MA 3021: Numerical Analysis I
Numerical Differentiation and Integration

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Introduction

- If the values of a function f are given at a few points $x_0, x_1, \cdots, x_n$, can that information be used to estimate a derivative $f'(c)$ or an integral $\int_a^b f(x)dx$?
- **Taylor's Theorem:** Let $f \in C^{n+1}[a, b]$ and $x_0 \in [a, b]$. Then for every $x \in [a, b]$, $\exists\ \xi(x)$ between x and x_0 such that

$$f(x) = P_n(x) + R_n(x),$$

where the n-th Taylor polynomial $P_n(x)$ is given by

$$P_n(x) = \sum_{k=0}^{n} \frac{1}{k!} f^{(k)}(x_0)(x - x_0)^k$$

and the remainder (error) term $R_n(x)$ is given by

$$R_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi(x))(x - x_0)^{n+1} \quad \text{(Lagrange's form).}$$

Numerical differentiation

- $f'(x_0) = \lim_{h\to 0} \frac{f(x_0+h)-f(x_0)}{h}$, if the limit exists. Intuitively, we have $f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$ if h is small.
- Assume that $h > 0$ and $f \in C^2[x_0, x_0+h]$. By Taylor's Theorem, we have

$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(\xi), \quad \text{for some } \xi \in (x_0, x_0+h).$$

- Rearranging the expansion, we obtain

$$f'(x_0) = \frac{1}{h}\Big(f(x_0+h) - f(x_0)\Big) - \frac{h}{2}f''(\xi).$$

- If the term $-\frac{h}{2}f''(\xi)$ is small, then we have an approximation of $f'(x_0)$,

$$f'(x_0) \approx \frac{1}{h}\Big(f(x_0+h) - f(x_0)\Big),$$

  called the forward-difference formula. The term "$-\frac{h}{2}f''(\xi)$" is called the truncation error, $O(h)$.
- When $h < 0$, we only have to change the assumption to $f \in C^2[x_0+h, x_0]$. ($\Rightarrow$ the backward-difference formula)

Higher order methods

- Assume that $h > 0$ and $f \in C^3[x_0 - h, x_0 + h]$.
  By Taylor's Theorem, we have

$$\begin{aligned} f(x_0 + h) &= f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(\xi_1), \\ f(x_0 - h) &= f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{6} f'''(\xi_2), \end{aligned}$$

  for some $\xi_1 \in (x_0, x_0 + h)$ and $\xi_2 \in (x_0 - h, x_0)$.
- After subtracting and rearranging, we have

$$f'(x_0) = \frac{1}{2h}\Big(f(x_0 + h) - f(x_0 - h)\Big) - \frac{h^2}{6}\frac{1}{2}\Big(f'''(\xi_1) + f'''(\xi_2)\Big).$$

- This is a more favorable result, because of the h^2 term in the error. Notice that, however, the presence of f''' in the error term.

Higher order methods (continued)

- From the Intermediate Value Theorem, we have that there is a $\xi \in (x_0 - h, x_0 + h)$, such that

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

Hence,

$$f'(x_0) = \frac{1}{2h}\Big(f(x_0 + h) - f(x_0 - h)\Big) - \frac{h^2}{6} f'''(\xi).$$

Therefore

$$f'(x_0) \approx \frac{1}{2h}\Big(f(x_0 + h) - f(x_0 - h)\Big),$$

which is a second-order formula, $O(h^2)$.

Approximation of $f''(x_0)$

Assume that $h > 0$ and $f \in C^4[x_0 - h, x_0 + h]$. From Taylor's Theorem, we have

$$\begin{aligned} f(x_0 + h) &= f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f^{(3)}(x_0) + \frac{h^4}{4!}f^{(4)}(\xi_1), \\ f(x_0 - h) &= f(x_0) - hf'(x_0) + \frac{h^2}{2!}f''(x_0) - \frac{h^3}{3!}f^{(3)}(x_0) + \frac{h^4}{4!}f^{(4)}(\xi_2), \end{aligned}$$

for some $\xi_1 \in (x_0, x_0 + h)$ and $\xi_2 \in (x_0 - h, x_0)$. After sum and rearrangement, we obtain the following central difference formula for the 2nd derivative:

$$\begin{aligned} f''(x_0) &= \frac{1}{h^2}\Big(f(x_0 + h) - 2f(x_0) + f(x_0 - h)\Big) - \frac{h^2}{12}\frac{1}{2}\Big(f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\Big) \\ &= \frac{1}{h^2}\Big(f(x_0 + h) - 2f(x_0) + f(x_0 - h)\Big) - \frac{h^2}{12}f^{(4)}(\xi), \end{aligned}$$

