

Numerical Differentiation and Integration

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Numerical Differentiation

$$f'(x_0) = \lim_{h \rightarrow 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

Question

How accurate is

$$\frac{f(x_0 + h) - f(x_0)}{h}?$$

Suppose a given function f has continuous first derivative and f'' exists. From Taylor's theorem

$$f(x + h) = f(x) + f'(x)h + \frac{1}{2}f''(\xi)h^2,$$

where ξ is between x and $x + h$, one has

$$f'(x) = \frac{f(x + h) - f(x)}{h} - \frac{h}{2}f''(\xi) = \frac{f(x + h) - f(x)}{h} + O(h).$$



Hence it is reasonable to use the approximation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

which is called forward finite difference, and the error involved is

$$|e| = \frac{h}{2} |f''(\xi)| \leq \frac{h}{2} \max_{t \in (x, x+h)} |f''(t)|.$$

Similarly one can derive the backward finite difference approximation

$$f'(x) \approx \frac{f(x) - f(x-h)}{h} \tag{1}$$

which has the same order of truncation error as the forward finite difference scheme.



The forward difference is an $O(h)$ scheme. An $O(h^2)$ scheme can also be derived from the Taylor's theorem

$$\begin{aligned}f(x+h) &= f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(\xi_1)h^3 \\f(x-h) &= f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(\xi_2)h^3,\end{aligned}$$

where ξ_1 is between x and $x+h$ and ξ_2 is between x and $x-h$. Hence

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{1}{6}[f'''(\xi_1) + f'''(\xi_2)]h^3$$

and

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{12}[f'''(\xi_1) + f'''(\xi_2)]h^2$$

Let

$$M = \max_{z \in [x-h, x+h]} f'''(z) \quad \text{and} \quad m = \min_{z \in [x-h, x+h]} f'''(z).$$



If f''' is continuous on $[x - h, x + h]$, then by the intermediate value theorem, there exists $\xi \in [x - h, x + h]$ such that

$$f'''(\xi) = \frac{1}{2}[f'''(\xi_1) + f'''(\xi_2)].$$

Hence

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6}f'''(\xi)h^2 = \frac{f(x+h) - f(x-h)}{2h} + O(h^2).$$

This is called center difference approximation and the truncation error is

$$|e| = \frac{h^2}{6}f'''(\xi)$$

Similarly, we can derive an $O(h^2)$ scheme from Taylor's theorem for $f''(x)$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{1}{12}f^{(4)}(\xi)h^2,$$

where ξ is between $x - h$ and $x + h$.



Polynomial Interpolation Method

Suppose that $(x_0, f(x_0)), (x_1, f(x_1)) \cdots, (x_n, f(x_n))$ have been given, we apply the Lagrange polynomial interpolation scheme to derive

$$P(x) = \sum_{i=0}^n f(x_i)L_i(x),$$

where

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

Since $f(x)$ can be written as

$$f(x) = \sum_{i=0}^n f(x_i)L(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x)w(x),$$

where

$$w(x) = \prod_{j=0}^n (x - x_j),$$



we have,

$$\begin{aligned} f'(x) &= \sum_{i=0}^n n f(x_i) L'_i(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w'(x) \\ &+ \frac{1}{(n+1)!} w(x) \frac{d}{dx} f^{(n+1)}(\xi_x). \end{aligned}$$

Note that

$$w'(x) = \sum_{j=0}^n \prod_{i=0, i \neq j}^n (x - x_i).$$

Hence a reasonable approximation for the first derivative of f is

$$f'(x) \approx \sum_{i=0}^n f(x_i) L'_i(x).$$

When $x = x_k$ for some $0 \leq k \leq n$,

$$w(x_k) = 0 \quad \text{and} \quad w'(x_k) = \prod_{i=0, i \neq k}^n (x_k - x_i).$$



Hence

$$f'(x_k) = \sum_{i=0}^n f(x_i)L'_i(x_k) + \frac{1}{(n+1)!}f^{(n+1)}(\xi_x) \prod_{i=0, i \neq k}^n (x_k - x_i), \quad (2)$$

which is called an $(n+1)$ -point formula to approximate $f'(x)$.

