where $h = (b-a)/n$. Note that both endpoints, $a = x_0$ and $b = x_n$, of the closed interval $[a,b]$ are included as nodes.

Theorem 7.1 (Closed Newton-Cotes Formulas) *For a given function $f(x)$ and closed interval $[a,b]$, the $(n+1)$-point closed Newton-Cotes method uses nodes*

$$x_i = a + ih, \quad i = 0, 1, \ldots, n, \quad h = \frac{b-a}{n}.$$

If n is even and $f \in C^{n+2}[a,b]$, then

$$\int_a^b f(x)\,dx = h\sum_{i=0}^{n} \alpha_i f(x_i) + \frac{h^{n+3}f^{(n+2)}(\xi)}{(n+2)!}\int_0^n t^2(t-1)\cdots(t-n)\,dt, \tag{7.38}$$

and if n is odd and $f \in C^{n+1}[a,b]$, then

$$\int_a^b f(x)\,dx = h\sum_{i=0}^{n} \alpha_i f(x_i) + \frac{h^{n+2}f^{(n+1)}(\xi)}{(n+1)!}\int_0^n t(t-1)\cdots(t-n)\,dt, \tag{7.39}$$

where $\xi \in (a,b)$ and

$$\alpha_i = \int_0^n \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{t-j}{i-j}\,dt, \qquad i = 0, 1, \ldots, n. \tag{7.40}$$

Consequently, the degree of accuracy is $n+1$ when n is an even integer, and n when n is an odd integer.

The weights α_i in the Newton-Cotes formula has the property

$$\sum_{i=0}^{n} \alpha_i = n. \tag{7.41}$$

This can be shown by applying the formula to $f(x) = 1$ with interpolating polynomial $P_n(x) = 1$. Let s be the common denominator of α_i, that is,

$$\alpha_i = \frac{\sigma_i}{s} \qquad (\Rightarrow \sigma_i = s\alpha_i)$$

such that σ_i are integers, then the formulation for approximating the definite integral can be expressed as

$$\int_a^b f(x)\,dx \approx h \sum_{i=0}^{n} \alpha_i f(x_i) = \frac{h}{s} \sum_{i=0}^{n} \sigma_i f(x_i). \tag{7.42}$$

Some of the most common closed Newton-Cotes formulas with their error terms are listed in the following table.

Name	n	s	σ_i	Error
Trapezoidal rule	1	2	$1, 1$	$-\frac{1}{12} f^{(2)}(\xi) h^3$
Simpson's rule	2	3	$1, 4, 1$	$-\frac{1}{90} f^{(4)}(\xi) h^5$
3/8-rule	3	$\frac{8}{3}$	$1, 3, 3, 1$	$-\frac{3}{80} f^{(4)}(\xi) h^5$
Milne's rule	4	$\frac{45}{2}$	$7, 32, 12, 32, 7$	$-\frac{8}{945} f^{(6)}(\xi) h^7$
	5	$\frac{288}{5}$	$19, 75, 50, 50, 75, 19$	$-\frac{275}{12096} f^{(6)}(\xi) h^7$
Weddle's rule	6	140	$41, 216, 27, 272, 27, 216, 41$	$-\frac{9}{1400} f^{(8)}(\xi) h^9$

Open Newton-Cotes Formulas

Another class of Newton-Cotes formulas is the open Newton-Cotes formulas in which the nodes

$$x_i = x_0 + ih, \quad i = 0, 1, \ldots, n, \quad \text{where } x_0 = a + h \text{ and } h = \frac{b-a}{n+2},$$

are used. This implies that $x_n = b - h$, and the endpoints, a and b, are not used. Hence we label $a = x_{-1}$ and $b = x_{n+1}$.