where at the last equality we use the Intermediate Value Theorem again. Thus, we have a second-order approximation of $f''(x_0)$

$$f''(x_0) \approx \frac{1}{h^2}\Big(f(x_0 + h) - 2f(x_0) + f(x_0 - h)\Big).$$

Richardson's extrapolation

- Richardson extrapolation is a general procedure to improve accuracy.
- Assume that f is sufficiently smooth and

$$\begin{aligned} f(x_0+h) &= \sum_{k=0}^{\infty} \frac{1}{k!} h^k f^{(k)}(x_0), \\ f(x_0-h) &= \sum_{k=0}^{\infty} \frac{1}{k!} (-1)^k h^k f^{(k)}(x_0). \end{aligned}$$

After subtraction and rearrangement, we obtain

$$f'(x_0) = \frac{1}{2h}\Big(f(x_0+h)-f(x_0-h)\Big)-\Big(\frac{h^2}{3!}f^{(3)}(x_0)+\frac{h^4}{5!}f^{(5)}(x_0)+\frac{h^6}{7!}f^{(7)}(x_0)+\cdots\Big).$$

or in an abstract form

$$M = N(h) + \Big(k_2 h^2 + k_4 h^4 + k_6 h^6 + \cdots\Big),$$

where $M := f'(x_0)$ and $N(h) := (f(x_0+h) - f(x_0-h))/(2h)$.

Richardson's extrapolation (continued)

- In general, suppose that

$$M = N(h) + \left(k_1 h + k_2 h^2 + k_3 h^3 + \cdots\right) \qquad \leftarrow (1).$$

$$\Rightarrow M - N(h) = O(h).$$

$$M = N(\frac{h}{2}) + k_1 \frac{h}{2} + k_2 \left(\frac{h}{2}\right)^2 + k_3 \left(\frac{h}{2}\right)^3 + \cdots \qquad \leftarrow (2).$$

$$2 \times (2) - (1) \Rightarrow M = 2N(\frac{h}{2}) - N(h) + k_2 \left(\frac{h^2}{2} - h^2\right) + k_3 \left(\frac{h^3}{4} - h^3\right) + \cdots$$

  Define

$$\begin{aligned} N_1(h) &:= N(h), \\ N_2(h) &:= N_1(\frac{h}{2}) + \left\{N_1(\frac{h}{2}) - N_1(h)\right\}. \end{aligned}$$

$$\Rightarrow M = N_2(h) - \tfrac{k_2}{2} h^2 - \tfrac{3k_3}{4} h^3 - \cdots \qquad \leftarrow (3).$$

$$\Rightarrow M - N_2(h) = O(h^2).$$

- This formula is the first step in Richardson extrapolation. It shows that a simple combination of $N_1(h)$ and $N_1(h/2)$ furnishes an estimate of M with an accuracy of $O(h^2)$.

Richardson's extrapolation (continued)

From (3), we have

$$M = N_2(\frac{h}{2}) - \frac{k_2}{8}h^2 - \frac{3k_3}{32}h^3 - \cdots \qquad \leftarrow (4).$$

$$4 \times (4) - (3) \Rightarrow 3M = 4N_2(\frac{h}{2}) - N_2(h) + \frac{3k_3}{8}h^3 + \cdots$$

$$\Rightarrow M = N_2(\frac{h}{2}) + \frac{1}{3}\left\{N_2(\frac{h}{2}) - N_2(h))\right\} + \frac{3k_3}{8}h^3 + \cdots$$

Define $N_3(h) = N_2(\frac{h}{2}) + \frac{1}{3}\{N_2(\frac{h}{2}) - N_2(h)\}$.

$\Rightarrow M - N_3(h) = O(h^3)$.

Richardson's extrapolation (continued)

Using the techniques, we have

$$
\begin{aligned}
N_4(h) &= N_3(\frac{h}{2}) + \frac{1}{7}\left\{N_3(\frac{h}{2}) - N_3(h)\right\}, \\
M - N_4(h) &= O(h^4), \\
N_5(h) &= N_4(\frac{h}{2}) + \frac{1}{15}\left\{N_4(\frac{h}{2}) - N_4(h)\right\}, \\
M - N_5(h) &= O(h^5), \\
&\vdots
\end{aligned}
$$

In general, if $M = N_1(h) + \sum_{j=1}^{m-1} k_j h^j + O(h^m)$ then for $j = 2, 3, \cdots, m$,

$$
\begin{aligned}
N_j(h) &= N_{j-1}(\frac{h}{2}) + \frac{1}{2^{j-1}-1}\left\{N_{j-1}(\frac{h}{2}) - N_{j-1}(h)\right\}, \\
M &= N_j(h) + O(h^j).
\end{aligned}
$$