- Three Point Formulas

Since

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

we have

$$L'_0(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}.$$

Similarly,

$$L'_1(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \quad \text{and} \quad L'_2(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}.$$



Hence

$$\begin{aligned} f'(x_j) &= f(x_0) \left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} \right] + f(x_1) \left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \right] \\ &+ f(x_2) \left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} \right] + \frac{1}{6} f^{(3)}(\xi_j) \prod_{k=0, k \neq j}^2 (x_j - x_k), \end{aligned}$$

for each $j = 0, 1, 2$. Assume that

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h, \text{ for some } h \neq 0.$$

Then

$$\begin{aligned} f'(x_0) &= \frac{1}{h} \left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2) \right] + \frac{h^2}{3} f^{(3)}(\xi_0), \\ f'(x_1) &= \frac{1}{h} \left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2) \right] - \frac{h^2}{6} f^{(3)}(\xi_1), \\ f'(x_2) &= \frac{1}{h} \left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2) \right] + \frac{h^2}{3} f^{(3)}(\xi_2). \end{aligned}$$



That is

$$f'(x_0) = \frac{1}{h} \left[-\frac{3}{2}f(x_0) + 2f(x_0 + h) - \frac{1}{2}f(x_0 + 2h) \right] + \frac{h^2}{3}f^{(3)}(\xi_0),$$

$$f'(x_0 + h) = \frac{1}{h} \left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0 + 2h) \right] - \frac{h^2}{6}f^{(3)}(\xi_1), \quad (3)$$

$$f'(x_0 + 2h) = \frac{1}{h} \left[\frac{1}{2}f(x_0) - 2f(x_0 + h) + \frac{3}{2}f(x_0 + 2h) \right] + \frac{h^2}{3}f^{(3)}(\xi_2) \quad (4)$$

Using the variable substitution x_0 for $x_0 + h$ and $x_0 + 2h$ in (3) and (4), respectively, we have

$$f'(x_0) = \frac{1}{2h} [-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\xi_0), \quad (5)$$

$$f'(x_0) = \frac{1}{2h} [-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

$$f'(x_0) = \frac{1}{2h} [f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(\xi_2). \quad (6)$$

Note that (6) can be obtained from (5) by replacing h with $-h$.



- Five-point Formulas

$$f'(x_0) = \frac{1}{12h} [f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi),$$

where $\xi \in (x_0 - 2h, x_0 + 2h)$ and

$$f'(x_0) = \frac{1}{12h} [-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5} f^{(5)}(\xi),$$

where $\xi \in (x_0, x_0 + 4h)$.



Round-off Error

Consider

$$f'(x_0) = \frac{1}{2h} [-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6} f^{(3)}(\xi_1),$$

where $\frac{h^2}{6} f^{(3)}(\xi_1)$ is called truncation error. Let $\tilde{f}(x_0 + h)$ and $\tilde{f}(x_0 - h)$ be the computed values of $f(x_0 + h)$ and $f(x_0 - h)$, respectively. Then

$$f(x_0 + h) = \tilde{f}(x_0 + h) + e(x_0 + h)$$

and

$$f(x_0 - h) = \tilde{f}(x_0 - h) + e(x_0 - h).$$

Therefore, the total error in the approximation

$$f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} = \frac{e(x_0 + h) - e(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1)$$

is due in part to round-off error and in the part to truncation error.



Assume that

$$|e(x_0 \pm h)| \leq \varepsilon \quad \text{and} \quad |f^{(3)}(\xi_1)| \leq M.$$

Then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} \right| \leq \frac{\varepsilon}{2h} + \frac{h^2}{6} M \equiv e(h).$$

Note that $e(h)$ attains its minimum at $h = \sqrt[3]{3\varepsilon/M}$.



Richardson's Extrapolation

Suppose $\forall h \neq 0$ we have a formula $N_1(h)$ that approximates an unknown value M

$$M - N_1(h) = K_1h + K_2h^2 + K_3h^3 + \dots, \quad (7)$$

for some unknown constants K_1, K_2, K_3, \dots . If $K_1 \neq 0$, then the truncation error is $O(h)$. For example,

$$f'(x) - \frac{f(x+h) - f(x)}{h} = -\frac{f''(x)}{2!}h - \frac{f'''(x)}{3!}h^2 - \frac{f^{(4)}(x)}{4!}h^3 - \dots.$$

Goal

Find an easy way to produce formulas with a higher-order truncation error.

Replacing h in (7) by $h/2$, we have

$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h}{2} + K_2\frac{h^2}{4} + K_3\frac{h^3}{8} + \dots.$$



Subtracting (7) with twice (8), we get

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \dots, \quad (9)$$

where

$$N_2(h) = 2N_1\left(\frac{h}{2}\right) - N_1(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right],$$

which is an $O(h^2)$ approximation formula.