Theorem 7.2 (Open Newton-Cotes Formulas) *For a given function $f(x)$ and closed interval $[a, b]$, the $(n+1)$-point open Newton-Cotes method uses nodes*

$$x_i = x_0 + ih, \quad i = 0, 1, \ldots, n, \quad \text{where } x_0 = a + h \text{ and } h = \frac{b-a}{n+2}.$$

If n is even and $f \in C^{n+2}[a, b]$, then

$$\int_a^b f(x)\,dx = h \sum_{i=0}^{n} \alpha_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2 (t-1) \cdots (t-n)\,dt, \tag{7.43}$$

and if n is odd and $f \in C^{n+1}[a, b]$, then

$$\int_a^b f(x)\,dx = h \sum_{i=0}^{n} \alpha_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t (t-1) \cdots (t-n)\,dt, \tag{7.44}$$

where $\xi \in (a, b)$ and

$$\alpha_i = \int_{-1}^{n+1} \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{t-j}{i-j}\,dt, \qquad i = 0, 1, \ldots, n. \tag{7.45}$$

Consequently, the degree of accuracy is $n+1$ when n is an even integer, and n when n is an odd integer.

The simplest open Newton-Cotes formula is choosing $n = 0$ and only using the midpoint $x_0 = \frac{a+b}{2}$. Then the coefficient and the error term can be computed easily as

$$\alpha_0 = \int_1^{-1} dt = 2, \quad \text{and} \quad \frac{h^3 f''(\xi)}{2!} \int_{-1}^{1} t^2 \, dt = \frac{1}{3} f''(\xi) h^3.$$

These gives the so-called Midpoint rule or Rectangular rule.

Midpoint Rule:

$$\int_a^b f(x)\,dx = 2hf(x_0) + \frac{1}{3} f''(\xi)h^3 = (b-a)f(\frac{a+b}{2}) + \frac{1}{3} f''(\xi)h^3, \qquad (7.46)$$

for some $\xi \in (a, b)$.

Analogous to the closed Newton-Cotes formulas, we list some of the commonly used open Newton-Cotes formulas in the following table.

Name	n	s	σ_i	Error
Midpoint rule	0	1	2	$\frac{1}{3} f^{(2)}(\xi)h^3$
	1	2	$3, 3$	$\frac{3}{4} f^{(2)}(\xi)h^3$
	2	3	$8, -4, 8$	$\frac{14}{45} f^{(4)}(\xi)h^5$
	3	24	$55, 5, 5, 55$	$\frac{95}{144} f^{(4)}(\xi)h^5$

Composite Newton-Cotes Forumlas

composite Simpson's rule

A composite rule is one obtained by applying an integration formula for a single interval to each subinterval of a partitioned interval. To illustrate the procedure, we choose an even integer n and partition the interval $[a, b]$ into n subintervals by nodes $x_0 < x_1 < \cdots < x_n = b$, and apply Simpson's rule on each consecutive pair of subintervals. With

$$h = \frac{b-a}{n} \quad \text{and} \quad x_j = a + jh, \quad j = 0, 1, \ldots, n,$$

we have on each interval $[x_{2j-2}, x_{2j}]$,

$$\int_{x_{2j-2}}^{x_{2j}} f(x)\,dx = \frac{h}{3}\left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\right] - \frac{h^5}{90} f^{(4)}(\xi_j),$$

for some $\xi_j \in (x_{2j-2}, x_{2j})$, provided that $f \in C^4[a, b]$.

The composite rule is obtained by summing up over the entire interval, that is,

$$\begin{aligned}
\int_a^b f(x)\,dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx \\
&= \sum_{j=1}^{n/2} \left[\frac{h}{3}\left(f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\right) - \frac{h^5}{90} f^{(4)}(\xi_j)\right] \\
&= \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2) + f(x_2) + 4f(x_3) + f(x_4) + f(x_4) + 4f(x_5)\right. \\
&\quad \left. + \cdots + f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \\
&= \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + 4f(x_5)\right. \\
&\quad \left. + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \\
&= \frac{h}{3}\left[f(x_0) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + f(x_n)\right] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j).
\end{aligned}$$

To estimate the error associated with approximation, since $f \in C^4[a,b]$, we have, by the Extreme Value Theorem,

$$\min_{x\in[a,b]} f^{(4)}(x) \le f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x),$$

for each $\xi_j \in (x_{2j-2}, x_{2j})$. Hence

$$\frac{n}{2}\min_{x\in[a,b]} f^{(4)}(x) \le \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \frac{n}{2}\max_{x\in[a,b]} f^{(4)}(x),$$

and

$$\min_{x\in[a,b]} f^{(4)}(x) \le \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x).$$

By the Intermediate Value Theorem, there exists $\mu \in (a,b)$ such that

$$f^{(4)}(\mu) = \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

Thus, by replacing $n = (b-a)/h$,

$$\sum_{j=1}^{n/2} f^{(4)}(\xi_j) = \frac{n}{2} f^{(4)}(\mu) = \frac{b-a}{2h} f^{(4)}(\mu).$$

Consequently, the composite Simpson's rule is derived.