Example

$$
\begin{aligned}
f'(x_0) &= \frac{1}{2h}\Big(f(x_0+h)-f(x_0-h)\Big) - \frac{1}{6}h^2 f^{(3)}(x_0) - \frac{1}{120}h^4 f^{(5)}(x_0) - \cdots \\
f'(x_0) &= N_1(h) + O(h^2). \\
f'(x_0) &= N_1(h) - \frac{1}{6}h^2 f^{(3)}(x_0) - \frac{1}{120}h^4 f^{(5)}(x_0) - \cdots \\
f'(x_0) &= N_1(\frac{h}{2}) - \frac{1}{24}h^2 f^{(3)}(x_0) - \frac{1}{1920}h^4 f^{(5)}(x_0) - \cdots \\
4f'(x_0) &= 4N_1(\frac{h}{2}) - \frac{1}{6}h^2 f^{(3)}(x_0) - \frac{1}{480}h^4 f^{(5)}(x_0) - \cdots \\
3f'(x_0) &= 4N_1(\frac{h}{2}) - N_1(h) + \frac{1}{160}h^4 f^{(5)}(x_0) - \cdots \\
f'(x_0) &= N_1(\frac{h}{2}) + \frac{1}{3}\left\{N_1(\frac{h}{2}) - N_1(h)\right\} + \frac{1}{480}h^4 f^{(5)}(x_0) - \cdots \\
f'(x_0) &:= N_2(h) + O(h^4).
\end{aligned}
$$

Another approach: differentiation via polynomial interpolation

- Suppose that $f \in C^2[a,b]$ and $x_0 \in (a,b)$. Suppose that $h \neq 0$ and small, $x_1 := x_0 + h \in [a,b]$. Then $\exists\ \xi(x) \in [a,b]$ such that

$$
\begin{aligned}
f(x) &= \frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1) + \frac{f''(\xi(x))}{2!}(x-x_0)(x-x_1) \\
&= \frac{x-x_0-h}{-h} f(x_0) + \frac{x-x_0}{h} f(x_0+h) + \frac{f''(\xi(x))}{2!}(x-x_0)(x-x_0-h)
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow f'(x) = -\frac{1}{h} f(x_0) + \frac{1}{h} f(x_0+h) + \frac{D_x f''(\xi(x))}{2!}(x-x_0)(x-x_0-h) \\
+ \frac{2(x-x_0)-h}{2!} f''(\xi(x)).
\end{aligned}
$$

- Hence we have $f'(x_0) = \dfrac{f(x_0+h)-f(x_0)}{h} - \dfrac{h}{2!} f''(\xi(x_0))$

$\Rightarrow f'(x_0) \approx \dfrac{f(x_0+h)-f(x_0)}{h}$ with error bound by $\frac{|h|}{2} M$,

$M := \max_{x \in [a,b]} |f''(x)|$.

$h > 0 \Rightarrow$ the forward-difference formula; $h < 0 \Rightarrow$ the backward-difference formula.

General case

Suppose that $x_0, x_1, \cdots, x_n \in I$ distinct & $f \in C^{n+1}(I)$. Then

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n), \text{ where } \xi(x) \in I.$$

$$\Rightarrow f'(x) = \sum_{k=0}^{n} f(x_k)L_k'(x) + D_x\left\{\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\right\}(x-x_0)(x-x_1)\cdots(x-x_n)$$

$$+\frac{f^{(n+1)}(\xi(x))}{(n+1)!}D_x\{(x-x_0)(x-x_1)\cdots(x-x_n)\}.$$

$$\Rightarrow f'(x_j) = \sum_{k=0}^{n} f(x_k)L_k'(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!}\prod_{k=0,k\neq j}^{n}(x_j - x_k).$$

We obtain an $(n+1)$-point formula.

Three point formula: x_0, x_1, x_2

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \Rightarrow L_0'(x) = \frac{(x-x_2)+(x-x_1)}{(x_0-x_1)(x_0-x_2)} = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)},$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \Rightarrow L_1'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)},$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \Rightarrow L_2'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}.$$

$$\Rightarrow f'(x_j) = \frac{2x_j-x_1-x_2}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{2x_j-x_0-x_2}{(x_1-x_0)(x_1-x_2)} f(x_1)$$

$$+ \frac{2x_j-x_0-x_1}{(x_2-x_0)(x_2-x_1)} f(x_2) + \frac{f^{(3)}(\xi_j)}{3!} \prod_{k=0, k\neq j}^{2} (x_j - x_k),$$

where $\xi_j := \xi(x_j)$.

