Numerical Analysis I
Numerical Differentiation and Integration

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[1] These slides are based on Prof. Tsung-Ming Huang(NTNU)'s original slides

Outline

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Numerical Differentiation

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

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

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

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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.

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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

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

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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

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

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we have,

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

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 $0 \le k \le n$,

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

Hence

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

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

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

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

$$
\begin{aligned}
f'(x_0) &= \frac{1}{h}\left[-\frac{3}{2}f(x_0)+2f(x_0+h)-\frac{1}{2}f(x_0+2h)\right]+\frac{h^2}{3}f^{(3)}(\xi_0), \\
f'(x_0+h) &= \frac{1}{h}\left[-\frac{1}{2}f(x_0)+\frac{1}{2}f(x_0+2h)\right]-\frac{h^2}{6}f^{(3)}(\xi_1), \qquad (3) \\
f'(x_0+2h) &= \frac{1}{h}\left[\frac{1}{2}f(x_0)-2f(x_0+h)+\frac{3}{2}f(x_0+2h)\right]+\frac{h^2}{3}f^{(3)}(\xi_2) \qquad (4)
\end{aligned}
$$

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

$$
\begin{aligned}
f'(x_0) &= \frac{1}{2h}\left[-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right]+\frac{h^2}{3}f^{(3)}(\xi_0), \qquad (5) \\
f'(x_0) &= \frac{1}{2h}\left[-f(x_0-h)+f(x_0+h)\right]-\frac{h^2}{6}f^{(3)}(\xi_1), \\
f'(x_0) &= \frac{1}{2h}\left[f(x_0-2h)-4f(x_0-h)+3f(x_0)\right]+\frac{h^2}{3}f^{(3)}(\xi_2). \qquad (6)
\end{aligned}
$$

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

- Five-point Formulas

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

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

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

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

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Round-off Error

Consider

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

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

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

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

Assume that

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

Then

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

Note that $e(h)$ attains its minimum at $h = \sqrt[3]{3\varepsilon/M}$.
In double precision arithmetics, for example, $\varepsilon \approx |f(x_0 \pm h)| \times 10^{-16}$. The minimum is $O(\sqrt[3]{M\varepsilon^2}) = O(10^{-10})$.

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Richardson's Extrapolation

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

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots, \quad (7)$$

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

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

Goal

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

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

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

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

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

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

$$M = N_2\left(\frac{h}{2}\right) - \frac{K_2}{8}h^2 - \frac{3K_3}{32}h^3 - \cdots . \tag{10}$$

Subtracting (9) from 4 times (10) gives

$$3M = 4N_2\left(\frac{h}{2}\right) - N_2(h) + \frac{3K_3}{8}h^3 + \cdots ,$$

which implies that

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

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

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

we have

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

and, consequently,

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

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

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

Subtracting (11) from 4 times (12) gives

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

where

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

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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

$$N_1(0.2) = \frac{f(2.0+0.2) - f(2.0-0.2)}{2h} = 22.414160,$$

$$N_1(0.1) = \frac{f(2.0+0.1) - f(2.0-0.1)}{h} = 22.228786.$$

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.

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$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^4)$
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: $N_4(h)$

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Remark

In practice, we are often encountered with the situation where the order of the numerical method is unknown. That is, the error expansion is of the form

$$M - N(h) = K_1 h^{p_1} + K_2 h^{p_2} + K_3 h^{p_3} + \cdots , \tag{13}$$

where $p_1, p_2, \cdots$ are unknown. Solving for the leading order p_1, together with the primary unknowns M and K_1, requires 3 equations, which can be obtained from, for example, the numerical results at h, $h/2$ and $h/4$:

$$\begin{aligned} M - N(h) &= K_1 h^{p_1} + \cdots , \\ M - N(\tfrac{h}{2}) &= K_1 \left(\tfrac{h}{2}\right)^{p_1} + \cdots , \\ M - N(\tfrac{h}{4}) &= K_1 \left(\tfrac{h}{4}\right)^{p_1} + \cdots \end{aligned} \tag{14}$$

The answer is given by

$$p_1 \approx \log_2 \frac{N(h) - N(\frac{h}{2})}{N(\frac{h}{2}) - N(\frac{h}{4})}$$

Once p_1 is known, Richardson extrapolation can be proceeded as before.