Composite Simpson's Rule:

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + f(b)\right] - \frac{b-a}{180} f^{(4)}(\mu)h^4,$$

where n is an even integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a,b)$.

Formula

2. Simpsons $\frac{1}{3}$ Rule

$$\int y dx = \frac{h}{3}\left(y_0 + 4\left(y_1 + y_3 + y_5 + ... + + y_{n-1}\right) + 2\left(y_2 + y_4 + y_6 + ... + y_{n-2}\right) + y_n\right)$$

Examples

1. Find Solution using Simpson's 1/3 rule

x	f(x)
1.4	4.0552
1.6	4.9530
1.8	6.0436
2.0	7.3891
2.2	9.0250

Solution:

The value of table for x and y

x	1.4	1.6	1.8	2	2.2
y	4.0552	4.953	6.0436	7.3891	9.025

Using Simpsons $\frac{1}{3}$ Rule

$$\int y dx = \frac{h}{3}\left[\left(y_0 + y_4\right) + 4\left(y_1 + y_3\right) + 2\left(y_2\right)\right]$$

$$\int y dx = \frac{0.2}{3}[(4.0552 + 9.025) + 4 \times (4.953 + 7.3891) + 2 \times (6.0436)]$$

$$\int y dx = \frac{0.2}{3}[(4.0552 + 9.025) + 4 \times (12.3421) + 2 \times (6.0436)]$$

$$\int y dx = 4.9691$$

Solution by Simpson's $\frac{1}{3}$ Rule is 4.9691

Composite Midpoint Rule:

$$\int_a^b f(x)\,dx = 2h\sum_{j=1}^{n/2} f(x_{2j-1}) - \frac{b-a}{6}f''(\mu)h^2,$$

where n is an even integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a, b)$.

To derive the composite Trapezoidal rule, we partition the interval $[a,b]$ by n equally spaced nodes $a = x_0 < x_1 < \cdots < x_n = b$, where n can be either odd or even. We then apply the trapezoidal rule on each subinterval $[x_{j-1}, x_j]$ and sum them up to obtain

$$\begin{aligned}
\int_a^b f(x)\,dx &= \sum_{j=1}^{n} \int_{x_{j-1}}^{x_j} f(x)\,dx \\
&= \sum_{j=1}^{n} \left[\frac{h}{2}\left(f(x_{j-1}) + f(x_j)\right) - \frac{h^3}{12} f''(\xi_j)\right] \\
&= \frac{h}{2}\left[f(x_0) + f(x_1) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + f(x_n)\right] - \frac{h^3}{12}\sum_{j=1}^{n} f''(\xi_j) \\
&= \frac{h}{2}\left[f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n)\right] - \frac{h^3}{12}\sum_{j=1}^{n} f''(\xi_j) \\
&= \frac{h}{2}\left[f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{h^3}{12}\sum_{j=1}^{n} f''(\xi_j) \\
&= \frac{h}{2}\left[f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12} f''(\mu) h^2,
\end{aligned}$$

where each $\xi_j \in (x_{j-1}, x_j)$ and $\mu \in (a,b)$.

Composite Trapezoidal Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12} f''(\mu) h^2,$$

where n is an integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a,b)$.

Formula

1. Trapezoidal Rule

$$\int y dx = \frac{h}{2}\left(y_0 + 2\left(y_1 + y_2 + y_3 + \ldots + y_{n-1}\right) + y_n\right)$$

1. Find Solution using Trapezoidal rule

x	f(x)
1.4	4.0552
1.6	4.9530
1.8	6.0436
2.0	7.3891
2.2	9.0250

Solution:

