數值分析 MA-3021

Chapter 4. Numerical Differentiation and Integration

Introduction

Question: 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 $\int_a^b f(x)\,dx$?

Theorem (Taylor's Theorem for functions of one variable)

Let $f \in C^{m+1}([a,b])$ and $x_0 \in [a,b]$. Then for every $x \in [a,b]$, there exists $\xi(x)$ between x and x_0 such that

$$f(x) = P_m(x) + R_m(x)\,,$$

where the m-th Taylor polynomial $P_m(x)$ is given by

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

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

$$R_m(x) = \frac{1}{(m+1)!} f^{(m+1)}(\xi(x))(x - x_0)^{m+1} \qquad \text{(Lagrange's form)}$$

§4.1 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,

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

   Rearranging the expansion, we obtain

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

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

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

   called the **forward-difference formula**. The term "$-\frac{h}{2} f''(\xi)$" is called the **truncation error** which is of order $\mathcal{O}(h)$.

§4.1 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.
3. Assume that $h<0$ and $f\in C^2([x_0+h, x_0])$. By Taylor's Theorem,

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

Rearranging the expansion, we obtain

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

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

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

called the **backward-difference formula**. The term "$-\frac{h}{2}f''(\xi)$" is called the **truncation error** which is of order $\mathcal{O}(h)$.

§4.1 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.

3. Assume that $h>0$ and $f\in C^2([x_0-h, x_0])$. By Taylor's Theorem,

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

   Rearranging the expansion, we obtain

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

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

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

   called the **backward-difference formula**. The term "$\frac{h}{2}f''(\xi)$" is called the **truncation error** which is of order $\mathcal{O}(h)$.

§4.1 Numerical Differentiation

- **Higher order methods**:

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

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

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

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

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.

§4.1 Numerical Differentiation

- **Higher order methods**:

3. 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 the **central difference formula for the 1st derivative** at x_0 and is a second-order formula, $\mathcal{O}(h^2)$.

§4.1 Numerical Differentiation

- **Approximation of $f''(x_0)$**: Assume that $h > 0$ and $f \in C^4([x_0 - h, x_0 + h])$. From Taylor's Theorem,

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

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:

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

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

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

§4.2 Richardson's Extrapolation

1. Richardson's 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

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

or in an abstract form

$$M=N(h)+\big(k_2h^2+k_4h^4+k_6h^6+\cdots\big),$$

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

§4.2 Richardson's Extrapolation

In general, suppose that a number M satisfies that

$$M = N(h) + k_1 h + k_2 h^2 + k_3 h^3 + \cdots \quad (\forall\, h \ll 1) \qquad (\star)$$

so that $M - N(h) = \mathcal{O}(h)$. Then

$$M = N(\tfrac{h}{2}) + k_1 \frac{h}{2} + k_2 \Big(\frac{h}{2}\Big)^2 + k_3 \Big(\frac{h}{2}\Big)^3 + \cdots . \qquad (\star')$$

Therefore, $2 \times (\star') - (\star)$ implies that

$$M = 2N(\tfrac{h}{2}) - N(h) + k_2 \Big(\frac{h^2}{2} - h^2\Big) + k_3 \Big(\frac{h^3}{4} - h^3\Big) + \cdots$$

Define

$$N_1(h) := N(h) \quad \text{and} \quad N_2(h) := N_1(\tfrac{h}{2}) + \Big\{ N_1(\tfrac{h}{2}) - N_1(h) \Big\}.$$

Then

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

which implies that $M - N_2(h) = \mathcal{O}(h^2)$.

§4.2 Richardson's Extrapolation

$$M = N_1(h) + k_1 h + k_2 h^2 + k_3 h^3 + \cdots \qquad (\star)$$

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

$(\star\star)$ is the first step in Richardson extrapolation. It shows that a simple combination of $N_1(h)$ and $N_1\left(\frac{h}{2}\right)$, $N_2(h) = 2N_1\left(\frac{h}{2}\right) - N_1(h)$, furnishes an estimate of M with an accuracy of $\mathcal{O}(h^2)$.

