6. Numerical Differentiation

Given: $f_i = f(x_i)$ for $i = 0,1,2,\cdots,N$

Find: An approximation of $f'(x)$ or $f'(x_i)$

§ Polynomial approximation

Step 1: approximate $f(x)$ by the polynomial of degree N

$$f(x) = \sum_{j=0}^{N} f_j L_{N,j}(x) + \frac{1}{(N+1)!} f^{(N+1)}(\xi(x)) \cdot \prod_{j=0}^{N}(x - x_j)$$

Step 2: take derivative with respect to x:

$$f'(x) = \sum_{j=0}^{N} f_j L'_{N,j}(x) + \frac{1}{(N+1)!}\frac{d}{dx}\left\{ f^{(N+1)}(\xi(x))\right\} \cdot \prod_{j=0}^{N}(x - x_j)$$

$$+ \frac{1}{(N+1)!} f^{(N+1)}(\xi(x)) \cdot \frac{d}{dx}\left\{\prod_{j=0}^{N}(x - x_j)\right\}$$

In particular, at $x = x_k$,

$$f'(x_k) = \sum_{j=0}^{N} f_j L'_{N,j}(x_k) + \frac{1}{(N+1)!}\frac{d}{dx}\left\{ f^{(N+1)}(\xi(x))\right\}_{x=x_k} \cdot \cancel{\prod_{j=0}^{N}(x_k - x_j)}$$

$$+ \frac{1}{(N+1)!} f^{(N+1)}(\xi(x_k)) \cdot \frac{d}{dx}\left\{\prod_{j=0}^{N}(x - x_j)\right\}_{x=x_k}$$

In remark, one may approximate $f'(x_k) \approx \sum_{j=0}^{N} f_j L'_{N,j}(x_k)$

with a truncation error $E_{tr} = \frac{1}{(N+1)!} f^{(N+1)}(\xi(x_k)) \cdot \prod_{\substack{j=0 \\ j\neq k}}^{N}(x_k - x_j)$

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§ Polynomial approximation

example: $N+1=3,\quad \{x_0, x_1, x_2\} = \{x_0, x_0+h, x_0+2h\}$

$$\left.\begin{aligned} L_{N,0}(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \\ L_{N,1}(x) &= \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \\ L_{N,2}(x) &= \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \end{aligned}\right\} \quad \begin{aligned} L'_{N,0}(x) &= \frac{(x-x_1)+(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-x_1)+(x-x_2)}{2h^2} \\ L'_{N,1}(x) &= \frac{(x-x_0)+(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-x_0)+(x-x_2)}{-h^2} \\ L'_{N,2}(x) &= \frac{(x-x_0)+(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-x_0)+(x-x_1)}{2h^2} \end{aligned}$$

Therefore,

$$f'(x_0) \approx \sum_{j=0}^{2} f_j L'_{N,j}(x_0) = f_0 \cdot \frac{-3h}{2h^2} + f_1 \cdot \frac{-2h}{-h^2} + f_2 \cdot \frac{-h}{2h^2} = \frac{1}{h}\left(-\frac{3}{2} f_0 + 2 f_1 - \frac{1}{2} f_2\right)$$

$$f'(x_1) \approx \sum_{j=0}^{2} f_j L'_{N,j}(x_1) = f_0 \cdot \frac{-h}{2h^2} + f_1 \cdot \frac{0}{-h^2} + f_2 \cdot \frac{h}{2h^2} = \frac{1}{2h}(f_2 - f_0)$$

---

truncation error $E_{tr} = \frac{1}{(N+1)!} f^{(N+1)}(\xi(x_k)) \cdot \prod_{\substack{j=0 \\ j\neq k}}^{N}(x_k - x_j)$

$$E_{tr}(x_0) = \frac{1}{3!} f^{(3)}(\xi(x_0)) \cdot \prod_{j=1}^{2}(x_0 - x_j)$$

$$= \frac{1}{6} f^{(3)}(\xi(x_0)) \cdot (x_0 - x_1)(x_0 - x_2)$$

$$= \frac{h^2}{3} f^{(3)}(\xi(x_0)) = O(h^2)$$ ~ 2nd order accuracy

$$E_{tr}(x_1) = \frac{1}{3!} f^{(3)}(\xi(x_1)) \cdot \prod_{\substack{j=0 \\ j\neq 1}}^{N}(x_1 - x_j)$$