The value of table for x and y

x	1.4	1.6	1.8	2	2.2
y	4.0552	4.953	6.0436	7.3891	9.025

Using Trapezoidal Rule

$$\int y dx = \frac{h}{2}\left[y_0 + y_4 + 2\left(y_1 + y_2 + y_3\right)\right]$$

$$\int y dx = \frac{0.2}{2}[4.0552 + 9.025 + 2 \times (4.953 + 6.0436 + 7.3891)]$$

$$\int y dx = \frac{0.2}{2}[4.0552 + 9.025 + 2 \times (18.3857)]$$

$$\int y dx = 4.9852$$

Solution by Trapezoidal Rule is 4.9852

Gaussian Quadrature

Gaussian Quadrature Rule: For a given function $f(x) \in C[-1,1]$ and integer n,

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_I),$$

where $x_0, x_1, \ldots, x_n$ are the roots of the $(n+1)$-st Lengendre polynomial p_{n+1}, and

$$c_i = \int_{-1}^{1} \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx. \qquad i = 0, 1, \ldots, n.$$

The following table give some frequently used values for x_i and c_i.

n	x_i	c_i
0	$x_0 = 0$	$c_0 = 2$
1	$x_0 = -0.5773502692$	$c_0 = c_1 = 1$
	$x_1 = 0.5773502692$	
2	$x_0 = -0.7745966692$	$c_0 = \frac{5}{9}$
	$x_1 = 0$	$c_1 = \frac{8}{9}$
	$x_2 = 0.7745966692$	$c_2 = \frac{5}{9}$
3	$x_0 = -0.8611363116$	$c_0 = 0.3478548451$
	$x_1 = -0.3399810436$	$c_1 = 0.6521451549$
	$x_2 = 0.3399810436$	$c_2 = 0.6521451549$
	$x_3 = 0.8611363116$	$c_3 = 0.3478548451$
4	$x_0 = -0.9061798459$	$c_0 = 0.2369268851$
	$x_1 = -0.5384693101$	$c_1 = 0.4786286705$
	$x_2 = 0$	$c_2 = \frac{128}{225} = 0.568888889$
	$x_3 = 0.5384693101$	$c_3 = 0.4786286705$
	$x_4 = 0.9061798459$	$c_4 = 0.2369268851$

A definite integral over an arbitrary interval $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using a simple change of variable technique:

$$t = \frac{2x - a - b}{b - a} \qquad \Longleftrightarrow \qquad x = \frac{1}{2}\left[(b-a)t + a + b\right].$$

Gaussian quadrature on arbitrary intervals

Use substitution or transformation to transform $\int_a^b f(x)dx$ into an integral defined over $[-1,1]$.
Let $x = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)t$, with $t \in [-1, 1]$
Then

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

The idea of Gaussian quadrature rule is not restricted to the use of the Lengendre polynomials. For a given weight function $w(x)$ and interval $[a,b]$, the nodes $x_0, x_1, \ldots, x_n$ can be chosen to be the roots of any monic polynomial q_{n+1} of degree $n+1$ which is w-orthogonal to Π_n in the sense that

$$\int_a^b q_{n+1}(x)p(x)w(x)\,dx = 0, \qquad \text{for all } p \in \Pi_n.$$

Note that in the Gaussian quadrature formulas the interval $[a,b]$ can be infinite, e.g., $[0,\infty)$ or $(-\infty,\infty)$. Some other important cases which lead to Gaussian integration rules are listed in the following table.

$[a,b]$	$w(x)$	Orthogonal polynomials
$[-1,1]$	$(1-x^2)^{-1/2}$	$T_n(x)$, Chebyshev polynomials
$[0,\infty)$	e^{-x}	$L_n(x)$, Laguerre polynomials
$(-\infty,\infty)$	e^{-x^2}	$H_n(x)$, Hermite polynomials

Trapezoidal Rule:

$$\int_a^b f(x)\,dx = \frac{1}{2}(b-a)\,[f(a)+f(b)] - \frac{h^3}{12}f''(\xi),$$

where $h = b - a$ and $\xi \in (a, b)$.

Simpson's Rule:

$$\int_a^b f(x)\,dx = \left(\frac{b-a}{2}\right)\left[\frac{1}{3}f(a) + \frac{4}{3}f(\frac{a+b}{2}) + \frac{1}{3}f(b)\right] + \frac{f^{(4)}(\xi)}{90}h^5,$$

Midpoint Rule:

$$\int_a^b f(x)\,dx = 2hf(x_0) + \frac{1}{3}f''(\xi)h^3 = (b-a)f(\frac{a+b}{2}) + \frac{1}{3}f''(\xi)h^3,$$

for some $\xi \in (a, b)$.

