Elements of Numerical Integration

The basic method involved in approximating the integration

$$\int_a^b f(x)\,dx, \tag{15}$$

is called numerical quadrature and uses a sum of the type

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i). \tag{16}$$

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

$$\begin{aligned}
\int_a^b f(x)\, dx &= \int_a^b P_n(x)\, dx + \int_a^b E_n(x)\, dx \\
&= \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)\, dx + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\zeta_x) \prod_{i=0}^{n} (x - x_i)
\end{aligned}$$

The quadrature formula is, therefore,

$$\int_a^b f(x)\, dx \approx \int_a^b P_n(x)\, dx = \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)\, dx \equiv \sum_{i=0}^{n} c_i f(x_i), \quad (18)$$

where

$$c_i = \int_a^b L_i(x)\, dx = \int_a^b \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\, dx. \quad (19)$$

Moreover, the error in the quadrature formula is given by

$$E = \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\zeta_x) \prod_{i=0}^{n} (x - x_i)\, dx, \tag{20}$$

for some $\zeta_x \in [a, b]$.

Let us consider formulas produced by using first and second Lagrange polynomials with equally spaced nodes. This gives the Trapezoidal rule and Simpson's rule, respectively.

Trapezoidal rule: Let $x_0 = a, x_1 = b, h = b - a$ and use the linear Lagrange polynomial:

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

Then

$$\begin{aligned} \int_a^b f(x)dx &= \int_{x_0}^{x_1} \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] dx \\ &\quad + \frac{1}{2} \int_{x_0}^{x_1} f''(\zeta(x))(x - x_0)(x - x_1)dx. \end{aligned} \tag{21}$$

Theorem (Weighted Mean Value Theorem for Integrals)

Suppose $f \in C[a,b]$, the Riemann integral of $g(x)$

$$\int_a^b g(x)dx = \lim_{\max \triangle x_i \to 0} \sum_{i=1}^{n} g(x_i)\triangle x_i,$$

exists and $g(x)$ does not change sign on $[a,b]$. Then $\exists\ c \in (a,b)$ with

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

Since $(x-x_0)(x-x_1)$ does not change sign on $[x_0,x_1]$, by the Weighted Mean Value Theorem, $\exists\ \zeta \in (x_0,x_1)$ such that

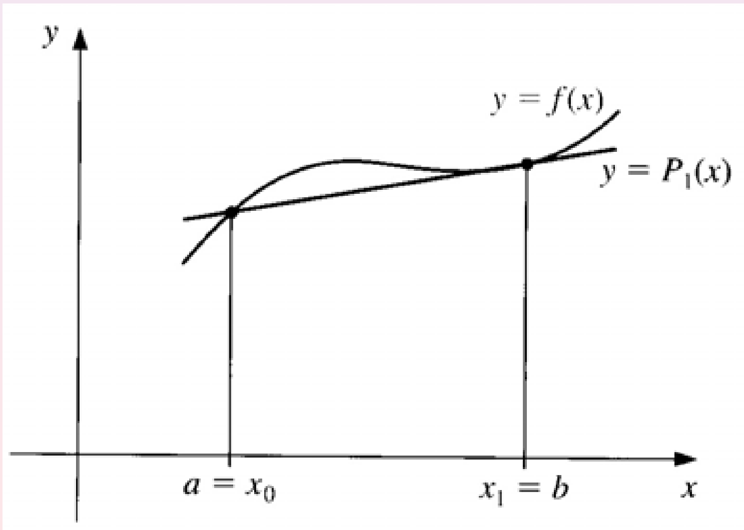
$$\int_{x_0}^{x_1} f''(\zeta(x))(x-x_0)(x-x_1)dx = f''(\zeta)\int_{x_0}^{x_1}(x-x_0)(x-x_1)dx$$

$$= f''(\zeta)\left[\frac{x^3}{3} - \frac{x_1+x_0}{2}x^2 + x_0x_1x\right]_{x_0}^{x_1} = -\frac{h^3}{6}f''(\zeta).$$

Consequently, Eq. (21) implies that

$$
\begin{aligned}
\int_a^b f(x)dx &= \left[\frac{(x-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} f(x_1)\right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\zeta) \\
&= \frac{x_1-x_0}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\zeta) \\
&= \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\zeta),
\end{aligned}
$$

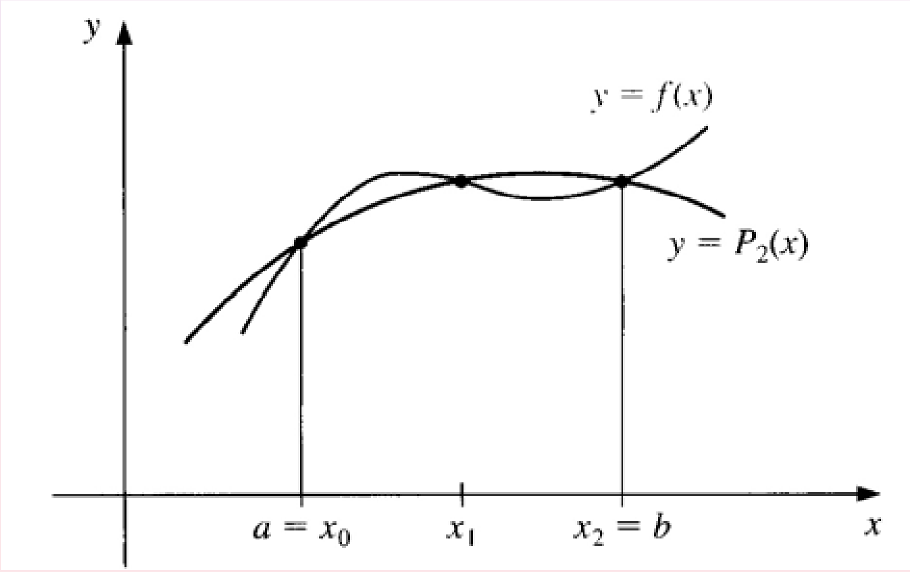
which is called the Trapezoidal rule.