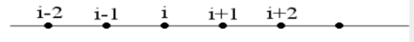
$$= \frac{1}{6} f^{(3)}(\xi(x_1)) \cdot (x_1 - x_0)(x_1 - x_2)$$

$$= -\frac{h^2}{6} f^{(3)}(\xi(x_1)) = O(h^2)$$

§ Finite Difference Approximation

Given: $f_i = f(x_i)$ for $x_i = a + i \times (b-a)/N, \quad i = 0,1,2,\cdots,N$

Find: $f'(x_i)$



Step 1: Taylor series expansion $f(x)$ about $x = x_i$

$$f(x) = f(x_i) + (x - x_i)\cdot f'(x_i) + \frac{1}{2}(x - x_i)^2 \cdot f''(x_i) + \frac{1}{6}(x - x_i)^3 \cdot f^{(3)}(x_i) + \frac{1}{24}(x - x_i)^4 \cdot f^{(4)}(x_i) + \cdots$$

$$f(x_{i+1}) = f_{i+1} = f_i + h \cdot f'(x_i) + \frac{1}{2}h^2 \cdot f''(x_i) + \frac{1}{6}h^3 \cdot f^{(3)}(x_i) + \frac{1}{24}h^4 \cdot f^{(4)}(x_i) + \cdots$$

(a) $$f(x_{i+1}) = f_{i+1} = f_i + h \cdot f'(x_i) + \frac{1}{2}h^2 \cdot f''(x_i) + \frac{1}{6}h^3 \cdot f^{(3)}(x_i) + \frac{1}{24}h^4 \cdot f^{(4)}(x_i) + \cdots$$

(b) $$f(x_{i-1}) = f_{i-1} = f_i - h \cdot f'(x_i) + \frac{1}{2}h^2 \cdot f''(x_i) - \frac{1}{6}h^3 \cdot f^{(3)}(x_i) + \frac{1}{24}h^4 \cdot f^{(4)}(x_i) + \cdots$$

From (a) or (b) or both

(a): $f_{i+1} - f_i = h \cdot f'(x_i) + \frac{1}{2}h^2 \cdot f''(x_i) + \cdots$

(b): $f_{i-1} - f_i = -h \cdot f'(x_i) + \frac{1}{2}h^2 \cdot f''(x_i) + \cdots$

(a) - (b): $f_{i+1} - f_{i-1} = 2h \cdot f'(x_i) + \frac{1}{3}h^3 \cdot f^{(3)}(x_i) + \cdots$

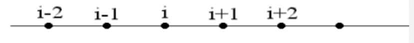
§ Finite Difference Approximation

(i) forward difference: $f'(x_i) = \dfrac{f_{i+1} - f_i}{h} - \dfrac{1}{2}h \cdot f''(x_i) + O(h^2)$

(ii) backward difference: $f'(x_i) = \dfrac{f_i - f_{i-1}}{h} + \dfrac{1}{2}h \cdot f''(x_i) + O(h^2)$

(iii) central difference: $f'(x_i) = \dfrac{f_{i+1} - f_{i-1}}{2h} \underbrace{- \dfrac{1}{6}h^2 \cdot f^{(3)}(x_i) + O(h^4)}_{\text{truncation error}}$

Using more points



(c): $$f(x_{i+2}) = f_{i+2} = f_i + 2h \cdot f'(x_i) + \frac{1}{2}\cdot 4h^2 \cdot f''(x_i) + \frac{1}{6}\cdot 8h^3 \cdot f^{(3)}(x_i) + \frac{1}{24}\cdot 16h^4 \cdot f^{(4)}(x_i) + \cdots$$

(d): $$f(x_{i-2}) = f_{i-2} = f_i - 2h \cdot f'(x_i) + \frac{1}{2}\cdot 4h^2 \cdot f''(x_i) - \frac{1}{6}\cdot 8h^3 \cdot f^{(3)}(x_i) + \frac{1}{24}\cdot 16h^4 \cdot f^{(4)}(x_i) + \cdots$$