Example

Let $N_1(h) = \dfrac{f(x_0+h) - f(x_0)}{h}$. Then $f'(x_0) = N_1(h) + \mathcal{O}(h)$. By Richards's extrapolation,

$$N_2(h) \equiv 2N_1\left(\frac{h}{2}\right) - N_1(h) = 2 \cdot \frac{f\left(x_0 + \frac{h}{2}\right) - f(x_0)}{h/2} - \frac{f(x_0+h) - f(x_0)}{h}$$

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

which provides an $\mathcal{O}(h^2)$ approximation of $f'(x_0)$.

§4.2 Richardson's Extrapolation

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Let $N_1(h) = \dfrac{f(x_0+h) - f(x_0)}{h}$. Then $f'(x_0) = N_1(h) + \mathcal{O}(h)$. By Richards's extrapolation,

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

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§4.2 Richardson's Extrapolation

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

Using $(\star\star)$ we have

$$M = N_2(\tfrac{h}{2}) - \frac{k_2}{8}h^2 - \frac{3k_3}{32}h^3 - \cdots; \qquad (\star\star')$$

thus $4 \times (\star\star') - (\star\star)$ implies that

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

or

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

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

$$M - N_3(h) = \mathcal{O}(h^3).$$

§4.2 Richardson's Extrapolation

Example

In previous example, we find that

$$N_2(h) = \frac{1}{h}\Big[-f(x_0+h) + 4f\Big(x_0+\frac{h}{2}\Big) - 3f(x_0)\Big]$$

provides an $\mathcal{O}(h^2)$ approximation of $f'(x_0)$. Therefore, the second step of Richard's extrapolation implies that

$$\begin{aligned}
N_3(h) &\equiv N_2(\tfrac{h}{2}) + \frac{1}{3}\Big\{N_2(\tfrac{h}{2}) - N_2(h))\Big\} = \frac{4}{3}N_2\big(\tfrac{h}{2}\big) - \frac{1}{3}N_2(h) \\
&= \frac{4}{3}\cdot\frac{2}{h}\Big[-f\Big(x_0+\frac{h}{2}\Big) + 4f\Big(x_0+\frac{h}{4}\Big) - 3f(x_0)\Big] \\
&\quad -\frac{1}{3}\cdot\frac{1}{h}\Big[-f(x_0+h) + 4f\Big(x_0+\frac{h}{2}\Big) - 3f(x_0)\Big] \\
&= \frac{1}{h}\Big[\frac{1}{3}f(x_0+h) - 4f\Big(x_0+\frac{h}{2}\Big) + \frac{32}{3}f\Big(x_0+\frac{h}{4}\Big) - 7f(x_0)\Big]
\end{aligned}$$

provides an $\mathcal{O}(h^3)$ approximation of $f'(x_0)$.

§4.2 Richardson's Extrapolation

In general, if a quantity M satisfies

$$M = N(h) + kh^m + \mathcal{O}(h^{m+1})$$

for some constant k, then

$$\begin{aligned} M - \Big\{N\big(\tfrac{h}{2}\big) + \frac{1}{2^m - 1}\Big[N\big(\tfrac{h}{2}\big) - N(h)\Big]\Big\} &= \frac{2^m}{2^m - 1}\big[M - N\big(\tfrac{h}{2}\big)\big] - \frac{1}{2^m - 1}\big[M - N(h)\big] \\ &= \frac{2^m}{2^m - 1}\Big[k\big(\tfrac{h}{2}\big)^m + \mathcal{O}(h^{m+1})\Big] - \frac{1}{2^m - 1}\Big[kh^m + \mathcal{O}(h^{m+1})\Big] \\ &= \mathcal{O}(h^{m+1}). \end{aligned}$$

In other words, if $N(h)$ is an order $\mathcal{O}(h^m)$ approximation of M, then

$$\widetilde{N}(h) = N\big(\tfrac{h}{2}\big) + \frac{1}{2^m - 1}\Big[N\big(\tfrac{h}{2}\big) - N(h)\Big]$$

is "likely" an order $\mathcal{O}(h^{m+1})$ approximation of M.