Composite Simpson's Rule:

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + f(b)\right] - \frac{b-a}{180}f^{(4)}(\mu)h^4, \tag{7.47}$$

where n is an even integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a, b)$.

Composite Trapezoidal Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}f''(\mu)h^2,$$

where n is an integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a, b)$.

Gaussian Quadrature Rule: For a given function $f(x) \in C[-1,1]$ and integer n,

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_I),$$

Adaptive Quadrature

Romberg Integration

Recall the trapezoidal rule integral formulation

$$\begin{aligned}\int_a^b f(x)\,dx &\approx T(n)\\ &= \frac{h}{2}[f(a) + 2f(a+h) + 2f(a+2h) + \cdots + 2f(a+(n-1)h) + f(a+nh)],\end{aligned}$$

where $h = \frac{b-a}{n}$. Observe in the following example that the interval $[a, b]$ is partitioned equally-spaced by $x_0 = a, x_1, x_2, x_3$, and $x_4 = b$.

Let $n = 2$ and $h = \frac{b-a}{2n}$. If we only consider the partitions by x_0, x_2, and x_4, and apply the Trapezoidal rule, we have the approximation

$$T(n) = \frac{2h}{2}[f(a) + 2f(a+2h) + f(a+4h)] = h[f(a) + 2f(a+2h) + f(a+4h)].$$

On the other hand, if we apply Trapezoidal rule to the partitions by all points x_0, x_1, x_2, x_3, and x_4, then we have

$$\begin{aligned} T(2n) &= \frac{h}{2}[f(a) + 2f(a+h) + 2f(a+2h) + 2f(a+3h) + f(a+4h)] \\ &= \frac{1}{2}T(n) + h[f(a+h) + f(a+3h)]. \end{aligned}$$

This observation shows that if we have computed $T(n)$ and the step size is halfed, we don't have to compute all the function values all over again, but just at those newly added points. In general, suppose $T(n)$ has been computed and the step size becomes $h = \frac{b-a}{2n}$, then

$$T(2n) = \frac{1}{2}T(n) + h\sum_{i=1}^{n} f(a + (2i-1)h).$$

With this idea in mind, we can apply the trapezoidal rule recursively, i.e., we partition the interval $[a, b]$ into 2^n subintervals with $n = 1, 2, 3, \ldots$, and the integral formulation becomes

$$T(2^n) = \frac{1}{2}T(2^{n-1}) + \frac{b-a}{2^n}\sum_{i=1}^{2^{n-1}} f(a + (2i-1)\frac{b-a}{2^n})$$

Algorithm **(Romberg Integration Algorithm)** *Use the Romberg algorithm to evaluate* $\int_a^b f(x)\,dx$.

$R(0,0) = \frac{1}{2}(b-a)[f(a)+f(b)]$
for $n = 1, 2, \ldots, M$ **do**
  $R(n,0) = \frac{1}{2}R(n-1,0) + \frac{b-a}{2^n}\sum_{i=1}^{2^{n-1}} f(a+(2i-1)\frac{b-a}{2^n})$
end for
for $k = 1, 2, \ldots, M$ **do**
  for $n = k, k+1, \ldots, M$ **do**
    $R(n,k) = R(n,k-1) + \frac{1}{4^k-1}[R(n,k-1) - R(n-1,k-1)]$
  end for
end for

Remarks

2. *M is modest, not too large.*
3. *No duplicate function evaluations in $R(0,0), R(1,0), \ldots, R(M,0)$.*
4. *No function evaluation is needed im computing $R(m,k)$ when $k \geq 1$.*

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

Method

Using $h_n = \frac{(b-a)}{2^n}$, the method can be inductively defined by

$$R(0,0) = h_0(f(a) + f(b))$$

$$R(n,0) = \tfrac{1}{2}R(n-1,0) + 2h_n \sum_{k=1}^{2^{n-1}} f(a + (2k-1)h_{n-1})$$

$$R(n,m) = R(n,m-1) + \tfrac{1}{4^m-1}(R(n,m-1) - R(n-1,m-1))$$

$$= \frac{1}{4^m-1}(4^m R(n,m-1) - R(n-1,m-1))$$

where $n \geq m$ and $m \geq 1$. In big O notation, the error for *R*(*n*, *m*) is:[3] $O\left(h_n^{2m+2}\right)$.