(c) − (d): $f_{i+2} - f_{i-2} = 4h \cdot f'(x_i) + \frac{8}{3}\cdot h^3 \cdot f^{(3)}(x_i) + \cdots$

$$\text{(iv)}\quad f'(x_i)=\frac{f_{i+1}-f_{i-2}}{4h}\underbrace{-\frac{2}{3}h^2\cdot f^{(3)}(x_i)+O(h^4)}_{\text{truncation error}}$$

$$\text{(iii) central difference:}\quad f'(x_i)=\frac{f_{i+1}-f_{i-1}}{2h}\underbrace{-\frac{1}{6}h^2\cdot f^{(3)}(x_i)+O(h^4)}_{\text{truncation error}}$$

$$4\times\text{(iii)}-\text{(iv)}:\quad 3f'(x_i)=4\cdot\frac{f_{i+1}-f_{i-1}}{2h}-\frac{f_{i+2}-f_{i-2}}{4h}+O(h^4)$$

$$\Rightarrow\quad f'(x_i)=\frac{f_{i-2}-8f_{i-1}+8f_{i+1}-f_{i+2}}{12h}+O(h^4)$$

---

§ Finite Difference Approximation

- second derivatives:

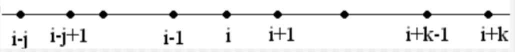
$$f_{i+1}=f_i+h\cdot f'(x_i)+\frac{1}{2}h^2\cdot f''(x_i)+\frac{1}{6}h^3\cdot f^{(3)}(x_i)+\frac{1}{24}h^4\cdot f^{(4)}(x_i)+\cdots$$

$$f_{i-1}=f_i-h\cdot f'(x_i)+\frac{1}{2}h^2\cdot f''(x_i)-\frac{1}{6}h^3\cdot f^{(3)}(x_i)+\frac{1}{24}h^4\cdot f^{(4)}(x_i)+\cdots$$

$$f_{i+1}+f_{i-1}=2f_i+h^2\cdot f''(x_i)+\frac{1}{12}h^4\cdot f^{(4)}(x_i)+O(h^6)$$

$$f''(x_i)=\frac{f_{i+1}-2f_i+f_{i-1}}{h^2}\underbrace{-\frac{1}{12}h^2\cdot f^{(4)}(x_i)+O(h^6)}_{\text{truncation error}}$$

IN GENERAL (e.g. higher order derivatives or higher order accuracy or even non-uniformly spaced grids)



- Select ***j*** points from LHS and ***k*** points from RHS to form the forumla:

$$f^{(m)}(x_i)=\alpha_{-j}f_{i-j}+\alpha_{-j+1}f_{i-j+1}+\cdots+\alpha_0 f_i+\cdots+\alpha_{k-1}f_{i+k-1}+\alpha_k f_{i+k}$$

$$\#\text{ of }\alpha\text{'s (degrees of freedom)}=(j+1+k);\quad \alpha\propto h^{-m}$$

- Taylor – seriers expand all f_j except f_i to obtain:

$$=\beta_0 f_i+\beta_1 f'(x_i)+\cdots+\beta_m f^{(m)}(x_i)+\cdots+\beta_{j+k}f^{(j+k)}(x_i)+O(\alpha h^{j+k+1})$$

$$\beta_i=\beta_i(\alpha)$$

$$f^{(m)}(x_i)\approx\alpha_{-j}f_{i-j}+\alpha_{-j+1}f_{i-j+1}+\cdots+\alpha_0 f_i+\cdots+\alpha_{k-1}f_{i+k-1}+\alpha_k f_{i+k}$$
$$=\beta_0 f_i+\beta_1 f'(x_i)+\cdots+\beta_m f^{(m)}(x_i)+\cdots+\beta_{j+k}f^{(j+k)}(x_i)+O(\alpha h^{j+k+1})$$

- choose $\{\alpha_i\}_{i=-j}^{k}$ such that

$$\begin{cases}\beta_m=1\\ \beta_i=0\quad\text{for } i=0,1,\cdots,j+k;\ \ i\neq m\end{cases}$$

- dimensional consistency: $\alpha_i=O(1/h^m)$

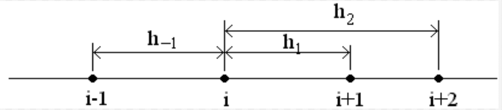
$$f^{(m)}(x_i)\approx\alpha_{-j}f_{i-j}+\alpha_{-j+1}f_{i-j+1}+\cdots+\alpha_0 f_i+\cdots+\alpha_{k-1}f_{i+k-1}+\alpha_k f_{i+k}$$