§4.2 Richardson's Extrapolation

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In other words, if $N(h)$ is an order $\mathcal{O}(h^m)$ approximation of M, then

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is "likely" an order $\mathcal{O}(h^{m+1})$ approximation of M.

§4.2 Richardson's Extrapolation

Example

From previous example we find that

$$N(h) \equiv \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}$$

is an order $\mathcal{O}(h^2)$ approximation of $f''(x_0)$ if $f \in C^4([x_0-h, x_0+h])$.

Then we expect that

$$\begin{aligned}\widetilde{N}(h) &= N\left(\tfrac{h}{2}\right) + \frac{1}{2^2-1}\left[N\left(\tfrac{h}{2}\right) - N(h)\right] \\ &= \frac{1}{h^2}\Big[-\frac{1}{3}f(x_0+h) + \frac{16}{3}f\left(x_0+\tfrac{h}{2}\right) - 10f(x_0) + \frac{16}{3}f\left(x_0-\tfrac{h}{2}\right) \\ &\qquad -\frac{1}{3}f(x_0-h)\Big]\end{aligned}$$

is a better approximation of $f''(x_0)$. This is true when $f \in C^5([x_0 - h, x_0 + h])$.

§4.2 Richardson's Extrapolation

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

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

If $f''(\xi(x))$ is differentiable, then

$$\begin{aligned} f'(x) &= -\frac{1}{h} f(x_0) + \frac{1}{h} f(x_0+h) + \frac{\frac{d}{dx} f''(\xi(x))}{2!}(x-x_0)(x-x_0-h) \\ &\quad + \frac{2(x-x_0)-h}{2!} f''(\xi(x))\,; \end{aligned}$$

thus $f'(x_0) = \dfrac{f(x_0+h)-f(x_0)}{h} - \dfrac{h}{2!} f''(\xi(x_0))$ which shows

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

§4.2 Richardson's Extrapolation

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

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

If $f''(\xi(x))$ is differentiable, then

$$\begin{aligned} f'(x) = -\frac{1}{h} f(x_0) + \frac{1}{h} f(x_0+h) + \frac{\frac{d}{dx} f''(\xi(x))}{2!}(x-x_0)(x-x_0-h) \\ + \frac{2(x-x_0)-h}{2!} f''(\xi(x))\,; \end{aligned}$$

thus $f'(x_0) = \dfrac{f(x_0+h)-f(x_0)}{h} - \dfrac{h}{2!} f''(\xi(x_0))$ which shows

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

§4.2 Richardson's Extrapolation

In general, suppose that $x_0, x_1, \cdots, x_n \in I$ are distinct $n+1$ points 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 $\xi(x) \in I$. If $f^{(n+1)}(\xi(x))$ is differentiable, then

$$f'(x) = \sum_{k=0}^{n} f(x_k) L'_k(x) + \frac{\frac{d}{dx} f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\frac{d}{dx}\{(x-x_0)(x-x_1)\cdots(x-x_n)\}$$

which shows

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

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

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where $\xi(x) \in I$. If $f^{(n+1)}(\xi(x))$ is differentiable, then

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

which shows

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

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

§4.2 Richardson's Extrapolation

Three point formula: x_0, x_1, x_2:

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

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

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

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

Therefore,

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

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

§4.2 Richardson's Extrapolation

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$$\Rightarrow L_0'(x) = \frac{(x-x_2)+(x-x_1)}{(x_0-x_1)(x_0-x_2)} = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)},$$
$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \Rightarrow L_1'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)},$$
$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \Rightarrow L_2'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}.$$

Therefore,

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

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

§4.2 Richardson's Extrapolation

The equal spaced case $x_0, x_1 = x_0 + h, x_2 = x_0 + 2h$: Using the three point formula,

