MA 1018: Introduction to Scientific Computing
Numerical Differentiation and Integration

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Introduction

1. If the values of 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 $\int_a^b f(x)\,dx$?
2. **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

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

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

Rearranging the expansion, we obtain

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

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

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

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

Higher order method

1. 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

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

2. 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.

The truncation error

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

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

Hence,

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

Therefore

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

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,

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

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 at x_0:

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

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

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

Richardson's extrapolation

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

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

After subtraction and rearrangement, we obtain

$$\begin{aligned} f'(x_0) &= \frac{1}{2h}\big(f(x_0+h) - f(x_0-h)\big) \\ &\quad - \left(\frac{h^2}{3!} f^{(3)}(x_0) + \frac{h^4}{5!} f^{(5)}(x_0) + \frac{h^6}{7!} f^{(7)}(x_0) + \cdots\right), \end{aligned}$$

or in an abstract form

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

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

Richardson's extrapolation (cont'd)

1. In general, suppose that

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

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

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

Define

$$N_1(h) := N(h) \quad \text{and} \quad N_2(h) := N_1(\frac{h}{2}) + \left\{N_1(\frac{h}{2}) - N_1(h)\right\}.$$

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

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

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

Richardson's extrapolation (cont'd)

From (3), we have

$$\begin{aligned} & M = N_2(\frac{h}{2}) - \frac{k_2}{8}h^2 - \frac{3k_3}{32}h^3 - \cdots \leftarrow (4) \\ & 4 \times (4) - (3) \Rightarrow 3M = 4N_2(\frac{h}{2}) - N_2(h) + \frac{3k_3}{8}h^3 + \cdots \\ & \Rightarrow M = N_2(\frac{h}{2}) + \frac{1}{3}\left\{N_2(\frac{h}{2}) - N_2(h))\right\} + \frac{3k_3}{8}h^3 + \cdots \end{aligned}$$

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 (cont'd)

Using the same techniques, we have

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

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

$$N_j(h) = N_{j-1}(\frac{h}{2}) + \frac{1}{2^{j-1}-1}\Big\{N_{j-1}(\frac{h}{2}) - N_{j-1}(h)\Big\},$$

$$M = N_j(h) + O(h^j).$$

Example

Below, we are going to derive an $O(h^4)$ approximation of $f'(x_0)$:

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

Differentiation via polynomial interpolation

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

$$f(x) = \frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1) + \frac{f''(\xi(x))}{2!}(x-x_0)(x-x_1)$$

$$= \frac{x-x_0-h}{-h} f(x_0) + \frac{x-x_0}{h} f(x_0+h) + \frac{f''(\xi(x))}{2!}(x-x_0)(x-x_0-h)$$

If $\frac{D_x f''(\xi(x))}{2!}$ exists $\Longrightarrow f'(x) = -\frac{1}{h} f(x_0) + \frac{1}{h} f(x_0+h)$

$$+ \frac{D_x f''(\xi(x))}{2!}(x-x_0)(x-x_0-h) + \frac{2(x-x_0)-h}{2!} f''(\xi(x)).$$

2. We have $f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2!} f''(\xi(x_0))$

$\Rightarrow f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$ with error bound $\frac{|h|}{2} \max_{x \in [a,b]} |f''(x)|$.

$h > 0$: the forward-difference formula
$h < 0$: the backward-difference formula

General case

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

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

where $\xi(x) \in I$.

$$\text{If } D_x\left\{\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\right\} \text{ exists } \Longrightarrow f'(x) = \sum_{k=0}^{n} f(x_k) L_k'(x)$$

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

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

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

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

Three point formula: x_0, x_1, x_2

First, we compute

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

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

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

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

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

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

Equal spaced

Consider the case of equal spaced: $x_0, x_1 = x_0 + h, x_2 = x_0 + 2h$. Then

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

These three formulas can be reformulated as

$$\begin{aligned}
f'(x_0) &= \frac{1}{2h}\left\{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right\} + \frac{1}{3}h^2 f^{(3)}(\xi_0), && (\star_1) \\
f'(x_0) &= \frac{1}{2h}\left\{-f(x_0-h) + f(x_0+h)\right\} - \frac{1}{6}h^2 f^{(3)}(\xi_1), \\
f'(x_0) &= \frac{1}{2h}\left\{f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right\} + \frac{1}{3}h^2 f^{(3)}(\xi_2). && (\star_2)
\end{aligned}$$

$(\star_2)$ and $(\star_2)$ are essentially the same! ($h > 0$ or $h < 0$, respectively)

Three-point and five-point formulas

1. **Three-point formula:**

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

2. **Five-point formula:**

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

Use Taylor's Theorem + extrapolation to derive $(\star)$

An alternative way to derive $(\star)$: Assume that $f \in C^5[x_0 - 2h, x + 2h]$ and $h > 0$. Then