$$=f^{(m)}(x_i)+O(\alpha h^{j+k+1})=f^{(m)}(x_i)+O(h^{j+k+1-m})$$

order $= j+k+1-m$

example: $m = 2, j = 1,$ and $k = 2$

$$f''(x_i) = \alpha_{-1} f_{i-1} + \alpha_0 f_i + \alpha_1 f_{i+1} + \alpha_2 f_{i+2}$$



define $h_{-1} = |x_{i-1} - x_i|$, $h_1 = |x_{i+1} - x_i|$, $h_2 = |x_{i+2} - x_i|$

$$f_{i-1} = f(x_{i-1}) = f(x_i - h_{-1}) = f_i - h_{-1} f_i' + \frac{h_{-1}^2}{2} f_i'' - \frac{h_{-1}^3}{6} f_i''' + O(h^4)$$

$$f_{i+1} = f(x_{i+1}) = f(x_i + h_1) = f_i + h_1 f_i' + \frac{h_1^2}{2} f_i'' + \frac{h_1^3}{6} f_i''' + O(h^4)$$

$$f_{i+2} = f(x_{i+2}) = f(x_i + h_2) = f_i + h_2 f_i' + \frac{h_2^2}{2} f_i'' + \frac{h_2^3}{6} f_i''' + O(h^4)$$

$$f''(x_i) = \alpha_{-1} f_{i-1} + \alpha_0 f_i + \alpha_1 f_{i+1} + \alpha_2 f_{i+2}$$

$$= \alpha_{-1} \left\{ f_i - h_{-1} f_i' + \frac{h_{-1}^2}{2} f_i'' - \frac{h_{-1}^3}{6} f_i''' + O(h^4) \right\}$$

$$+ \alpha_0 f_i$$

$$+ \alpha_1 \left\{ f_i + h_1 f_i' + \frac{h_1^2}{2} f_i'' + \frac{h_1^3}{6} f_i''' + O(h^4) \right\}$$

$$+ \alpha_2 \left\{ f_i + h_2 f_i' + \frac{h_2^2}{2} f_i'' + \frac{h_2^3}{6} f_i''' + O(h^4) \right\}$$

$$= \overset{\beta_0 = 0}{\boxed{(\alpha_{-1} + \alpha_0 + \alpha_1 + \alpha_2)}} f_i + \overset{\beta_1 = 0}{\boxed{(-\alpha_{-1} h_{-1} + \alpha_1 h_1 + \alpha_2 h_2)}} f_i'$$

$$+ \overset{\beta_2 = 1}{\boxed{\frac{(\alpha_{-1} h_{-1}^2 + \alpha_1 h_1^2 + \alpha_2 h_2^2)}{2}}} f_i'' + \overset{\beta_3 = 0}{\boxed{\frac{(-\alpha_{-1} h_{-1}^3 + \alpha_1 h_1^3 + \alpha_2 h_2^3)}{2}}} f_i''' + O(\alpha h^4)$$

$$f''(x_i) = \alpha_{-1} f_{i-1} + \alpha_0 f_i + \alpha_1 f_{i+1} + \alpha_2 f_{i+2} + O(\alpha h^4) \quad \text{if}$$

$$\begin{cases} \beta_0 = \alpha_{-1} + \alpha_0 + \alpha_1 + \alpha_2 = 0 \\ \beta_1 = -\alpha_{-1} h_{-1} + \alpha_1 h_1 + \alpha_2 h_2 = 0 \\ \beta_2 = \dfrac{\alpha_{-1} h_{-1}^2 + \alpha_1 h_1^2 + \alpha_2 h_2^2}{2} = 1 \\ \beta_3 = -\alpha_{-1} h_{-1}^3 + \alpha_1 h_1^3 + \alpha_2 h_2^3 = 0 \end{cases} \quad O(h^2) \quad \to \alpha \sim O(h^{-2})$$

- special case: uniformly spaced nodes: $h_{-1} = h_1 = h$ and $h_2 = 2h$

$$\begin{cases} \alpha_{-1} + \alpha_0 + \alpha_1 + \alpha_2 = 0 \\ -\alpha_{-1} + \alpha_1 + 2\alpha_2 = 0 \\ \alpha_{-1} + \alpha_1 + 4\alpha_2 = 2/h^2 \\ -\alpha_{-1} + \alpha_1 + 8\alpha_2 = 0 \end{cases} \Rightarrow \begin{cases} \alpha_{-1} = 1/h^2 \\ \alpha_0 = -2/h^2 \\ \alpha_1 = 1/h^2 \\ \alpha_2 = 0 \end{cases}$$