Equal spaced: $x_0, x_1 = x_0 + h, x_2 = x_0 + 2h$

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

$\Longrightarrow$

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

Formula $(*)$ and formula $(**)$ are essentially the same! ($h > 0$ or $h < 0$, respectively)

Three-point and five-point formulas

- **Three-point formula:**

$$
\begin{aligned}
f'(x_0) &= \frac{1}{2h}\{-3f(x_0)+4f(x_0+h)-f(x_0+2h)\}+\frac{1}{3}h^2 f^{(3)}(\xi_0),\\
&\quad \text{for some } \xi_0 \text{ between } x_0 \text{ and } x_0+2h,\\
f'(x_0) &= \frac{1}{2h}\{f(x_0+h)-f(x_0-h)\}-\frac{1}{6}h^2 f^{(3)}(\xi_1),\\
&\quad \text{for some } \xi_1 \text{ between } x_0-h \text{ and } x_0+h.
\end{aligned}
$$

- **Five-point formula:**

$$
\begin{aligned}
f'(x_0) &= \frac{1}{12h}\{f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)\}+\frac{h^4}{30}f^{(5)}(\xi)\\
&\quad \text{for some } \xi \text{ between } x_0-2h \text{ and } x_0+2h, \leftarrow (\bigstar)\\
f'(x_0) &= \frac{1}{12h}\{-25f(x_0)+48f(x_0+h)-36f(x_0+2h)\\
&\qquad +16f(x_0+3h)-3f(x_0+4h)\}+\frac{h^4}{5}f^{(5)}(\xi),\\
&\quad \text{for some } \xi \text{ between } x_0 \text{ and } x_0+4h.
\end{aligned}
$$

Use Taylor's Theorem + extrapolation to derive (★)

$$
\begin{aligned}
f(x_0+h) &= f(x_0)+hf'(x_0)+\frac{h^2}{2!}f''(x_0)+\frac{h^3}{3!}f^{(3)}(x_0)+\frac{h^4}{4!}f^{(4)}(x_0)+\frac{h^5}{120}f^{(5)}(\xi_1),\\
f(x_0-h) &= f(x_0)-hf'(x_0)+\frac{h^2}{2!}f''(x_0)-\frac{h^3}{3!}f^{(3)}(x_0)+\frac{h^4}{4!}f^{(4)}(x_0)-\frac{h^5}{120}f^{(5)}(\xi_2),
\end{aligned}
$$

where ξ_1 between x_0 and x_0+h, ξ_2 between x_0 and x_0-h.

$$\Rightarrow f(x_0+h)-f(x_0-h)=2hf'(x_0)+\frac{h^3}{3}f'''(x_0)+\frac{h^5}{120}\left\{f^{(5)}(\xi_1)+f^{(5)}(\xi_2)\right\},$$

$$\Rightarrow f'(x_0)=\frac{1}{2h}\{f(x_0+h)-f(x_0-h)\}-\frac{h^2}{6}f'''(x_0)-\frac{h^4}{120}f^{(5)}(\widetilde{\xi}),\leftarrow (Eqn1)$$

Replace h by $2h$,

$$\Rightarrow f'(x_0)=\frac{1}{4h}\{f(x_0+2h)-f(x_0-2h)\}-\frac{4h^2}{6}f'''(x_0)-\frac{16h^4}{120}f^{(5)}(\widehat{\xi}),\leftarrow (Eqn2)$$

where $\widetilde{\xi}$ between x_0-h and x_0+h, $\widehat{\xi}$ between x_0-2h and x_0+2h.

Use Taylor's Theorem + extrapolation to derive (★) (continued)

$4 \times (Eqn1) - (Eqn2) \Rightarrow 3f'(x_0) =$
$$\frac{2}{h}\{f(x_0+h) - f(x_0-h)\} - \frac{1}{4h}\{f(x_0+2h) - f(x_0-2h)\} - \frac{h^4}{30}f^{(5)}(\widetilde{\xi}) + \frac{2h^4}{15}f^{(5)}(\widehat{\xi}).$$

If $f \in C^5[x_0 - 2h, x + 2h]$ $(h > 0)$ then we have

$$\frac{4h^4}{30}f^{(5)}(\widehat{\xi}) - \frac{h^4}{30}f^{(5)}(\widetilde{\xi}) = \frac{h^4}{30}\{4f^{(5)}(\widehat{\xi}) - f^{(5)}(\widetilde{\xi})\} = \frac{h^4}{30}3f^{(5)}(\xi) \quad \text{(why?)}.$$

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

for some $\xi \in [x_0 - 2h, x_0 + 2h]$.