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

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

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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

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

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

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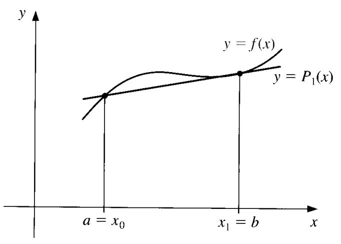
Consequently, Eq. (21) implies that

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

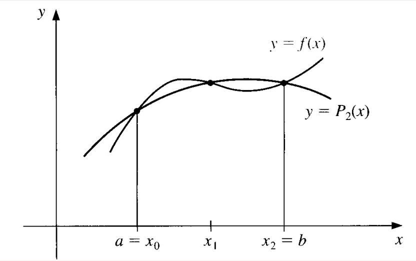
which is called the Trapezoidal rule.



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 $x = x_0 + th$,

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

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

it implies that

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

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

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

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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 p such that the formula is exact for x^k, when $k = 0, 1, \ldots, p$.

- The Trapezoidal and Simpson's rules have degrees of precision 1 and 3, respectively.
- The degree of accuracy of a quadrature formula is p if and only if the error $E = 0$ for all polynomials $P(x)$ of degree less than or equal to p, but $E \neq 0$ for some polynomials of degree $p + 1$.

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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.

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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

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

and the general Newton-Cotes formula has the form

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

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.

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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:

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

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

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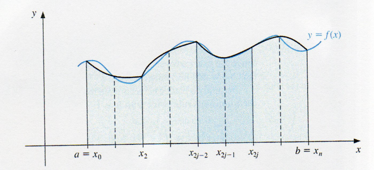
Composite Numerical Integration

- 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.



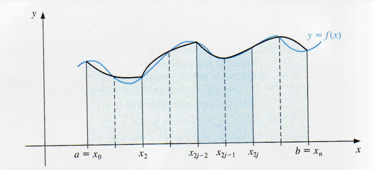
To illustrate the procedure, we choose an even integer n and partition the interval $[a, b]$ into n subintervals by nodes $a = x_0 < x_1 < \cdots < x_n = b$, and apply Simpson's rule on each consecutive pair of subintervals. With

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

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,

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx \\ &= \sum_{j=1}^{n/2} \left[\frac{h}{3} \left(f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j}) \right) - \frac{h^5}{90} f^{(4)}(\xi_j) \right] \\ &= \frac{h}{3} \left[f(x_0) + 4f(x_1) + f(x_2) \right. \\ &\quad + f(x_2) + 4f(x_3) + f(x_4) \\ &\quad + f(x_4) + 4f(x_5) + f(x_6) \\ &\qquad \vdots \\ &\quad \left. + f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \right] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j)\end{aligned}$$

Hence

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

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

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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 $\mu \in (a, b)$.

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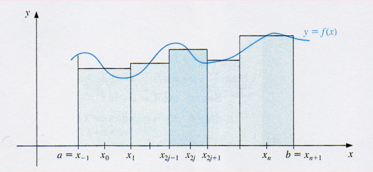
The composite Midpoint rule can be derived in a similar way, except the midpoint rule is applied on each subinterval $[x_{2j-1}, x_{2j+1}]$ instead. That is,

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

Note that n must again be even. Consequently,

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



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 $\mu \in (a, b)$.

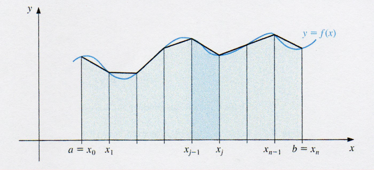
Composite Midpoint Rule

$$\int_a^b f(x)\, dx = 2h \sum_{j=1}^{n/2} f(x_{2j}) + \frac{b-a}{6} f''(\mu) h^2, \tag{29}$$

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 $[a, b]$ by n equally spaced nodes $a = x_0 < x_1 < \cdots < x_n = b$, where n can be either odd or even. Apply the trapezoidal rule on $[x_{j-1}, x_j]$ and sum them up to obtain

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



Hence,

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

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

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Composite Trapezoidal Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12} f''(\mu)h^2, \qquad (30)$$

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

Newton-Cotes formulas:

- The choice of nodes $x_0, x_1, \ldots, x_n$ was made *a priori*.
- Use values of the function at equally spaced points.
- Once the nodes were fixed, the coefficients were determined, e.g., by integrating the fundamental Lagrange polynomials of degree n.
- These formulas are exact for polynomials of degree $\leq n$ $(n+1$, if n is even).