(central difference)

$$f''(x_i) = \frac{f_{i-1} - 2 f_i + f_{i+1}}{h^2} + O(h^2)$$

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§ Finite Difference Approximation

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2)$$

- unavoidable rounding error: $f_{i+1} = fl(f_{i+1}) + e_{i+1}$

$$f_{i-1} = fl(f_{i-1}) + e_{i-1}$$

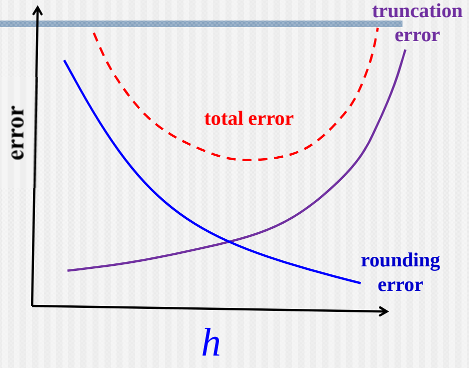
$$\text{output}(f_i') = \frac{fl(f_{i+1}) - fl(f_{i-1})}{2h} = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{e_{i+1} - e_{i-1}}{2h}$$

$$= f_i' + O(h^2) - \frac{e_{i+1} - e_{i-1}}{2h}$$

= exact value + truncation error + rounding error

↓ as h ↓ ↑ as h ↓

§ Finite Difference Approximation



§ Numerical Integration

Given: $\{(x_i, f_i)\}_{i=1}^{N}$ Want: $I=\int_a^b f(x)\,dx$

- polynomial approximation (global)

$$f(x)\approx P_{N-1}(x)=\sum_{i=1}^{N} f_i L_{N-1,i}(x)$$

$$I=\int_a^b f(x)\,dx\approx\sum_{i=1}^{N} f_i\int_a^b L_{N-1,i}(x)\,dx\ =\sum_{i=1}^{N} c_i f_i$$

$$c_i\equiv\int_a^b L_{N-1,i}(x)\,dx$$

§ Numerical Integration --- given $f(x)$ for $a\leqq x\leqq b$

$$I=\int_a^b f(x)\,dx\approx\sum_{i=1}^{N} c_i f(x_i)$$

Question: What a choice of the nodes $\{x_i\}_{i=1}^{N}$ and a choice of the

coefficients $\{c_i\}_{i=1}^{N}$ will give a "best" approximation?

- A “best” choice is recognized as the one that produces the exact result for the largest class of polynomials, Π(*R*).

For any $f(x)\in\Pi(R)$, then $I=\int_a^b f(x)\,dx=\sum_{i=1}^{N} c_i f(x_i)$ instead of "≈"

§ Numerical Integration --- given $f(x)$ for $a\leqq x\leqq b$

$$I=\int_a^b f(x)\,dx\approx\sum_{i=1}^{N} c_i f(x_i)$$

- degrees of freedom = 2*N*
- candidate of the largest class of polynomials : $\Pi_{2N-1}(R)$

  i.e. polynomials of degree $\leqq 2N-1$

$$P_{2N-1}(x)=a_{2N-1}x^{2N-1}+a_{2N-2}x^{2N-2}+\cdots+a_1x+a_0\ =\sum_{m=0}^{2N-1} a_m x^m$$

$$\int_a^b P_{2N-1}(x)\,dx=\sum_{i=1}^{N} c_i P_{2N-1}(x_i)$$

$$\sum_{m=0}^{2N-1}\int_a^b a_m x^m dx=\sum_{i=1}^{N} c_i\left(\sum_{m=0}^{2N-1} a_m x_i^m\right)$$

$$\sum_{m=0}^{2N-1} a_m \left(\int_a^b x^m dx \right) = \sum_{m=0}^{2N-1} a_m \left(\sum_{i=1}^{N} c_i x_i^m \right)$$

"=" must hold for arbitrary a_m, m=0,1,…,2N–1

$$\sum_{i=1}^{N} c_i x_i^m = \int_a^b x^m dx = \frac{b^{m+1} - a^{m+1}}{m+1}$$

for $m = 0,1,2,\cdots,2N-1$

~ 2N nonlinear equations for 2N unknowns ~

- With the solutions of the above system of equations, we intend to approximate
$$I = \int_a^b f(x)dx \approx \sum_{i=1}^{N} c_i f(x_i)$$
for any given function $f(x)$.