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

Therefore,

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right]+\frac{1}{3}h^2f^{(3)}(\xi_0), \quad (\star)$$
$$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h)+f(x_0+h)\right]-\frac{1}{6}h^2f^{(3)}(\xi_1),$$
$$f'(x_0) = \frac{1}{2h}\left[f(x_0-2h)-4f(x_0-h)+3f(x_0)\right]+\frac{1}{3}h^2f^{(3)}(\xi_2). \quad (\star\star)$$

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

§4.2 Richardson's Extrapolation

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

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

Therefore,

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

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

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

§4.2 Richardson's Extrapolation

- **Three-point formula:**

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

for some ξ_0 between x_0 and x_0+2h,

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

for some ξ_1 between x_0-h and x_0+h.

- **Five-point formula:**

$$f'(x_0) = \frac{1}{12h}\Big[f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)\Big] + \frac{h^4}{30}f^{(5)}(\xi) \quad \text{for some } \xi \text{ between } x_0-2h \text{ and } x_0+2h, \qquad (\diamond)$$

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

for some ξ between x_0 and x_0+4h.

§4.2 Richardson's Extrapolation

We can also apply Taylor's Theorem and extrapolation to obtain ($\diamond$): if f is 5 times continuously differentiable in the interval of interest,

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

where $\xi_\pm$ between x_0 and $x_0 \pm h$. Therefore,

$$f(x_0+h) - f(x_0-h) = 2hf'(x_0) + \frac{h^3}{3}f'''(x_0) + \frac{h^5}{120}\Big[f^{(5)}(\xi_+) + f^{(5)}(\xi_-)\Big]$$

which implies that

$$f'(x_0) = \frac{1}{2h}\Big[f(x_0+h) - f(x_0-h)\Big] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(\tilde{\xi}). \qquad (\square)$$

Replacing h by $2h$ in ($\square$), we have

$$f'(x_0) = \frac{1}{4h}\Big[f(x_0+2h) - f(x_0-2h)\Big] - \frac{4h^2}{6}f'''(x_0) - \frac{16h^4}{120}f^{(5)}(\hat{\xi}), \quad (\square\square)$$

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

§4.2 Richardson's Extrapolation

We can also apply Taylor's Theorem and extrapolation to obtain ($\diamond$): if f is 5 times continuously differentiable in the interval of interest,

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where $\xi_\pm$ between x_0 and $x_0 \pm h$. Therefore,

$$f(x_0+h) - f(x_0-h) = 2hf'(x_0) + \frac{h^3}{3}f'''(x_0) + \frac{h^5}{120}\left[f^{(5)}(\xi_+) + f^{(5)}(\xi_-)\right]$$

which implies that

$$f'(x_0) = \frac{1}{2h}\Big[f(x_0+h) - f(x_0-h)\Big] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(\tilde{\xi}). \qquad (\square)$$

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§4.2 Richardson's Extrapolation

$$f'(x_0) = \frac{1}{2h}\Big[f(x_0+h)-f(x_0-h)\Big]-\frac{h^2}{6}f'''(x_0)-\frac{h^4}{120}f^{(5)}(\tilde{\xi}), \qquad (\square)$$

$$f'(x_0) = \frac{1}{4h}\Big[f(x_0+2h)-f(x_0-2h)\Big]-\frac{4h^2}{6}f'''(x_0)-\frac{16h^4}{120}f^{(5)}(\hat{\xi}). \qquad (\square\square)$$

Cancelling out the h^4 terms: $4 \times (\square) - (\square\square)$ implies that

$$3f'(x_0) = \frac{2}{h}\Big[f(x_0+h)-f(x_0-h)\Big] - \frac{1}{4h}\Big[f(x_0+2h)-f(x_0-2h)\Big] - \frac{h^4}{30}f^{(5)}(\tilde{\xi}) + \frac{2h^4}{15}f^{(5)}(\hat{\xi}).$$

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

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

To see the exact remainder, we can apply the Cauchy Mean Value Theorem to the quotient

$$\frac{12hf'(x_0)-\Big[f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)\Big]}{12h^5}.$$

§4.3 Numerical Integration

Let $x_0, x_1, \cdots, x_n \in [a, b]$ be $n+1$ distinct nodes, and $f : [a, b] \to \mathbb{R}$ be Riemann integrable.