This approach is convenient when the formulas are combined to form the composite rules, but the restriction may decrease the accuracy of the approximation.

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Gaussian quadrature

1. Chooses the points for evaluation in an optimal, rather than pre-fixed or equally-spaced, way.
2. The nodes $x_0, x_1, \ldots, x_n \in [a, b]$ and the coefficients $c_0, c_1, \ldots, c_n$ are chosen to minimize the expected error obtained in the approximation

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i) \tag{31}$$

3. Produce the exact result for the largest class of polynomials, that is, the choice which gives the greatest degree of precision.

The coefficients $c_0, c_1, \ldots, c_n$ are arbitrary, and the nodes $x_0, x_1, \ldots, x_n$ are restricted only in $[a, b]$. These give $2n + 2$ degrees of freedom. Thus we can expect that the quadrature formula of (31) can be discovered that will be exact for polynomials of degree $\leq 2n + 1$.

Suppose we want to determine c_0, c_1, x_0 and x_1 so that

$$\int_{-1}^{1} f(x)dx \approx c_0 f(x_0) + c_1 f(x_1) \tag{32}$$

gives the exact result whenever $f(x)$ is a polynomial of degree $2 \times 2 - 1 = 3$ or less, i.e.,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

Since

$$\begin{aligned} & \int (a_0 + a_1 x + a_2 x^2 + a_3 x^3) dx \\ = \; & a_0 \int 1 dx + a_1 \int x dx + a_2 \int x^2 dx + a_3 \int x^3 dx, \end{aligned}$$

this is equivalent to show that (32) gives exact results when $f(x)$ is $1, x, x^2$ and x^3. Hence

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$$
\begin{aligned}
c_0 + c_1 &= \int_{-1}^{1} 1 dx = 2, \\
c_0 x_0 + c_1 x_1 &= \int_{-1}^{1} x dx = 0, \\
c_0 x_0^2 + c_1 x_1^2 &= \int_{-1}^{1} x^2 dx = \frac{2}{3}, \\
c_0 x_0^3 + c_1 x_1^3 &= \int_{-1}^{1} x^3 dx = 0.
\end{aligned}
$$

It implies that

$$
c_0 = 1,\ c_1 = 1,\ x_0 = -\frac{\sqrt{3}}{3},\ x_1 = \frac{\sqrt{3}}{3}
$$

which gives

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

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Theorem

Suppose that $x_0, x_1, \ldots, x_n$ are the roots of the $(n+1)$-st Lengendre polynomial p_{n+1}, and that for each $i = 0, 1, \ldots, n$,

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

If $f(x)$ is any polynomial of degree $\leq 2n+1$, then

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

Gaussian Quadrature Rule

$$\int_{-1}^{1} f(x) \, dx \approx \sum_{i=0}^{n} c_i f(x_i), \tag{33}$$

Orthogonalization and Legendre polynomials

Definition

1. In a inner-product space, we say f is orthogonal to g, and write $f \perp g$ if $\langle f, g \rangle = 0$.
2. We write $f \perp G$ if $f \perp g$ for all $g \in G$.
3. We say that a finite or infinite sequence of vectors $f_1, f_2, \ldots$ in an inner-product space is orthogonal if $\langle f_i, f_j \rangle = 0$ for all $i \neq j$, and orthonormal if $\langle f_i, f_j \rangle = \delta_{ij}$.

The space of continuous functions on $[a, b]$ with inner-product defined as

$$\langle f, g \rangle = \int_a^b f(x)g(x)\, dx, \tag{34}$$

is an inner-product space.