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§ Alternative way to solve $\{x_i\}_{i=1}^{N}$ and $\{c_i\}_{i=1}^{N}$

Let $f(x) \in \Pi_{2N-1}(R)$ and $f(x_i) = f_i$. Then $f(x)$ can be written as

$$f(x) = P_{N-1}(x) + \phi_N(x) \sum_{m=0}^{N-1} \alpha_m x^m$$

$$\phi_N(x) = \prod_{i=1}^{N} (x - x_i)$$

$$P_{N-1}(x) = \sum_{i=1}^{N} f(x_i) \cdot L_{N-1,i}(x) = \sum_{i=1}^{N} f(x_i) \cdot \frac{\phi_N(x)}{(x - x_i)\phi'_N(x_i)}$$

= the unique polynomial of degree N–1 passing through the N points

$$\phi'_N(x) = \sum_{k=1}^{N} \prod_{\substack{j=1 \\ j \neq k}}^{N} (x - x_j) \quad \Rightarrow \quad \phi'_N(x_i) = \sum_{k=1}^{N} \prod_{\substack{j=1 \\ j \neq k}}^{N} (x_i - x_j) = \prod_{\substack{j=1 \\ j \neq i}}^{N} (x_i - x_j)$$

" best choice" : $\sum_{i=1}^{N} c_i f(x_i) = \int_a^b f(x)dx$

$$= \int_a^b P_{N-1}(x)dx + \int_a^b \left(\sum_{m=0}^{N-1} \alpha_m x^m \right) \phi_N(x)dx$$

Without loss of generality, we assume [a,b]=[–1,1].

$$\sum_{i=1}^{N} c_i f(x_i) = \int_{-1}^{1} \sum_{i=1}^{N} f(x_i) \cdot \frac{\phi_N(x)}{(x - x_i)\phi'_N(x_i)} dx + \int_{-1}^{1} \left(\sum_{m=0}^{N-1} \alpha_m x^m \right) \phi_N(x)dx$$

$$= \sum_{i=1}^{N} f(x_i) \cdot \int_{-1}^{1} \frac{\phi_N(x)}{(x - x_i)\phi'_N(x_i)} dx + \int_{-1}^{1} \left(\sum_{m=0}^{N-1} \alpha_m x^m \right) \phi_N(x)dx$$

$$= \sum_{i=1}^{N} c_i f(x_i) + \boxed{\int_{-1}^{1} \left(\sum_{m=0}^{N-1} \alpha_m x^m \right) \phi_N(x)dx}$$

$= 0$ for any polynomial of deg ree $\leq N-1$

$\Rightarrow$ $\phi_N(x)$ is the N^{th} polynomial that is orthogonal to

all polynomials of degree $\leq N-1$

$\Rightarrow$ $\phi_N(x)$ is the Legendre polynomial of degree N

§ Gaussian-Legendre quadrature method (–1 $\leqq x \leqq$ 1)

For any arbitrary given function $f(x)$:

$$I = \int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{N} c_i f(x_i)$$

$$\phi_N(x) = \prod_{i=1}^{N} (x - x_i) = L_N(x) \text{ (Legendre polynomial)}$$

$$c_i = \int_{-1}^{1} \frac{L_N(x)}{(x - x_i)L'_N(x_i)} dx$$

- "=" instead of "$\approx$" when $f(x)$ is a polynomial of degree $\leq 2N-1$

§ Legendre polynomials $L_N(x)$

- a polynomial of degree N
- $L_0(x)=1$

  $L_1(x)=x$

  $L_2(x)=\frac{3}{2}x^2-\frac{1}{2}$

  $nL_n(x)=(2n-1)xL_{n-1}(x)-(n-1)L_{n-2}(x)$
- orthogonal to any polynomial of degree $\le N-1$

  $$\int_{-1}^{1}P_{N-1}(x)L_N(x)dx=0$$
- $\int_{-1}^{1}L_n(x)L_m(x)dx=\frac{2}{2n+1}\delta_{nm}$