Goal: Find a_i's such that $\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$.

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

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

thus we expect that $a_i = \int_a^b L_i(x)dx$.

§4.3 Numerical Integration

- **Trapezoidal rule**:

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

$$\begin{aligned}
\int_a^b f(x)dx &= \int_{x_0}^{x_1} \left[\frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1)\right] dx \\
&\quad + \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)dx \\
&= \left[\frac{(x-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} f(x_1)\right]\Bigg|_{x=x_0}^{x=x_1} + \frac{f''(\xi)}{2}\int_{x_0}^{x_1}(x-x_0)(x-x_1)dx \\
&\quad \text{for some } \xi \in (x_0, x_1) \\
&= \frac{1}{2}(x_1-x_0)f(x_1) - \frac{1}{2}(x_0-x_1)f(x_0) + \frac{1}{2}f''(\xi)\left[\frac{x^3}{3} - \frac{(x_0+x_1)x^2}{2} + x_0x_1x\right]\Bigg|_{x=x_0}^{x=x_1} \\
&= \frac{1}{2}(x_1-x_0)\Big[f(x_0)+f(x_1)\Big] + \frac{1}{2}f''(\xi)\left(\frac{-1}{6}\right)(x_1-x_0)^3 \\
&= \frac{h}{2}\Big[f(x_0)+f(x_1)\Big] - \frac{1}{12}h^3 f''(\xi).
\end{aligned}$$

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

§4.3 Numerical Integration

- **Simpson's rule**:

Let $x_0 = a, x_1 = a+h, x_2 = b, h = (b-a)/2$. If $f \in C^3([x_0, x_2])$, then

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} \Big[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \Big] dx + \int_{x_0}^{x_2} \frac{f^{(3)}(\xi(x))}{3!}(x-x_0)(x-x_1)(x-x_2)dx$$

$$= \frac{h}{3}\Big[f(x_0)+4f(x_1)+f(x_2)\Big] + \int_{x_0}^{x_2} \frac{f^{(3)}(\xi(x))}{3!}(x-x_0)(x-x_1)(x-x_2)dx$$

for some $\xi \in [x_0, x_2]$; thus Simpson's Rule has $\mathcal{O}(h^4)$ error term.

§4.3 Numerical Integration

- **Alternative approach: Taylor's Theorem**

Let $x, x_1 \in [x_0, x_2]$. If $f \in C^2([x_0, x_2])$, there exists $\xi(x) \in (x_0, x_2)$ such that

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

Then

$$\int_{x_0}^{x_2} f(x)dx = \left[f(x_1)(x-x_1) + \frac{f'(x_1)}{2}(x-x_1)^2\right]\Big|_{x=x_0}^{x=x_2} + \frac{1}{2}\int_{x_0}^{x_2} f''(\xi(x))(x-x_1)^2 dx$$

and Intermediate Value Theorem implies that

$$\int_{x_0}^{x_2} f''(\xi(x))(x-x_1)^2 dx = f''(\xi_1)\int_{x_0}^{x_2}(x-x_1)^2 dx = \frac{f''(\xi_1)}{3}(x-x_1)^3\Big|_{x=x_0}^{x=x_2}$$

for some $\xi_1 \in (x_0, x_2)$. Therefore, we obtain the **Midpoint Rule**:

$$\int_{x_0}^{x_2} f(x)dx = 2hf\left(\frac{x_0+x_2}{2}\right) + \frac{h^3}{24}f''(\xi_1), \qquad h = x_2 - x_0.$$

§4.3 Numerical Integration

- **Alternative approach: Taylor's Theorem**

Similarly, if $f \in C^4([x_0, x_2])$, there exists $\xi(x) \in (x_0, x_2)$ such that