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

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

$$\Rightarrow f(x_0 + h) - f(x_0 - h) = 2hf'(x_0) + \frac{h^3}{3}f^{(3)}(x_0) + \frac{h^5}{120}\left\{f^{(5)}(\xi_1) + f^{(5)}(\xi_2)\right\},$$
$$\Rightarrow f'(x_0) = \frac{1}{2h}\left\{f(x_0 + h) - f(x_0 - h)\right\} - \frac{h^2}{6}f^{(3)}(x_0) - \frac{h^4}{120}f^{(5)}(\tilde{\xi}), \qquad (1)$$

Replacing h by $2h$, we have

$$\Rightarrow f'(x_0) = \frac{1}{4h}\left\{f(x_0 + 2h) - f(x_0 - 2h)\right\} - \frac{4h^2}{6}f^{(3)}(x_0) - \frac{16h^4}{120}f^{(5)}(\hat{\xi}), \quad (2)$$

where $\tilde{\xi}$ between $x_0 - h$ and $x_0 + h$, $\hat{\xi}$ between $x_0 - 2h$ and $x_0 + 2h$.

Use Taylor's Theorem + extrapolation to derive $(\star)$ (cont'd)

Performing "$4 \times (1) - (2)$", we obtain

$$\begin{aligned} 3f'(x_0) &= \frac{2}{h}\Big\{f(x_0+h) - f(x_0-h)\Big\} \\ &\quad - \frac{1}{4h}\Big\{f(x_0+2h) - f(x_0-2h)\Big\} - \frac{h^4}{30}f^{(5)}(\tilde{\xi}) + \frac{2h^4}{15}f^{(5)}(\hat{\xi}). \end{aligned}$$

The error term can be expressed as

$$\frac{4h^4}{30}f^{(5)}(\hat{\xi}) - \frac{h^4}{30}f^{(5)}(\tilde{\xi}) = \frac{h^4}{30}\{4f^{(5)}(\hat{\xi}) - f^{(5)}(\tilde{\xi})\} = O(h^4).$$

Therefore, we have

$$f'(x_0) = \frac{1}{12h}\Big\{f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\Big\} + O(h^4).$$

Homework

The forward-difference formula can be expressed as

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

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

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} \left\{ \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \right\} dx$$
$$+ \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\,dx$$
$$= \left(\frac{(x - x_1)^2}{2(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{2(x_1 - x_0)} f(x_1) \right)\Bigg|_{x_0}^{x_1} + \frac{f''(\xi)}{2} \int_{x_0}^{x_1} (x - x_0)(x - x_1)\,dx,$$

for some $\xi \in (x_0, x_1)$

$$= \frac{(x_1 - x_0)}{2} f(x_1) - \frac{(x_0 - x_1)}{2} f(x_0) + \frac{1}{2} f''(\xi) \left(\frac{x^3}{3} - \frac{(x_0 + x_1)x^2}{2} + x_0 x_1 x \right)\Bigg|_{x_0}^{x_1}$$
$$= \frac{1}{2}(x_1 - x_0)(f(x_0) + f(x_1)) + \frac{1}{2} f''(\xi)\left(\frac{-1}{6}\right)(x_1 - x_0)^3$$
$$= \frac{h}{2}\Big\{ f(x_0) + f(x_1) \Big\} - \frac{1}{12} h^3 f''(\xi).$$

If $f(x)$ is a polynomial with degree$(f) \leq 1$, then the trapezoidal rule gives exact result! *The error is large if the interval size is large.*

Error term in the trapezoid rule

- **The error term in the trapezoid rule:** Assume that $f \in C^2[a,b]$. Using the error term in the Lagrange interpolation and the mean-value theorem for integrals, we have

$$\int_a^b f(x) - p_2(x)\,dx = \int_a^b f''(\xi_x)\frac{(x-a)(x-b)}{2}\,dx$$

$$= \frac{1}{2}f''(\xi)\int_a^b x^2 - (a+b)x + ab\,dx = \cdots = -\frac{1}{12}(b-a)^3 f''(\xi),$$

where $f''(\xi_x) = 2(f(x) - p(x))/(x^2 - (a+b)x + ab)$ is continuous on (a,b) and can be continuously extended to $[a,b]$ by using the L'Hospital rule to calculate $\lim_{x\to a^+} f''(\xi_x)$ and $\lim_{x\to b^-} f''(\xi_x)$.

- **The mean-value theorem for integrals**: *Assume that $u \in C[a,b]$, $v \in \mathcal{R}[a,b]$ and v doesn't change sign on $[a,b]$. Then $\exists\ \xi \in (a,b)$ such that $\int_a^b u(x)v(x)\,dx = u(\xi)\int_a^b v(x)\,dx$.*

Simpson's rule

Let $x_0 = a, x_1 = a + h, x_2 = b$, and $h = (b - a)/2$. 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 to derive Simpson's rule

Let $x \in [x_0, x_2]$. Then by Taylor's Theorem, $\exists\, \xi(x) \in (x_0, x_2)$ such that

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

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

$$
\begin{aligned}
\because\ \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4 dx = \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4 dx \\
= \frac{f^{(4)}(\xi_1)}{24\times 5}(x-x_1)^5\Big|_{x_0}^{x_2}, \text{ for some } \xi_1 \in (x_0, x_2).
\end{aligned}
$$

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

Simpson's rule/degree of precision

Applying the central difference formula to $f''(x_1)$, we have

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

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, $k = 0 : n$.