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Definition

$\{\phi_0, \phi_1, \ldots, \phi_n\}$, where $\phi_i \in C[a,b]$ for all $i = 0, 1, \ldots, n$, is said to be an orthogonal set of functions if

$$\langle \phi_i, \phi_j \rangle = \int_a^b \phi_i(x)\phi_j(x)\,dx = \begin{cases} 0, & \text{when } i \neq j, \\ \alpha_i > 0, & \text{when } i = j. \end{cases}$$

If, in addition, $\alpha_i = 1$ for all i, then the set is said to be orthonormal.

Definition

Legendre polynomials: Gram-Schmidt process applied to $1, x, x^2, \cdots$.

$$
\begin{aligned}
p_0(x) &= 1 \\
p_1(x) &= x - \frac{\langle x, p_0 \rangle}{\langle p_0, p_0 \rangle} p_0 = x \\
p_2(x) &= x^2 - \frac{\langle x^2, p_0 \rangle}{\langle p_0, p_0 \rangle} p_0 - \frac{\langle x^2, p_1 \rangle}{\langle p_1, p_1 \rangle} p_1 = x^2 - \frac{1}{3} \\
&\cdots
\end{aligned}
$$

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Corollary

For any $n > 0$*, the set of Legendre polynomials* $\{p_0, p_1, \ldots, p_n\}$ *defined above is linearly independent and*

$$\langle q, p_n \rangle = \int_a^b q(x) p_n(x)\, dx = 0$$

for any polynomial $q(x)$ *with* $\deg(q(x)) \le n - 1$.

Let Π_n denote the set of polynomials of degree at most n, that is,

$$\Pi_n = \{p(x) \,|\, p(x) \text{ is a polynomial and } \deg(p) \le n\}.$$

Theorem

Let $q(x)$ be any nonzero polynomial of degree $n+1$, and $q(x) \perp \Pi_n$. If $x_0, x_1, \ldots, x_n$ are the roots of $q(x)$ in $[a,b]$, and

$$c_i = \int_a^b \prod_{\substack{j=0 \\ j \ne i}}^{n} \frac{x - x_j}{x_i - x_j}\, dx,$$

then

$$\int_a^b p(x)\, dx = \sum_{i=0}^{n} c_i p(x_i), \quad \text{for any } \; p \in \Pi_{2n+1}.$$

That is, the quadrature rule is exact for any polynomial of degree $\le 2n+1$.

Proof: For any polynomial $p \in \Pi_{2n+1}$, we can write

$$p(x) = q(x)t(x) + r(x),$$

where $t(x), r(x) \in \Pi_n$. Since $x_0, x_1, \ldots, x_n$ are roots of $q(x)$, we have

$$p(x_i) = q(x_i)t(x_i) + r(x_i) = r(x_i), \qquad i = 0, 1, \ldots, n.$$

By assumption, $q \perp \Pi_n$, we have

$$\langle q, t \rangle = \int_a^b q(x)t(x)\,dx = 0.$$

Since $r(x) \in \Pi_n$, it can be expressed exactly in the Lagrange form

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

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Hence

$$\begin{aligned}
\int_a^b p(x)\,dx &= \int_a^b q(x)t(x)\,dx + \int_a^b r(x)\,dx \\
&= \int_a^b r(x)\,dx = \int_a^b \sum_{i=0}^{n} r(x_i) \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\,dx \\
&= \sum_{i=0}^{n} r(x_i) \int_a^b \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\,dx \\
&= \sum_{i=0}^{n} p(x_i) \int_a^b \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\,dx \\
&= \sum_{i=0}^{n} c_i p(x_i).
\end{aligned}$$

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If the interval $[a, b]$ is $[-1, 1]$, then we can obtain a set of orthogonal polynomials called the Lengendre polynomials. The first few Lengendre polynomials are

$$
\begin{aligned}
p_0(x) &= 1 \\
p_1(x) &= x \\
p_2(x) &= x^2 - \frac{1}{3} \\
p_3(x) &= x^3 - \frac{3}{5}x \\
p_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{35} \\
p_5(x) &= x^5 - \frac{10}{9}x^3 + \frac{5}{21}x
\end{aligned}
$$

Gaussian Quadrature Rule

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

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i), \qquad (35)$$

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

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

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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	$x_0 = -0.9061798459$	$c_0 = 0.2369268851$
	$x_1 = -0.5384693101$	$c_1 = 0.4786286705$
	$x_2 = 0$	$c_2 = \frac{128}{225} = 0.568888889$
	$x_3 = 0.5384693101$	$c_3 = 0.4786286705$
	$x_4 = 0.9061798459$	$c_4 = 0.2369268851$