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

Then

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

and Intermediate Value Theorem implies that

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

Therefore,

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

§4.3 Numerical Integration

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

The central difference scheme

$$f''(x_1) = \frac{f(x_1+h) - 2f(x_1) + f(x_1-h)}{h^2} - \frac{f^{(4)}(\xi_2)}{12}h^2$$

then implies that

$$\begin{aligned}\int_{x_0}^{x_2} f(x)dx &= 2hf(x_1) + \frac{h^3}{3}\Big[\frac{f(x_1+h)-2f(x_1)+f(x_1-h)}{h^2} - \frac{f^{(4)}(\xi_2)}{12}h^2\Big] \\ &\quad + \frac{f^{(4)}(\xi_1)}{120} \cdot 2h^5 \\ &= \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2)\Big] - \frac{h^5}{12}\Big[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\Big] \\ &\text{``}=\text{''} \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2)\Big] - \frac{h^5}{90}f^{(4)}(\xi)\end{aligned}$$

for some $\xi \in (x_0, x_2)$. This gives Simpson's Rule for numerical integration.

§4.3 Numerical Integration

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

The central difference scheme

$$f''(x_1) = \frac{f(x_1+h) - 2f(x_1) + f(x_1-h)}{h^2} - \frac{f^{(4)}(\xi_2)}{12} h^2$$

then implies that

$$\begin{aligned}
\int_{x_0}^{x_2} f(x)dx &= 2hf(x_1) + \frac{h^3}{3}\left[\frac{f(x_1+h)-2f(x_1)+f(x_1-h)}{h^2} - \frac{f^{(4)}(\xi_2)}{12} h^2\right] \\
&\quad + \frac{f^{(4)}(\xi_1)}{120} \cdot 2h^5 \\
&= \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2)\Big] - \frac{h^5}{12}\left[\frac{1}{3} f^{(4)}(\xi_2) - \frac{1}{5} f^{(4)}(\xi_1)\right] \\
&\text{``=''}\ \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2)\Big] - \frac{h^5}{90} f^{(4)}(\xi)
\end{aligned}$$

for some $\xi \in (x_0, x_2)$. This gives Simpson's Rule for numerical integration.

§4.3 Numerical Integration

To see the "correct" error bound for Simpson's rule, we let F be an anti-derivative of f and consider the error function

$$g(h) = \int_{x_1-h}^{x_1+h} f(x)\,dx - \frac{h}{3}\left[f(x_1-h)+4f(x_1)+f(x_1+h)\right].$$

Then $g(0) = g'(0) = g''(0) = g'''(0) = 0$; thus the Cauchy Mean Value Theorem implies that

$$\frac{g(h)}{h^5} = \frac{g'(h_1)}{5h_1^4} = \frac{g''(h_2)}{20h_2^3} = \frac{g'''(h_3)}{60h_3^2} = -\frac{f'''(x_1+h_3) - f'''(x_1-h_3)}{180h_3}$$
$$= -\frac{f^{(4)}(\xi)}{90}$$

for some ξ between 0 and h; thus $g(h) = -\dfrac{f^{(4)}(\xi)}{90}h^5$.

§4.3 Numerical Integration

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

§4.3 Numerical Integration

Composite numerical integration:

1. Large integration interval $\Longrightarrow$ large h $\Longrightarrow$ inaccurate; small h $\Longrightarrow$ high-degree polynomial $\Longrightarrow$ inaccurate.
2. Idea: piecewise approach + low-order Newton-cotes formulas.

Composite Simpson's rule: Let n be an even integer. Divide $[a, b]$ into n sub-intervals with equal length and define $h = \dfrac{b-a}{n}$ as well as $x_j = a + jh$ for $j = 0, 1, \cdots, n$. Then

$$\begin{aligned}\int_a^b f(x)dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx \\ &= \sum_{j=1}^{n/2} \left\{ \frac{h}{3}\Big[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\Big] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\}\end{aligned}$$

§4.3 Numerical Integration

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$$\int_a^b f(x)dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx$$

$$= \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2) + f(x_2) + 4f(x_3) + f(x_4)$$

$$+ \cdots + f(x_{n-2} + 4f(x_{n-1}) + f(x_n)\Big] - \frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

§4.3 Numerical Integration

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

§4.3 Numerical Integration

$$\int_a^b f(x)dx = \frac{h}{3}\Big[f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\Big] - \frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

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

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

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

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

here we have used $h = \frac{b-a}{n}$ to conclude the last equality.