Example

The forward-difference formula can be expressed as

$$f'(x_0) = \frac{1}{h}\{f(x_0+h) - f(x_0)\} - \frac{h}{2}f''(x_0) - \frac{h^2}{6}f'''(x_0) + O(h^3).$$

Use extrapolation to derive an $O(h^3)$ formula for $f'(x_0)$.

Numerical integration

Numerical quadrature: $\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$.

Let $x_0, x_1, \cdots, x_n \in [a, b]$ be $n+1$ distinct nodes.

Let $P_n(x) = \sum_{i=0}^{n} f(x_i)L_i(x)$ be the nth Lagrange polynomial. Then

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

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

Trapezoidal rule

Let $x_0 = a, x_1 = b, h = b - a$. Then

$$
\begin{aligned}
& \int_a^b f(x)dx \\
= \; & \int_{x_0}^{x_1} \left\{ \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \right\} dx + \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)dx \\
= \; & \left(\frac{(x - x_1)^2}{2(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{2(x_1 - x_0)} f(x_1) \right)\Bigg|_{x_0}^{x_1} + \frac{1}{2} f''(\xi) \int_{x_0}^{x_1} (x - x_0)(x - x_1)dx, \\
& \qquad for\ some\ \xi \in (x_0, x_1) \\
= \; & \frac{1}{2}(x_1 - x_0)f(x_1) - \frac{1}{2}(x_0 - x_1)f(x_0) + \frac{1}{2} f''(\xi) \left(\frac{x^3}{3} - \frac{(x_0 + x_1)x^2}{2} + x_0 x_1 x \right)\Bigg|_{x_0}^{x_1} \\
= \; & \frac{1}{2}(x_1 - x_0)(f(x_0) + f(x_1)) + \frac{1}{2} f''(\xi)(\frac{-1}{6})(x_1 - x_0)^3 \\
= \; & \frac{h}{2}\{f(x_0) + f(x_1)\} - \frac{1}{12} h^3 f''(\xi).
\end{aligned}
$$

Remark: If $f(x)$ is a polynomial with degree$(f) \leq 1$, then the Trapezoidal Rule gives exact result!

Simpson's rule

Let $x_0 = a, x_1 = a + h, x_2 = b, h = (b - a)/2$. Then

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_2}\left\{\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1)\right. \\ &\quad \left. + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)\right\}dx \\ &\quad + \int_{x_0}^{x_2}\frac{f^{(3)}(\xi(x))}{3!}(x-x_0)(x-x_1)(x-x_2)dx \\ &\Longrightarrow O(h^4) \text{ error term.}\end{aligned}$$

Alternative approach: Taylor's Theorem

Let $x \in [x_0, x_2]$. Then $\exists\ \xi(x) \in (x_0, x_2)$ such that

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

$$\Longrightarrow \int_{x_0}^{x_2} f(x)dx = \left(f(x_1)(x - x_1) + \frac{f'(x_1)}{2}(x - x_1)^2 + \frac{f''(x_1)}{6}(x - x_1)^3 + \frac{f'''(x_1)}{24}(x - x_1)^4 \right)_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx.$$

$$\because\ \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx = \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2} (x - x_1)^4 dx = \frac{f^{(4)}(\xi_1)}{24 \times 5}(x - x_1)^5 \Big|_{x_0}^{x_2},$$

for some $\xi_1 \in (x_0, x_2)$.

$$\therefore \int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{120}2h^5.$$

Simpson's rule/degree of precision

$$
\begin{aligned}
\int_{x_0}^{x_2} f(x)dx &= 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}\Big(f(x_0) - 2f(x_1) + f(x_2)\Big) - \frac{h^2}{12}f^{(4)}(\xi_2)\right\} \\
&\qquad + \frac{f^{(4)}(\xi_1)}{60}h^5 \\
&= \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) - \frac{h^5}{12}\left\{\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\right\} \\
&= \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) - \frac{h^5}{90}f^{(4)}(\xi), \quad \text{for some } \xi \in (x_0, x_2).
\end{aligned}
$$

Definition: The degree of accuracy (precision) of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, $k = 0, 1, \cdots, n$.

Note: Trapezoidal rule: degree of precision $= 1$;
Simpson's rule: degree of precision $= 3$.

