Numerical Analysis I
Numerical Differentiation and Integration

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Fall 2010

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

Outline

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

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

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,

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

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

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

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

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

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

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

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

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 $O(\sqrt[3]{M\varepsilon^2}) = O(10^{-10})$.

Richardson's Extrapolation

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

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

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

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

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,

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

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

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

Subtracting (11) from 4 times (12) gives

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

where

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

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

$$\begin{aligned} N_1(0.2) &= \frac{f(2.0+0.2) - f(2.0-0.2)}{2h} = 22.414160, \\ N_1(0.1) &= \frac{f(2.0+0.1) - f(2.0-0.1)}{h} = 22.228786. \end{aligned}$$

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: $N_4(h)$

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

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

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

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

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

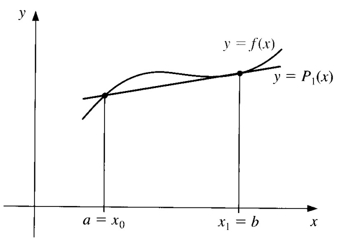
$$\int_{x_0}^{x_1} f''(\zeta(x))(x - x_0)(x - x_1)dx = f''(\zeta) \int_{x_0}^{x_1} (x - x_0)(x - x_1)dx$$

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

Consequently, Eq. (21) implies that

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

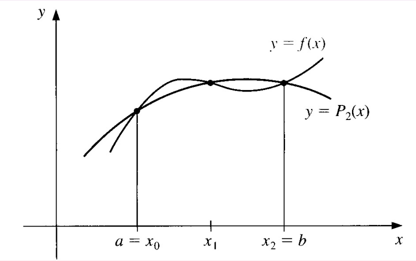
which is called the Trapezoidal rule.



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

$$\begin{aligned} P_2(x) &= f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \\ &\quad + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \end{aligned}$$

to interpolate $f(x)$, then



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

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

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

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

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

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

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

- $n = 2$: 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

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

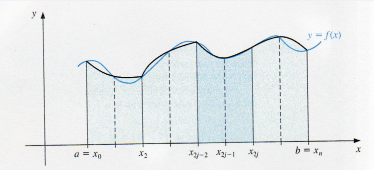
These gives the so-called Midpoint rule or Rectangular rule.
Midpoint Rule:

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

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

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.



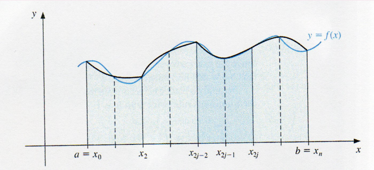
To illustrate the procedure, we choose an even integer n and partition the interval $[a, b]$ into n subintervals by nodes $a = x_0 < x_1 < \cdots < x_n = b$, and apply Simpson's rule on each consecutive pair of subintervals. With

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

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,

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

Hence

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

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

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

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

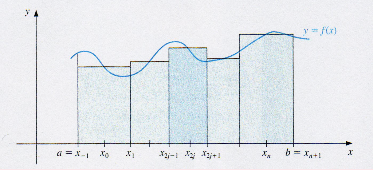
where n is an even integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a, b)$.

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,

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

Note that n must again be even. Consequently,

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



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

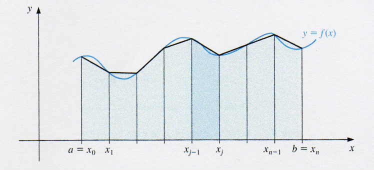
Composite Midpoint Rule

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

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

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.

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_1, c_2, x_1 and x_2 so that

$$\int_{-1}^{1} f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) \qquad (32)$$

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

$$\begin{aligned} c_1 + c_2 &= \int_{-1}^{1} 1 dx = 2, \\ c_1 x_1 + c_2 x_2 &= \int_{-1}^{1} x dx = 0, \\ c_1 x_1^2 + c_2 x_2^2 &= \int_{-1}^{1} x^2 dx = \frac{2}{3}, \\ c_1 x_1^3 + c_2 x_2^3 &= \int_{-1}^{1} x^3 dx = 0. \end{aligned}$$

It implies that

$$c_1 = 1, \; c_2 = 1, \; x_1 = -\frac{\sqrt{3}}{3}, \; x_2 = \frac{\sqrt{3}}{3}$$

which gives

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

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.

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 $1, x, x^2, \cdots$.

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

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,

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

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

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

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 $\leq 2n+1$.

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

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

Hence

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

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,

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

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

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

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

Additional Properties of Legendre Polynomials

- Alternative definitions:
- Other normalizations are possible.