$$nL_n(x)=(2n-1)xL_{n-1}(x)-(n-1)L_{n-2}(x)$$

$$L_n(x)=a_nx^n+a_{n-1}x^{n-1}+\cdots+a_1x+a_0$$

$$L_{n-1}(x)=b_{n-1}x^{n-1}+b_{n-2}x^{n-2}+\cdots+b_1x+b_0$$

$$L_{n-2}(x)=c_{n-2}x^{n-2}+c_{n-3}x^{n-3}+\cdots+c_1x+c_0$$

$$n\left(a_nx^n+a_{n-1}x^{n-1}+\cdots+a_1x+a_0\right)$$

$$=\begin{Bmatrix}(2n-1)\left(b_{n-1}x^n+b_{n-2}x^{n-1}+\cdots+b_1x^2+b_0x\right)\\ -(n-1)\left(c_{n-2}x^{n-2}+c_{n-3}x^{n-3}+\cdots+c_1x+c_0\right)\end{Bmatrix}$$

$$n\left(a_nx^n+a_{n-1}x^{n-1}+\cdots+a_1x+a_0\right)=\begin{Bmatrix}(2n-1)\left(b_{n-1}x^n+b_{n-2}x^{n-1}+\cdots+b_1x^2+b_0x\right)\\ -(n-1)\left(c_{n-2}x^{n-2}+c_{n-3}x^{n-3}+\cdots+c_1x+c_0\right)\end{Bmatrix}$$

$x^n:\quad na_n=(2n-1)b_{n-1}$

$x^{n-1}:\quad na_{n-1}=(2n-1)b_{n-2}$

$x^{n-2}:\quad na_{n-2}=(2n-1)b_{n-3}-(n-1)c_{n-2}$

$x^k:\quad na_k=(2n-1)b_{k-1}-(n-1)c_k\quad\text{for }1\le k\le n-2$

$x^0:\quad na_0=-(n-1)c_0$

```
REAL*8 :: A(0:N),B(0:N),C(0:N-1)
C(0)=0
C(1)=1
B(0)=-0.5d0
B(1)=0
B(2)=1.5d0
```

$L_1(x)$

$L_2(x)$

```
DO m=3,N
   tmpB=2d0*DBLE(m)-1d0
   tmpC=DBLE(m)-1d0
   A(m)=tmpB*B(m-1)
   A(m-1)=tmpB*B(m-2)
   DO k=m-2,1,-1
      A(k)=tmpB*B(k-1)-tmpC*C(k)
   ENDDO
   A(0)=-tmpC*C(0)
   C(0:m-1)=B(0:m-1)
   B(0:m)=A(0:m)/DBLE(m)
ENDDO
A(0:N)=B(0:N)
```

$ma_m=(2m-1)b_{m-1}$

$ma_{m-1}=(2m-1)b_{m-2}$

$ma_k=(2m-1)b_{k-1}-(m-1)c_k$

$ma_0=-(m-1)c_0$

$$c_i = \int_{-1}^{1} \frac{L_N(x)}{(x-x_i)L_N'(x_i)}dx$$

- $\int_{-1}^{1} L_n(x)L_m(x)dx = \frac{2}{2n+1}\delta_{nm}$

$$= \frac{1}{L_N'(x_i)}\int_{-1}^{1} P_{N-1}(x)dx$$

$$= \frac{1}{L_N'(x_i)}\int_{-1}^{1}\sum_{k=0}^{N-1} a_k L_k(x)dx$$

$$= \frac{1}{L_N'(x_i)}\sum_{k=0}^{N-1} a_k \int_{-1}^{1} L_k(x)dx$$

$$= \frac{1}{L_N'(x_i)}\sum_{k=0}^{N-1} a_k \int_{-1}^{1} L_k(x)L_0(x)dx$$

$$= \frac{1}{L_N'(x_i)}\sum_{k=0}^{N-1} a_k \cdot 2\delta_{k0}$$

$$= \frac{2a_0}{L_N'(x_i)}$$

---

§ Weighted Gaussian quadrature methods

Given: $f(x)$ and $\omega(x)$ for $a \le x \le b$

Want: $\{x_i\}_{i=1}^{N}$ and $\{c_i\}_{i=1}^{N}$ such that $\int_a^b \omega(x) f(x)dx \approx \sum_{i=1}^{N} c_i f(x_i)$

Theorem: Let ω(x) be a positive weight function and $\phi_N(x)$ be a nonzero polynomial of degree N that is ω-orthogonal to $\Pi_{N-1}(R)$, i.e.

$$\int_a^b \omega(x)\phi_N(x)P_{N-1}(x)dx = 0$$

Then, $\{x_i\}_{i=1}^{N}$ are the zeros of $\phi_N(x)$ and $c_i = \int_a^b \frac{\omega(x)\phi_N(x)}{(x-x_i)\phi_N'(x_i)}dx$