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

Midpoint rule

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

1. Intuition:

$$\int_a^b f(x)dx \approx \int_a^b f(x_0)\,dx = f(x_0)(b-a) = f(\frac{a+b}{2})(b-a).$$

2. Based on Taylor's Theorem:

$$\int_a^b f(x)dx \approx \int_a^b f(x_0) + f'(x_0)(x-x_0)dx$$
$$= f(\frac{a+b}{2})(b-a) + \frac{f'(x_0)}{2}(x - \frac{a+b}{2})^2\Big|_a^b = f(\frac{a+b}{2})(b-a) + 0.$$
$$f(x) - \big(f(x_0) + f'(x_0)(x-x_0)\big) = \frac{f''(\xi(x))}{2!}(x-x_0)^2.$$
$$\Longrightarrow \int_a^b f(x)dx - f(\frac{a+b}{2})(b-a) = \int_a^b \frac{f''(\xi(x))}{2!}(x-x_0)^2 dx$$
$$= \frac{f''(\xi)}{2!}\int_a^b (x-x_0)^2 dx = \frac{f''(\xi)}{6}\,\frac{(b-a)^3}{4} = \frac{f''(\xi)}{24}(b-a)^3,\ \xi \in (a,b).$$

Composite numerical integration

1. Large integration interval $\Longrightarrow$ large h $\Longrightarrow$ inaccurate; small h $\Longrightarrow$ high-degree polynomial $\Longrightarrow$ inaccurate.

2. **Example:** Using Simpson's rule with $h = 2$, we have

$$\int_0^4 e^x dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958...$$

(exact value $= 53.59815...$)

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

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

Composite Simpson's rule (cont'd)

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

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

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

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

1. **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
$$\int_a^b f(x)dx = \frac{h}{3}\left\{f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right\} - \frac{(b-a)}{180}h^4 f^{(4)}(\mu).$$
2. **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
$$\int_a^b f(x)dx = \frac{h}{2}\left\{f(x_0) + 2\sum_{j=1}^{n-1} f(x_j) + f(x_n)\right\} - \frac{(b-a)}{12}h^2 f''(\mu).$$
3. **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

1. Degree of precision + use values of function at equally spaced points, e.g. the trapezoidal rule.

2. **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 $i = 1 : n$ to be determined $\Longrightarrow 2n$ parameters.

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

3. **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$(f) \leq 3 \ \ (= 2n - 1)$.

Example (cont'd)

We determine $c_1, c_2 \in \mathbb{R}$ and $x_1, x_2 \in [-1, 1]$ such that the formula gives exact value when $f(x) = 1, x, x^2, x^3$.

$$2 = \int_{-1}^{1} 1dx = c_1 f(x_1) + c_2 f(x_2) = c_1 + c_2 \qquad (f(x) = 1),$$

$$0 = \int_{-1}^{1} xdx = c_1 f(x_1) + c_2 f(x_2) = c_1 x_1 + c_2 x_2 \qquad (f(x) = x),$$

$$\frac{2}{3} = \int_{-1}^{1} x^2 dx = c_1 f(x_1) + c_2 f(x_2) = c_1 x_1^2 + c_2 x_2^2 \qquad (f(x) = x^2),$$

$$0 = \int_{-1}^{1} x^3 dx = c_1 f(x_1) + c_2 f(x_2) = c_1 x_1^3 + c_2 x_2^3 \qquad (f(x) = x^3).$$

$$\Longrightarrow c_1 + c_2 = 2, \quad c_1 x_1 + c_2 x_2 = 0, \quad c_1 x_1^2 + c_2 x_2^2 = \tfrac{2}{3}, \quad c_1 x_1^3 + c_2 x_2^3 = 0.$$

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

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

This formula has degree of precision 3.

Legendre polynomials

In Chapter 8, some Legendre polynomials are given by

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

The Legendre polynomials have the following properties:

- 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 0. e.g., $p_2(x) = x^2 - \frac{1}{3}$ has roots $\frac{-\sqrt{3}}{3}$ and $\frac{\sqrt{3}}{3}$.

Theorem on Gaussian quadrature

Theorem: *Suppose that* $x_1, x_2, \cdots, x_n$ *are the roots of the nth Legendre polynomial* $p_n(x)$*. For* $i = 1, 2, \cdots, n$*, define*

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

If $p(x)$ *is a polynomial and degree*$(p(x)) \leq 2n - 1$*. 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$(R(x)) \leq n - 1$. Then $R^{(n)}(x) = 0$ and by the Lagrange interpolating theorem, we have

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

Therefore,

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

Proof of the theorem on Gaussian quadrature (con'd)

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$(Q(x)) \leq n - 1$

$$\therefore \int_{-1}^{1} Q(x)p_n(x)\, dx = 0$$

$\because$ x_i is a root of $p_n(x)$ for $i = 1 : n$

$$\therefore p(x_i) = Q(x_i)p_n(x_i) + R(x_i) = R(x_i)$$

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

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

This completes the proof. $\square$

Change of variables

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

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

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

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