Replacing h in (9) by $h/2$, we get

$$M = N_2\left(\frac{h}{2}\right) - \frac{k_2}{8}h^2 - \frac{3K_3}{32}h^3 - \dots. \quad (10)$$

Subtracting (9) from 4 times (10) gives

$$3M = N_2\left(\frac{h}{2}\right) - N_2(h) + \frac{3K_3}{8}h^3 + \dots,$$

which implies that

$$M = \left[N_2\left(\frac{h}{2}\right) + \frac{N_2(h/2) - N_2(h)}{3} \right] + \frac{K_3}{8}h^3 + \dots \equiv N_3(h) + \frac{K_3}{8}h^3 + \dots$$

Using induction, M can be approximated by

$$M = N_m(h) + O(h^m),$$

where

$$N_m(h) = N_{m-1}\left(\frac{h}{2}\right) + \frac{N_{m-1}(h/2) - N_{m-1}(h)}{2^{m-1} - 1}.$$

Centered difference formula. From the Taylor's theorem

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \frac{h^5}{5!}f^{(5)}(x) + \dots$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \frac{h^5}{5!}f^{(5)}(x) + \dots$$

we have

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2h^3}{3!}f'''(x) + \frac{2h^5}{5!}f^{(5)}(x) + \dots$$



and, consequently,

$$\begin{aligned} f'(x_0) &= \frac{f(x_0+h) - f(x_0-h)}{2h} - \left[\frac{h^2}{3!} f'''(x_0) + \frac{h^4}{5!} f^{(5)}(x_0) + \dots \right], \\ &\equiv N_1(h) - \left[\frac{h^2}{3!} f'''(x_0) + \frac{h^4}{5!} f^{(5)}(x_0) + \dots \right]. \end{aligned} \quad (11)$$

Replacing h in (11) by $h/2$ gives

$$f'(x_0) = N_1\left(\frac{h}{2}\right) - \frac{h^2}{24} f'''(x_0) - \frac{h^4}{1920} f^{(5)}(x_0) - \dots \quad (12)$$

Subtracting (11) from 4 times (12) gives

$$f'(x_0) = N_2(h) + \frac{h^4}{480} f^{(5)}(x_0) + \dots,$$

where

$$N_2(h) = \frac{1}{3} \left[4N_1\left(\frac{h}{2}\right) - N_1(h) \right] = N_1\left(\frac{h}{2}\right) + \frac{N_1(h/2) - N_1(h)}{3}.$$



In general,

$$f'(x_0) = N_j(h) + O(h^{2j})$$

with

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}.$$

Example

Suppose that $x_0 = 2.0$, $h = 0.2$ and $f(x) = xe^x$. Compute an approximated value of $f'(2.0) = 22.16716829679195$ to six decimal places.

Solution. By centered difference formula, we have

$$N_1(0.2) = \frac{f(0.2 + h) - f(0.2 - h)}{2h} = 22.414160,$$

$$N_1(0.1) = \frac{f(0.1 + h) - f(0.1 - h)}{2h} = 22.228786.$$



It implies that

$$N_2(0.2) = N_1(0.1) + \frac{N_1(0.1) - N_1(0.2)}{3} = 22.166995$$

which does not have six decimal digits. Adding $N_1(0.05) = 22.182564$, we get

$$N_2(0.1) = N_1(0.05) + \frac{N_1(0.05) - N_1(0.1)}{3} = 22.167157$$

and

$$N_3(0.2) = N_2(0.1) + \frac{N_2(0.1) - N_2(0.2)}{15} = 22.167168$$

which contains six decimal digits.



$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^4)$
1: $N_1(h) = N(h)$			
2: $N_1(h/2) = N(h/2)$	3: $N_2(h)$		
4: $N_1(h/4) = N(h/4)$	5: $N_2(h/2)$	6: $N_3(h)$	
7: $N_1(h/8) = N(h/8)$	8: $N_2(h/4)$	9: $N_3(h/2)$	10: $N_4(h)$



Elements of Numerical Integration

The basic method involved in approximating the integration

$$\int_a^b f(x) dx, \quad (13)$$

is called numerical quadrature and uses a sum of the type

$$\int_a^b f(x) dx \approx \sum_{i=0}^n c_i f(x_i). \quad (14)$$

The method of quadrature in this section is based on the polynomial interpolation. We first select a set of distinct nodes $\{x_0, x_1, \dots, x_n\}$ 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

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

The quadrature formula is, therefore,

$$\int_a^b f(x) dx \approx \int_a^b P_n(x) dx = \sum_{i=0}^n f(x_i) \int_a^b L_i(x) dx \equiv \sum_{i=0}^n c_i f(x_i), \quad (16)$$

where

$$c_i = \int_a^b L_i(x) dx = \int_a^b \prod_{\substack{j=0 \\ j \neq i}}^n \frac{x - x_j}{x_i - x_j} dx. \quad (17)$$