§4.3 Numerical Integration

$$\int_a^b f(x)dx = \frac{h}{3}\Big[f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\Big] - \frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

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

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

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

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

here we have used $h = \frac{b-a}{n}$ to conclude the last equality.

§4.3 Numerical Integration

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

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here we have used $h = \dfrac{b-a}{n}$ to conclude the last equality.

§4.3 Numerical Integration

Example (Composite Simpson's rule)

Find $\int_0^4 e^x\,dx$ using Simpson's rule. We note that the exact value of this integral is $e^4 - 1 = 53.59815...$.

- $(h = 2)$: $\int_0^4 e^x dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958...$
- $(h = 1)$:
$$\int_0^4 e^x dx = \int_0^2 e^x dx + \int_2^4 e^x dx$$
$$\approx \frac{1}{3}(e^0 + 4e^1 + e^2) + \frac{1}{3}(e^2 + 4e^3 + e^4) = 53.86385\cdots.$$
- $(h = 1/2)$:
$$\int_0^4 e^x dx = \int_0^1 e^x dx + \cdots + \int_3^4 e^x dx$$
$$\approx \frac{1}{6}(e^0 + 4e^{0.5} + e^1) + \cdots + \frac{1}{6}(e^3 + 4e^{3.5} + e^4)$$
$$= 53.61622\cdots.$$

§4.3 Numerical Integration

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 there 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 there exists $\mu \in (a,b)$ such that

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

§4.3 Numerical Integration

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

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

§4.4 Gauss Quadrature

1. Previous quadrature formula of numerical integration use values of function at equally spaced points.
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 $i = 1, 2, \cdots, n$. There are $2n$ parameters to choose, so the greatest degree of precision $\leqslant 2n - 1$.

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$(f) \leqslant 3\,(= 2n - 1)$; that is, gives exact value when $f(x) = 1, x, x^2, x^3$.

§4.4 Gauss Quadrature

Example (Cont'd)

The quadrature formula gives exact value for $f(x) = 1, x, x^2, x^3$:

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

Solving for c_1, c_2, x_1, x_2, (assuming $x_1 < x_2$) we obtain that

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

thus the 2-point Gauss quadrature formula is

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

This formula has degree of precision 3.

§4.4 Gauss Quadrature

Definition

The Legendre polynomial of degree n is the polynomial

$$p_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}\left[(x^2-1)^n\right].$$

- Some Legendre polynomials are given by

$$p_0(x) = 1, \qquad p_1(x) = x, \qquad p_2(x) = \frac{1}{2}(3x^2-1),$$
$$p_3(x) = \frac{1}{2}(5x^3-3x), \quad p_4(x) = \frac{1}{8}(35x^4-30x^2+3), \quad \cdots$$

- 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 less than n.
- The roots of $p_n(x)$ are distinct, lie in $(-1,1)$, and have a symmetry with respect to 0.

§4.4 Gauss Quadrature

- $\int_{-1}^{1} p(x)p_n(x)dx = 0$ if p is a polynomial of degree less than n.

Proof.