The zeroeth extrapolation, $R(n, 0)$, is equivalent to the trapezoidal rule with $2^n + 1$ points; the first extrapolation, $R(n, 1)$, is equivalent to Simpson's rule with $2^n + 1$ points. The second extrapolation, $R(n, 2)$, is equivalent to Boole's rule with $2^n + 1$ points. The further extrapolations differ from Newton-Cotes formulas. In particular further Romberg extrapolations expand on Boole's rule in very slight ways, modifying weights into ratios similar as in Boole's rule. In contrast, further Newton-Cotes methods produce increasingly differing weights, eventually leading to large positive and negative weights. This is indicative of how large degree interpolating polynomial Newton-Cotes methods fail to converge for many integrals, while Romberg integration is more stable.

By labelling our $O(h^2)$ approximations as $A_0\left(\frac{h}{2^n}\right)$ instead of $R(n,0)$, we can perform Richardson extrapolation with the error formula defined below:

$$\int_a^b f(x)\,dx = A_0\left(\frac{h}{2^n}\right) + a_0\left(\frac{h}{2^n}\right)^2 + a_1\left(\frac{h}{2^n}\right)^4 + a_2\left(\frac{h}{2^n}\right)^6 + \cdots$$

Once we have obtained our $O(h^{2(m+1)})$ approximations $A_m\left(\frac{h}{2^n}\right)$, we can label them as $R(n,m)$.

Composite Trapezoidal Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12} f''(\mu)h^2,$$

where n is an integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a, b)$.

Romberg integration example

Consider

$$\int_1^2 \frac{1}{x} dx = \ln 2.$$

We will use this integral to illustrate how Romberg integration works. First, compute the trapezoid approximations starting with $n = 2$ and doubling n each time:

$n = 1: \ R_1^0 = \left(1 + \frac{1}{2}\right)\frac{1}{2} = 0.75;$

$n = 2: \ R_2^0 = 0.5\left(\frac{1}{1.5}\right) + \frac{0.5}{2}(1 + \frac{1}{2}) = 0.708333333$

$n = 4: \ R_3^0 = 0.25\left(\frac{1}{1.25} + \frac{1}{1.5} + \frac{1}{1.75}\right) + \frac{0.25}{2}(1 + \frac{1}{2}) = 0.69702380952$

$n = 8: \ R_4^0 = 0.69412185037$

$n = 16: R_5^0 = 0.69314718191.$

Next we use the formula:

$$R_k^i = \frac{4^i R_k^{i-1} - R_{k-1}^{i-1}}{4^i - 1}$$

Next we use the formula:

$$R_k^i = \frac{4^i R_k^{i-1} - R_{k-1}^{i-1}}{4^i - 1}$$

The easiest way is to keep track of computations is to build a table of the form:

$$\begin{array}{ccccc}
R_1^0 & & & & \\
R_2^0 & R_2^1 & & & \\
R_3^0 & R_3^1 & R_3^2 & & \\
R_4^0 & R_4^1 & R_4^2 & R_4^3 & \\
R_5^0 & R_5^1 & R_5^2 & R_5^3 & R_5^3
\end{array}$$

Starting with the first column (which we just computed), all other entries can be easily computed. For example starting with R_1^0, R_2^0 we find

$$R_2^1 = \frac{4R_2^0 - R_1^0}{3} = 0.694444$$

$$R_3^1 = \frac{4R_3^0 - R_2^0}{3} = 0.693253; \quad R_3^2 = \frac{16R_3^1 - R_2^1}{15} = 0.69317460$$

and so on. Every entry depends only on its left and left-top neighbour. Continuing in this way, we get the following table:

and so on. Every entry depends only on its left and left-top neighbour. Continuing in this way, we get the following table:

0.75000000000				
0.70833333333	**0.69**444444444			
0.69702380952	**0.693**25396825	**0.6931**7460317		
0.69412185037	**0.6931**5453065	**0.69314**790148	**0.69314**747764	
0.69339120220	**0.69314**765281	**0.693147**19429	**0.693147**18307	**0.6931471819**1

The correct digits are shown in bold (the exact answer to 15 digits is given by $\ln 2 = 0.693147180559945$). Here is the table listing error $R_i^k - \ln 2$.