Moreover, the error in the quadrature formula is given by

$$E = \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\zeta_x) \prod_{i=0}^n (x - x_i) dx, \quad (18)$$

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

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



(19)

Theorem (Weighted Mean Value Theorem for Integrals)

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

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

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

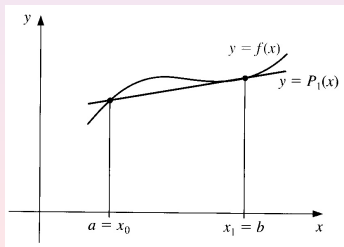
$$\begin{aligned} \int_{x_0}^{x_1} f''(\zeta(x))(x - x_0)(x - x_1)dx &= f''(\zeta) \int_{x_0}^{x_1} (x - x_0)(x - x_1)dx \\ &= f''(\zeta) \left[\frac{x^3}{3} - \frac{x_1 + x_0}{2}x^2 + x_0x_1x \right]_{x_0}^{x_1} = -\frac{h^3}{6} f''(\zeta). \end{aligned}$$



Consequently, Eq. (19) implies that

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

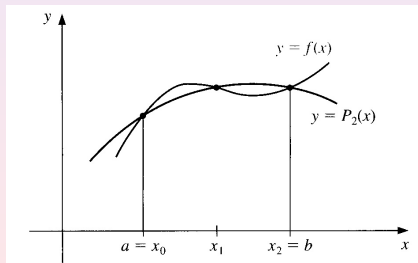
which is called the Trapezoidal rule.



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



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

Since, letting $x = x_0 + th$,

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

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



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

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.

Deriving Simpson's rule in this way, however, 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 . Then for each $x \in [a, b]$, there exists $\zeta_x \in (a, b)$ such that

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2$$



Then

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

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

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

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

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

This gives the Simpson's rule formulation.



If $|f^{(n+1)}(x)| \leq M$ on $[a, b]$, then

$$\left| \int_a^b f(x) dx - \sum_{i=0}^n c_i f(x_i) \right| \leq \frac{M}{(n+1)!} \int_a^b \prod_{i=0}^n (x - x_i) dx. \quad (20)$$

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

$$x_i = \frac{a+b}{2} + \frac{b-a}{2} \cos \left[\frac{(i+1)\pi}{n+2} \right], \quad i = 0, 1, \dots, n. \quad (21)$$

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

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

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

$$\int_a^b f(x) dx \approx f(x_0)(b-a) + \sum_{i=1}^n f[x_0, x_1, \dots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j) dx. \quad (22)$$



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

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 $k = 0, 1, \dots, n$.

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 .

A quadrature formula of the form (14) is called a Newton-Cotes formula if the nodes $\{x_0, x_1, \dots, x_n\}$ are equally spaced. Consider a uniform partition of the closed interval $[a, b]$ by

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



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 (17) gives

$$c_i = \int_a^b L_i(x) dx = \int_0^n \varphi_i(t) h dt = h \int_0^n \prod_{\substack{j=0 \\ j \neq i}}^n \frac{t - j}{i - j} dt, \quad (23)$$

and the general Newton-Cotes formula has the form

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

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

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

and

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

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

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

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:

$$\int_a^b f(x) dx = \frac{1}{2}(b - a) [f(a) + f(b)] - \frac{h^3}{12} f''(\xi), \quad (25)$$



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.

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

$$c_0 = h \int_0^2 \frac{t-1}{0-1} \cdot \frac{t-2}{0-2} dt = \frac{h}{2} \int_0^2 (t^2 - 3t + 2) dt = \frac{h}{3},$$

$$c_1 = h \int_0^2 \frac{t-0}{1-0} \cdot \frac{t-2}{1-2} dt = -h \int_0^2 (t^2 - 2t) dt = \frac{4h}{3},$$

$$c_2 = h \int_0^2 \frac{t-0}{2-0} \cdot \frac{t-1}{2-1} dt = \frac{h}{2} \int_0^2 (t^2 - t) dt = \frac{h}{3},$$



and

$$\int_a^b P_2(x) dx = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2) = h \left[\frac{1}{3} f(a) + \frac{4}{3} f\left(\frac{a+b}{2}\right) + \frac{1}{3} f(b) \right]$$

gives the so-called Simpson's rule. Deriving the formulation this way, however, the error term

$$\frac{1}{6} \int_a^b f^{(3)}(\zeta_x)(x-x_0)(x-x_1)(x-x_2) dx$$

provides only an $O(h^4)$ formulation involving $f^{(3)}$. A higher order error analysis can be derived by 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