Romberg Integration

Recall the trapezoidal rule integral formulation

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

where $h = \frac{b-a}{n}$. 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

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

• If we apply Trapezoidal rule by x_0, x_1, x_2, x_3, and x_4, then we have

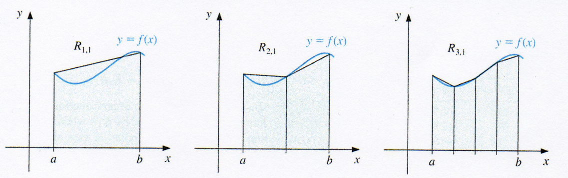
$$\begin{aligned}T(2n) &= \frac{h}{2}[f(a) + 2f(a+h) + 2f(a+2h) + 2f(a+3h) + f(a+4h)] \\ &= \frac{1}{2}T(n) + h[f(a+h) + f(a+3h)].\end{aligned}$$

This observation shows that

- if we have computed $T(n)$ and the step size is half, 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

$$T(2n) = \frac{1}{2}T(n) + h\sum_{i=1}^{n} f(a + (2i-1)h). \tag{36}$$

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 $n = 1, 2, 3, \ldots$,



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and the integral formulation becomes

$$T(2^n) = \frac{1}{2}T(2^{n-1}) + \frac{b-a}{2^n}\sum_{i=1}^{2^{n-1}} f(a + (2i-1)\frac{b-a}{2^n}). \qquad (37)$$

Let

$$R_{k,1} = T(2^k).$$

If $f \in C^\infty[a,b]$, then

$$\int_a^b f(x)dx - R_{k,1} = K_1 h_k^2 + \sum_{i=2}^{\infty} K_i h_k^{2^i}, \qquad (38)$$

where each K_i is independent of h_k and depends only on $f^{(2i-1)}(a)$ and $f^{(2i-1)}(b)$. Replacing h_k with $h_{k+1} = h_k/2$, we get

$$\int_a^b f(x)dx - R_{k+1,1} = \frac{K_1 h_k^2}{4} + \sum_{i=2}^{\infty} \frac{K_i h_k^{2^i}}{4^i}. \qquad (39)$$

Subtracting Eq. (38) from 4 times Eq. (39), we have

$$\int_a^b f(x)dx - \left[R_{k+1,1} + \frac{R_{k+1,1} - R_{k,1}}{3}\right] = -\frac{K_2}{4}h_k^4 + \sum_{i=3}^{\infty} \frac{K_i}{3}\left(\frac{1-4^{i-1}}{4^{i-1}}\right) h_k^{2}$$

Define

$$R_{k,2} = R_{k,1} + \frac{R_{k,1} - R_{k-1,1}}{3}, \quad \text{for } k = 2, 3, \ldots, n.$$

Apply the extrapolation procedure to those values. Continuing this notation, we have, for each $k = 2, 3, 4, \ldots, n$ and $j = 2, \ldots, k$, an $O(h_k^{2j})$ approximation formula defined by

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}.$$

This is called the Romberg algorithm.

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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 $n = 1, 2, \ldots, M$

$\quad R(n,0) = \frac{1}{2}R(n-1,0) + \frac{b-a}{2^n}\sum_{i=1}^{2^{n-1}} f(a+(2i-1)\frac{b-a}{2^n})$

End for

For $k = 1, 2, \ldots, M$

$\quad$ For $n = k, k+1, \ldots, M$

$\quad\quad R(n,k) = R(n,k-1) + \frac{1}{4^k-1}[R(n,k-1) - R(n-1,k-1)]$

$\quad$ End for

End for

Theorem

If $f \in C[a,b]$, *then for each column* k,

$$\lim_{n\to\infty} R(n,k) = \int_a^b f(x)\,dx. \tag{40}$$

Moreover, if $f \in C^{2m}[a,b]$, *then* $R(n,m)$ *converges to* $\int_a^b f(x)\,dx$ *with a rate of* $O(h^{2m})$, *where* $h = \frac{b-a}{2^n}$.