Since p_n is a polynomial of degree n, $\{p_0, p_1, \cdots, p_n\}$ is linearly independent. If p is a polynomial of degree less than n, then

$$p(x) = c_0 p_0(x) + c_1 p_1(x) + \cdots + c_{n-1} p_{n-1}(x)$$

for some constants $c_0, c_1, \cdots, c_{n-1}$. Therefore, it suffices to show that $\int_{-1}^{1} p_k(x)p_n(x)\,dx = 0$ for all $0 \leqslant k \leqslant n$. Note that

$$\frac{d^{n-j}}{dx^{n-1}}\Big|_{x=\pm 1}(x^2-1)^n = 0 \quad \text{for all } 1 \leqslant j \leqslant n.$$

Integrating by parts, we find that for $1 \leqslant j \leqslant n$,

$$\begin{aligned}\int_{-1}^{1} p_k(x)p_n(x)\,dx &= \frac{1}{2^{n+k}n!k!}\int_{-1}^{1}\frac{d^k}{dx^k}(x^2-1)^k\frac{d^n}{dx^n}(x^2-1)^n\,dx \\ &= \frac{(-1)^j}{2^{n+k}n!k!}\int_{-1}^{1}\frac{d^{k+j}}{dx^{k+j}}(x^2-1)^k\frac{d^{n-j}}{dx^{n-j}}(x^2-1)^n\,dx = 0\,.\end{aligned}$$

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□

§4.4 Gauss Quadrature

- The roots of $p_n(x)$ are distinct, lie in $(-1, 1)$.

Proof.

Assume the contrary that p_n has m pairwise different zeroes x_1, x_2, $\cdots$, x_m of **odd multiplicity** in $(-1, 1)$ (that is, p_n changes sign in x_j for $j = 1, 2, \cdots, m$) with $0 \leqslant m < n$. Since $\int_{-1}^{1} p_n(x)\, dx = 0$, we must have $m \geqslant 1$. Consider the polynomial $z(x) = (x - x_1)(x - x_2)\cdots(x - x_m)$. Then

1. The function $f(x) = z(x)p_n(x)$ is sign-definite in $(-1, 1)$; thus $\int_{-1}^{1} z(x)p_n(x)\, dx \neq 0$.
2. $\int_{-1}^{1} z(x)p_n(x)\, dx = 0$ since $\text{degree}(z) < n$.

Clearly ① and ② contradict each other; thus we conclude that the roots of p_n are distinct and lie in $(-1, 1)$. □

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§4.4 Gauss Quadrature

Theorem

Let $x_0, x_1, x_2, \cdots, x_n$ be roots of the Legendre polynomial p_{n+1}, and $L_{n,i}$ be the Lagrange polynomial of degree n satisfying $L_{n,i}(x_j) = \delta_{ij}$. If p is a polynomial and $degree(p) < 2(n+1)$, then

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

where $c_i = \displaystyle\int_{-1}^{1} L_{n,i}(x)\, dx$.

Recall that for given $n+1$ distinct points $x_0, x_1, \cdots, x_n$, the Lagrange polynomial $L_{n,i}$ is a polynomial of degree n defined by

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

Any polynomial p of degree n can be expressed as

$$p(x) = \sum_{i=0}^{n} L_{n,i}(x) p(x_i).$$

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§4.4 Gauss Quadrature

Proof.

Let p be a polynomial of degree $< 2(n+1)$. Then the division algorithm implies that

$$p(x) = q(x)p_{n+1}(x) + r(x)\,,$$

where q, r are polynomials satisfying degree$(q) \leqslant n$ and degree$(r) \leqslant n$. Since r is a polynomial of degree $\leqslant n$,

$$r(x) = \sum_{i=0}^{n} L_{n,i}(x) r(x_i) = \sum_{i=0}^{n} L_{n,i}(x) p(x_i)\,.$$

Therefore,

$$p(x) = q(x)p_{n+1}(x) + \sum_{i=0}^{n} L_{n,i}(x) p(x_i);$$

thus the fact that $\int_{-1}^{1} q(x)p_{n+1}(x)\,dx = 0$ further implies that

$$\int_{-1}^{1} p(x)\,dx = \sum_{i=0}^{n}\Big(\int_{-1}^{1} L_{n,i}(x)\,dx\Big)p(x_i) = \sum_{i=0}^{n} c_i p(x_i)\,. \qquad \square$$

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§4.4 Gauss Quadrature

Remark: To find $\int_a^b f(x)\,dx$, we make the substitution of variable

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

and find that

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

Example

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