5.7e-02				
1.5e-02	1.3e-03			
3.9e-03	1.1e-04	2.7e-05		
9.7e-04	7.4e-06	7.2e-07	3.0e-07	
2.4e-04	4.7e-07	1.4e-08	2.5e-09	1.4e-09

Note that each successive iteration yields around two extra digits (*why*?). The final iteration only required $n = 16$ function evaluations, plus $O(\ln n)$ arithmetic operations to build the table.

Example 2. Consider $\int_1^3 (x^6 - x^2 \sin(2x))dx = 317.3442466$. Compare results from the closed Newton-Cotes formula with n=1, the open Newton-Cotes formula with n =1 and Gaussian quadrature when n = 2.

Solution:

(a) n = 1 closed Newton-Cotes formula (Trapezoidal rule):

$$\int_1^3 x^6 - x^2 \sin(2x)\, dx \approx \frac{2}{2}[f(1) + f(3)] = 731.605$$

(b) n = 1 open Newton-Cotes formula:

$h = \frac{3-1}{1+2} = \frac{2}{3}$. Nodes are: $x_{-1} = 1, x_0 = \frac{5}{3}, x_1 = \frac{7}{3}, x_2 = 3.$

$$\int_1^3 x^6 - x^2 \sin(2x)\, dx \approx \frac{3}{2} h \left[f\left(\frac{5}{3}\right) + f\left(\frac{7}{3}\right)\right] = 188.786$$

(c) n = 2 Gaussian quadrature:

Example 1. **a)** Use Simpson's rule to approximate $\int_0^4 e^x dx$. The exact value is 53.59819. **b)** Divide [0,4] into [0,1] + [1,2] + [2,3] + [3,4]. Use Simpson's rule to approximate $\int_0^1 e^x dx$, $\int_1^2 e^x dx$, $\int_2^3 e^x dx$ and $\int_3^4 e^x dx$. Then approximate $\int_0^4 e^x dx$ by adding approximations for $\int_0^1 e^x dx$, $\int_1^2 e^x dx$, $\int_2^3 e^x dx$ and $\int_3^4 e^x dx$. Compare with accurate value.

Solution:

a) $h = \frac{4-0}{2}$. $\int_0^4 e^x dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958.$

Error= |53.59819 -56.76958| = 3.17143

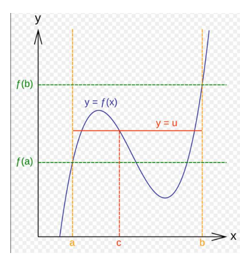
b) $\int_0^4 e^x dx = \int_0^1 e^x dx + \int_1^2 e^x dx + \int_2^3 e^x dx + \int_3^4 e^x dx \approx \frac{0.5}{3}(e^0 + 4e^{0.5} + e^1) + \frac{0.5}{3}(e^1 + 4e^{1.5} + e^2) + \frac{0.5}{3}(e^2 + 4e^{2.5} + e^3) + \frac{0.5}{3}(e^3 + 4e^{3.5} + e^4) = 53.61622$

Error=|53.59819 -53.61622| = 0.01807

Intermediate value theorem

In mathematical analysis, the **intermediate value theorem** states that if f is a continuous function whose domain contains the interval $[a, b]$, then it takes on any given value between $f(a)$ and $f(b)$ at some point within the interval.

Theorem [edit]



The intermediate value theorem states the following:

Consider an interval $I = [a, b]$ of real numbers $\mathbb{R}$ and a continuous function $f : I \to \mathbb{R}$. Then

- *Version I.* if u is a number between $f(a)$ and $f(b)$, that is,

  $$\min(f(a), f(b)) < u < \max(f(a), f(b)),$$

  then there is a $c \in (a, b)$ such that $f(c) = u$.
- *Version II.* the image set $f(I)$ is also a closed interval, and it contains $\big[\min(f(a), f(b)), \max(f(a), f(b))\big]$.

Remark: *Version II* states that the set of function values has no gap. For any two function values $c, d \in f(I)$ with $c < d$ all points in the interval $[c, d]$ are also function values,

$$[c, d] \subseteq f(I).$$

A subset of the real numbers with no internal gap is an interval. *Version I* is naturally contained in *Version II*.