The $(n+1)$-point closed Newton-Cotes formula

Let $a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b$ be the uniform grid points of $[a, b]$ with $h = \dfrac{b-a}{n}$. Then

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

$$a_i := \int_{x_0}^{x_n} L_i(x)dx = \int_{x_0}^{x_n} \left\{ \prod_{j=0, j\neq i}^{n} \frac{(x - x_j)}{(x_i - x_j)} \right\} dx.$$

Theorem: the $(n+1)$-point closed Newton-Cotes formula

- If n is even and $f \in C^{n+2}[a, b]$ then $\exists\ \xi \in (a, b)$ such that
$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)dt.$$
- If n is odd and $f \in C^{n+1}[a, b]$ then $\exists\ \xi \in (a, b)$ such that
$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)dt.$$

Examples

- $n = 1$: trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}\{f(x_0) + f(x_1)\} - \frac{h^3}{12} f''(\xi) \text{ for some } \xi \in (x_0, x_1).$$

- $n = 2$: Simpson's rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\{f(x_0) + 4f(x_1) + f(x_2)\} - \frac{h^5}{90} f^{(4)}(\xi) \text{ for some } \xi \in (x_0, x_2).$$

- $n = 3$: Simpson's three-eight rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}\{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\} - \frac{3h^5}{80} f^{(4)}(\xi) \text{ for some } \xi \in (x_0, x_3).$$

- $n = 4$:

$$\int_{x_0}^{x_4} f(x)dx = \frac{2h}{45}\{7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)\} - \frac{8h^7}{945} f^{(6)}(\xi) \text{ for some } \xi \in (x_0, x_4).$$

The $(n+1)$-point open Newton-Cotes formula

Let $a = x_{-1} < x_0 < x_1 < \cdots < x_{n-1} < x_n < x_{n+1} = b$ be the uniform grid points of $[a,b]$ with $h = \dfrac{b-a}{n+2}$. Then use $\{x_0, x_1, \cdots, x_n\}$ to find the Lagrange interpolating polynomial.

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

Theorem: the $(n+1)$-point open Newton-Cotes formula

- If n is even and $f \in C^{n+2}[a,b]$ then $\exists\ \xi \in (a,b)$ such that
$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)dt.$$
- If n is odd and $f \in C^{n+1}[a,b]$ then $\exists\ \xi \in (a,b)$ such that
$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)dt.$$

Examples

- $n = 0$: midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi) \text{ for some } \xi \in (x_{-1}, x_1).$$

- $n = 1$:

$$\int_{x_{-1}}^{x_2} f(x)dx = \frac{3h}{2}\{f(x_0) + f(x_1)\} + \frac{3h^3}{4} f''(\xi) \text{ for some } \xi \in (x_{-1}, x_2).$$

- $n = 2$:

$$\int_{x_{-1}}^{x_3} f(x)dx = \frac{4h}{3}\{2f(x_0) - f(x_1) + 2f(x_2)\} + \frac{14h^5}{45} f^{(4)}(\xi) \text{ for some } \xi \in (x_{-1}, x_3).$$

- $n = 4$:

$$\int_{x_{-1}}^{x_4} f(x)dx = \frac{5h}{24}\{11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)\} + \frac{95h^5}{144} f^{(4)}(\xi) \text{ for some } \xi \in (x_{-1}, x_4).$$

Midpoint rule

Consider the smooth function f on $[a,b]$. Let $x_0 = \dfrac{a+b}{2}$.

- Intuition: $\displaystyle\int_a^b f(x)dx \approx \int_a^b f(x_0)dx = f(x_0)(b-a) = f(\frac{a+b}{2})(b-a)$.
- Based on Taylor's Theorem:

$$\begin{aligned}
\int_a^b f(x)dx &\approx \int_a^b f(x_0) + f'(x_0)(x-x_0)dx \\
&= f(\frac{a+b}{2})(b-a) + \frac{f'(x_0)}{2}(x - \frac{a+b}{2})^2\Big|_a^b \\
&= f(\frac{a+b}{2})(b-a) + 0.
\end{aligned}$$

- $f(x) - \Big(f(x_0) + f'(x_0)(x-x_0)\Big) = \dfrac{f''(\xi(x))}{2!}(x-x_0)^2$.

$$\Longrightarrow \int_a^b f(x)dx - f(\frac{a+b}{2})(b-a) = \int_a^b \frac{f''(\xi(x))}{2!}(x-x_0)^2dx$$

$$= \frac{f''(\xi)}{2!}\int_a^b (x-x_0)^2dx = \frac{f''(\xi)}{6}\frac{(b-a)^3}{4} = \frac{f''(\xi)}{24}(b-a)^3,\ \xi \in (a,b).$$