If we choose $x_0 = a$, $x_1 = \frac{1}{2}(a+b)$, $x_2 = b$, $h = (b-a)/2$, and the second order Lagrange polynomial

$$P_2(x) = f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

to interpolate $f(x)$, then



$$
\begin{aligned}
\int_a^b f(x)dx &= \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \right. \\
&\quad \left. + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx \\
&\quad + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\zeta(x)) dx.
\end{aligned}
$$

Since, letting $x = x_0 + th$,

$$
\begin{aligned}
\int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} dx &= h \int_0^2 \frac{t-1}{0-1} \cdot \frac{t-2}{0-2}\, dt \\
&= \frac{h}{2} \int_0^2 (t^2 - 3t + 2)\, dt = \frac{h}{3}, \\
\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} dx &= h \int_0^2 \frac{t-0}{1-0} \cdot \frac{t-2}{1-2}\, dt \\
&= -h \int_0^2 (t^2 - 2t)\, dt = \frac{4h}{3},
\end{aligned}
$$

$$
\begin{aligned}
\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx &= h\int_0^2 \frac{t-0}{2-0}\cdot\frac{t-1}{2-1}\,dt \\
&= \frac{h}{2}\int_0^2 (t^2-t)\,dt = \frac{h}{3},
\end{aligned}
$$

it implies that

$$
\begin{aligned}
\int_a^b f(x)dx &= h\left[\frac{1}{3}f(x_0)+\frac{4}{3}f(x_1)+\frac{1}{3}f(x_2)\right] \\
&\quad + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\zeta(x))dx,
\end{aligned}
$$

which is called the Simpson's rule and provides only an $O(h^4)$ error term involving $f^{(3)}$. A higher order error analysis can be derived by expanding f in the third Taylor's formula about x_1. $\forall\ x \in [a,b]$, $\exists\ \zeta_x \in (a,b)$ such that

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

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

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

It can show that there exists $\xi \in (a, b)$ such that

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

This gives the Simpson's rule formulation.

Definition

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 Trapezoidal and Simpson's rules have degrees of precision one and three, respectively.
- 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 $n + 1$.

Newton-Cotes Formulas

Definition (Newton-Cotes formula)

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.

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 (19) gives

$$c_i = \int_a^b L_i(x)\, dx = \int_0^n \varphi_i(t) h\, dt = h \int_0^n \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{t - j}{i - j}\, dt, \tag{22}$$

and the general Newton-Cotes formula has the form

$$\int_a^b f(x)\, dx = h \sum_{i=0}^{n} f(x_i) \int_0^n \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{t - j}{i - j}\, dt + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\zeta_x) \prod_{i=0}^{n} (x - x_i) \tag{23}$$

Theorem (Closed Newton-Cotes Formulas)

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point closed Newton-Cotes formula with $x_0 = a, x_n = b$ and $h = (b-a)/n$. If n is even and $f \in C^{n+2}[a,b]$, then

$$\int_a^b f(x)\,dx = h\sum_{i=0}^{n} \alpha_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!}\int_0^n t^2(t-1)\cdots(t-n)\,dt, \tag{24}$$

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

$$\int_a^b f(x)\,dx = h\sum_{i=0}^{n} \alpha_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!}\int_0^n t(t-1)\cdots(t-n)\,dt, \tag{25}$$

where $\xi \in (a,b)$ and $\alpha_i = \int_0^n \prod_{j=0,\ j\neq i}^{n} \frac{t-j}{i-j}\,dt$ for $i = 0, 1, \ldots, n$.

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

- $n = 1$: Trapezoidal rule

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

- $n = 2$: Simpson's rule

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

- 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.
- The degree of accuracy of Trapezoidal rule is one.
- The Simpson's rule is an $O(h^5)$ scheme and the degree of accuracy is three.

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

$$x_i = x_0 + ih, \quad i = 0, 1, \ldots, n,$$

where

$$x_0 = a + h \quad \text{and} \quad h = \frac{b-a}{n+2},$$

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 $b = x_{n+1}$. The formulas become

$$\int_a^b f(x)dx = \int_{x_{-1}}^{x_{n+1}} f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i),$$

where

$$a_i = \int_a^b L_i(x)dx.$$

The following theorem summarizes the open Newton-Cotes formulas.

Theorem (Open Newton-Cotes Formulas)

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ *denotes the* $(n+1)$*-point open Newton-Cotes formula with* $x_{-1} = a$, $x_{n+1} = b$ *and* $h = (b-a)/(n+2)$. *If* n *is even and* $f \in C^{n+2}[a,b]$, *then*

$$\int_a^b f(x)\,dx = h\sum_{i=0}^{n} \alpha_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!}\int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt, \tag{26}$$

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

$$\int_a^b f(x)\,dx = h\sum_{i=0}^{n} \alpha_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!}\int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt, \tag{27}$$

where $\xi \in (a,b)$ *and* $\alpha_i = \int_{-1}^{n+1} \prod_{j=0, j\neq i}^{n} \frac{t-j}{i-j}\,dt$ *for* $i = 0, 1, \ldots, n$.

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:

$$\int_a^b f(x)\,dx = 2hf(x_0) + \frac{1}{3} f''(\xi)h^3 = (b-a)f(\frac{a+b}{2}) + \frac{1}{3} f''(\xi)h^3, \quad (28)$$

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