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

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

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

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:

$$\int_a^b f(x) dx = \left(\frac{b-a}{2} \right) \left[\frac{1}{3} f(a) + \frac{4}{3} f\left(\frac{a+b}{2}\right) + \frac{1}{3} f(b) \right] + \frac{f^{(4)}(\xi)}{90} h^5, \quad (26)$$

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 $i = 0, 1, \dots, n$, 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. The following theorem details the Newton-Cotes formulas and the associated error analysis.



Theorem (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

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

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

$$\int_a^b f(x) dx = h \sum_{i=0}^n \alpha_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n) dt, \quad (27)$$

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

$$\int_a^b f(x) dx = h \sum_{i=0}^n \alpha_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n) dt, \quad (28)$$

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

$$f^{(n)} \leftarrow \frac{n}{t-i}$$

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

$$\sum_{i=0}^n \alpha_i = n. \quad (30)$$

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,

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

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

$$\int_a^b f(x) dx \approx h \sum_{i=0}^n \alpha_i f(x_i) = \frac{h}{s} \sum_{i=0}^n \sigma_i f(x_i). \quad (31)$$

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	$-\frac{9}{1400}f^{(8)}(\xi)h^9$

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

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

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 $b = x_{n+1}$. The following theorem summarizes the open Newton-Cotes formulas.



Theorem (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

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

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

$$\int_a^b f(x) dx = h \sum_{i=0}^n \alpha_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n + 2)!} \int_{-1}^{n+1} t^2(t - 1) \cdots (t - n) dt, \quad (32)$$

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

$$\int_a^b f(x) dx = h \sum_{i=0}^n \alpha_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n + 1)!} \int_{-1}^{n+1} t(t - 1) \cdots (t - n) dt, \quad (33)$$

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

$$f^{n+1} \frac{n}{t - i}$$

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:

$$\int_a^b f(x) dx = 2hf(x_0) + \frac{1}{3} f''(\xi) h^3 = (b-a)f\left(\frac{a+b}{2}\right) + \frac{1}{3} f''(\xi) h^3, \quad (35)$$

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	$\frac{95}{144} f^{(4)}(\xi) h^5$

It is obvious that the Newton-Cotes formulas are generally not suitable for numerical integration over large interval. Higher degree formulas would be required, and the coefficients in these formulas are difficult to obtain. Also the Newton-Cotes formulas which are based on polynomial interpolation would be inaccurate over a large interval because of the oscillatory nature of high-degree polynomials. Now we discuss a piecewise approach, called composite rule, to numerical integration over large interval that uses the low-order Newton-Cotes formulas.

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 $x_0 < x_1 < \dots < x_n = b$, and apply Simpson's

rule on each consecutive pair of subintervals. With

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

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

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

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,

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



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

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

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

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

and

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

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:

$$\int_a^b f(x) dx = \frac{h}{3} \left[f(a) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + 2 \sum_{j=1}^{(n/2)-1} f(x_{2j}) + f(b) \right] - \frac{b-a}{180} f^{(4)}(\mu) \quad (36)$$

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

The composite Midpoint rule can be derived in a similar way, except the midpoint rule is applied on each subinterval $[x_{2j-1}, x_{2j}]$ instead. That is,

$$\int_{x_{2j-2}}^{x_{2j}} f(x) dx = 2hf(x_{2j-1}) + \frac{h^3}{3} f''(\xi_j), \quad j = 1, 2, \dots, \frac{n}{2}.$$



Note that n must again be even. Consequently,

$$\int_a^b f(x) dx = 2h \sum_{j=1}^{n/2} f(x_{2j-1}) + \frac{h^3}{3} \sum_{j=1}^{n/2} f''(\xi_j).$$

The error term can be written as

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

for some $\mu \in (a, b)$. Therefore, the composite Midpoint rule has the following formulation.

Composite Midpoint Rule:

$$\int_a^b f(x) dx = 2h \sum_{j=1}^{n/2} f(x_{2j-1}) - \frac{b-a}{6} f''(\mu) h^2, \quad (37)$$

where n is an even integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \dots, n$, 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

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



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

Composite Trapezoidal Rule

$$\int_a^b f(x) dx = \frac{h}{2} \left[f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b) \right] - \frac{b-a}{12} f''(\mu) h^2, \quad (38)$$

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