Composite numerical integration

- Large integration interval $\Longrightarrow$ large h $\Longrightarrow$ inaccurate; small h $\Longrightarrow$ high-degree polynomial $\Longrightarrow$ inaccurate.
- Idea: piecewise approach + low-order Newton-cotes formulas.
- **Example:** Using Simpson's rule with $h = 2$, we have

$$\int_0^4 e^x\,dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958\cdots \quad (\textit{exact value} \ = 53.59815\cdots)$$

Composite Simpson's rule:

- $(h = 1)$ $\displaystyle\int_0^4 e^x\,dx = \int_0^2 e^x\,dx + \int_2^4 e^x\,dx \approx$
  $\displaystyle\frac{1}{3}(e^0 + 4e^1 + e^2) + \frac{1}{3}(e^2 + 4e^3 + e^4) = 53.86385\cdots.$
- $(h = 1/2)$ $\displaystyle\int_0^4 e^x\,dx = \int_0^1 e^x\,dx + \cdots + \int_3^4 e^x\,dx \approx$
  $\displaystyle\frac{1}{6}(e^0 + 4e^{1/2} + e^1) + \cdots + \frac{1}{6}(e^3 + 4e^{3.5} + e^4) = 53.61622\cdots.$

Composite Simpson's rule

Let n be an even integer. Divide $[a, b]$ into n subintervals.

Let $h = \dfrac{b-a}{n}$ and $x_j = a + jh$ for $j = 0, 1, \cdots, n$. Then

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

Composite Simpson's rule (continued)

If $f \in C^4[a,b]$ then $\min\limits_{x\in[a,b]} f^{(4)}(x) \le f^{(4)}(\xi_j) \le \max\limits_{x\in[a,b]} f^{(4)}(x)$.

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

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

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

$$f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \Longrightarrow \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = \frac{h^5 n}{180} f^{(4)}(\mu).$$

$$\because h = \frac{b-a}{n} \Rightarrow n = \frac{b-a}{h}$$

$$\Rightarrow \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = \frac{h^5(b-a)}{180h} f^{(4)}(\mu) = \frac{(b-a)}{180} h^4 f^{(4)}(\mu).$$

Composite rules

- **The composite Simpson's rule:** Let n be an even integer, $h = \frac{b-a}{n}$, $x_0 = a < x_1 < \cdots < x_n = b$ and $x_j = a + jh$. If $f \in C^4[a,b]$ then $\exists\ \mu \in (a,b)$ such that

$$\int_a^b f(x)dx = \frac{h}{3}\left\{ f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right\} - \frac{(b-a)}{180}h^4 f^{(4)}($$

- **The composite trapezoidal rule:** Let $h = \frac{b-a}{n}$, $x_0 = a < x_1 < \cdots < x_n = b$ and $x_j = a + jh$. If $f \in C^2[a,b]$ then $\exists\ \mu \in (a,b)$ such that

$$\int_a^b f(x)dx = \frac{h}{2}\left\{ f(x_0) + 2\sum_{j=1}^{n-1} f(x_j) + f(x_n)\right\} - \frac{(b-a)}{12}h^2 f''(\mu).$$

- **The composite midpoint rule:** Let n be an even integer, $h = \frac{b-a}{n+2}$, $x_{-1} = a < x_0 < x_1 < \cdots < x_n < x_{n+1} = b$ and $x_j = a + (j+1)h$. If $f \in C^2[a,b]$ then $\exists\ \mu \in (a,b)$ such that

$$\int_a^b f(x)dx = 2h\sum_{j=0}^{n/2} f(x_{2j}) + \frac{(b-a)}{6}h^2 f''(\mu).$$

Gaussian quadrature

- Degree of precision + use values of function at equally spaced points, e.g. the trapezoidal rule.
- **Gaussian quadrature:** $\int_a^b f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i)$, where $c_i \in \mathbb{R}$ and $x_i \in [a, b]$ for $i = 1, 2, \cdots, n \Longrightarrow 2n$ parameters to choose.

  The greatest degree of precision $\leq 2n - 1$.

Example

Let $[a, b] = [-1, 1]$ and $n = 2$. We want to determine $c_1, c_2 \in \mathbb{R}$, $x_1, x_2 \in [-1, 1]$ such that

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

and gives exact value whenever $f(x)$ is a polynomial with degree$(f) \leq 3 (= 2n - 1)$. $\Longleftrightarrow$ gives exact value when $f(x) = 1, x, x^2, x^3$.

Example (continued)

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

$\Longrightarrow$

$$\begin{aligned}
&c_1 + c_2 = 2,\\
&c_1x_1 + c_2x_2 = 0,\\
&c_1x_1^2 + c_2x_2^2 = \frac{2}{3},\\
&c_1x_1^3 + c_2x_2^3 = 0.
\end{aligned}$$

$\Longrightarrow c_1 = 1, c_2 = 1, x_1 = \dfrac{-\sqrt{3}}{3}, x_2 = \dfrac{\sqrt{3}}{3}.$

$\Longrightarrow \displaystyle\int_{-1}^{1} f(x)dx \approx 1f(\frac{-\sqrt{3}}{3}) + 1f(\frac{\sqrt{3}}{3}).$ This formula has degree of precision 3.

Legendre polynomials

(Chapter 8) Some Legendre polynomials are given by

$$p_0(x) = 1, \qquad p_1(x) = x, \qquad p_2(x) = x^2 - \frac{1}{3},$$
$$p_3(x) = x^3 - \frac{3}{5}x, \qquad p_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}, \qquad \cdots$$

- For each n, $p_n(x)$ is a polynomial of degree n.
- $\int_{-1}^{1} p(x)p_n(x)dx = 0$ whenever $p(x)$ is a polynomial of degree $\leq n-1$.
- The roots of $p_n(x)$ are distinct, lie in $(-1, 1)$, have a symmetry with respect to the origin. e.g., $p_2(x) = x^2 - \frac{1}{3}$ has roots $\frac{-\sqrt{3}}{3}$ and $\frac{\sqrt{3}}{3}$.

Theorem

Suppose that $x_1, x_2, \cdots, x_n$ are the roots of the nth Legendre polynomial $p_n(x)$. For $i = 1, 2, \cdots, n$, $c_i := \int_{-1}^{1} \prod_{j=1, j\neq i}^{n} \left(\frac{x - x_j}{x_i - x_j} \right) dx$. If $p(x)$ is a polynomial and degree$(p(x)) < 2n$. Then $\int_{-1}^{1} p(x)dx = \sum_{i=1}^{n} c_i p(x_i)$.

Proof: Let $R(x)$ be a polynomial and degree$(R(x)) \leq n - 1$. Let $x_1, x_2, \cdots, x_n$ be the roots of the nth Legendre polynomial $p_n(x)$. Then

$$R(x) = \sum_{i=1}^{n} \left(\prod_{j=1, j\neq i}^{n} \frac{x - x_j}{x_i - x_j} R(x_i) \right) + nth\ derivative\ of\ R(x) =$$

$$\sum_{i=1}^{n} \left(\prod_{j=1, j\neq i}^{n} \frac{x - x_j}{x_i - x_j} R(x_i) \right) + 0.$$

$$\int_{-1}^{1} R(x)dx = \int_{-1}^{1} \sum_{i=1}^{n} \left(\prod_{j=1, j\neq i}^{n} \frac{x - x_j}{x_i - x_j} R(x_i) \right) dx$$

$$= \sum_{i=1}^{n} \left(\int_{-1}^{1} \prod_{j=1, j\neq i}^{n} \frac{x - x_j}{x_i - x_j} dx \right) R(x_i) = \sum_{i=1}^{n} c_i R(x_i).$$

Proof (continued)

Let $p(x)$ be a polynomial with degree$(p(x)) \leq 2n-1$.

Then $p(x) = Q(x)p_n(x) + R(x)$ for some $Q(x)$ and $R(x)$

with degree$(Q(x)) \leq n-1$ and degree$(R(x)) \leq n-1$.

$\because$ degree$(Q(x)) \leq n-1 \quad \therefore \displaystyle\int_{-1}^{1} Q(x)p_n(x)dx = 0$.

$\because x_i$ is a root of $p_n(x)$ for $i = 1, 2, \cdots, n \quad \therefore p(x_i) = Q(x_i)p_n(x_i) + R(x_i) = R(x_i)$.

$$\Longrightarrow \int_{-1}^{1} p(x)dx = \int_{-1}^{1} \Big(Q(x)p_n(x) + R(x)\Big)dx = \int_{-1}^{1} R(x)dx$$

$$= \sum_{i=1}^{n} c_i R(x_i) = \sum_{i=1}^{n} c_i p(x_i).$$

This completes the proof.

Concluding remarks

Change of variables: $\int_a^b f(x)dx \to \int_{-1}^1 \widetilde{f}(t)dt.$

$$t = \frac{2x - a - b}{b - a} \iff x = \frac{1}{2}\Big((b-a)t + a + b\Big).$$

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

Example: $\int_1^{1.5} e^{-x^2}dx = \int_{-1}^1 e^{-\left(\frac{1}{2}(0.5t+2.5)\right)^2}\frac{0.5}{2}dt = \frac{1}{4}\int_{-1}^1 e^{-\frac{(t+5)^2}{16}}dt.$