---

§ Weighted Gaussian quadrature methods

- $\omega(x)=1$, $(a,b)=(-1,1)$: $\phi_N(x)=L_N(x)$ (Legendre)
- $\omega(x)=1/\sqrt{1-x^2}$, $(a,b)=(-1,1)$: $\phi_N(x)=T_N(x)$ (Chebychev)
- $\omega(x)=\exp(-x^2)$, $(a,b)=(-\infty,\infty)$: $\phi_N(x)=H_N(x)$ (Hermite)

Theorem:

- The quadrature formula holds exactly for all $f(x)\in\Pi_{2N-1}(R)$.
- For $f \in C^{2N}[a,b]$, the error term is

$$\frac{f^{(2N)}(\xi)}{(2N)!}\int_a^b \phi_N^2(x)\omega(x)dx \quad \text{for some } a<\xi<b$$

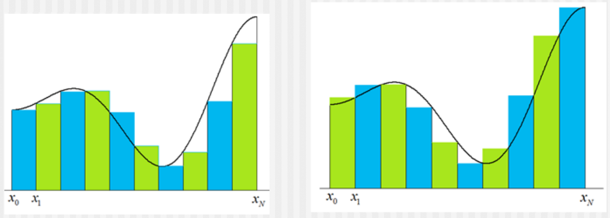
---

§ Piecewise approaches

Given: $f_i = f(x_i)$ for $a = x_0 < x_1 < x_2 < \cdots < x_{N-1} < x_N = b$

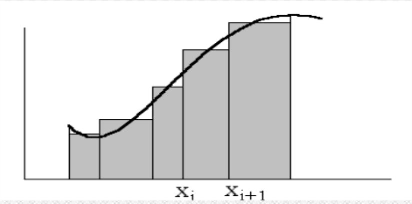
Want: $I = \int_a^b f(x)dx$

Simpliest way: $I \approx \sum_{i=0}^{N-1} f_i(x_{i+1}-x_i)$ or $\sum_{i=1}^{N} f_i(x_i - x_{i-1})$



§ Piecewise approaches

- rectangular rule



$$I=\int_a^b f(x)\,dx=\sum_{i=0}^{N-1}\left(\int_{x_i}^{x_{i+1}} f(x)\,dx\right)\approx\sum_{i=0}^{N-1}\left\{f\left(\frac{x_i+x_{i+1}}{2}\right)(x_{i+1}-x_i)\right\}$$

- error analysis: define $\bar{x}_i=(x_i+x_{i+1})/2$

for $x\in[x_i,x_{i+1}]$: $f(x)=f(\bar{x}_i)+(x-\bar{x}_i)f'(\bar{x}_i)+\dfrac{(x-\bar{x}_i)^2}{2}f''(\bar{x}_i)+O(\Delta x^3)$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx=\int_{x_i}^{x_{i+1}}\left\{f(\bar{x}_i)+\cancel{(x-\bar{x}_i)f'(\bar{x}_i)}+\frac{(x-\bar{x}_i)^2}{2}f''(\bar{x}_i)+\cancel{O(\Delta x^3)}\right\}dx$$

$$=f(\bar{x}_i)(x_{i+1}-x_i)+\frac{f''(\bar{x}_i)}{24}\cdot(x_{i+1}-x_i)^3+O(\Delta x^5)$$

$$I=\int_a^b f(x)\,dx=\sum_{i=0}^{N-1}\left(\int_{x_i}^{x_{i+1}} f(x)\,dx\right)$$

$$=\sum_{i=0}^{N-1}\left\{f(\bar{x}_i)(x_{i+1}-x_i)+\frac{f''(\bar{x}_i)}{24}\cdot(x_{i+1}-x_i)^3+O(\Delta x^5)\right\}$$

$$=\sum_{i=0}^{N-1}\left\{f(\bar{x}_i)(x_{i+1}-x_i)+O(\Delta x^3)\right\}$$

$$=\sum_{i=0}^{N-1}\left\{f(\bar{x}_i)(x_{i+1}-x_i)\right\}+N\cdot O(\Delta x^3)$$

total truncation error $\sim\dfrac{(b-a)}{\Delta x}\cdot O(\Delta x^3)\sim(b-a)O(\Delta x^2)$

Problem: We have $f(x_i)$ but not $f(\bar{x}_i)$.

Solution: make sure $x_i=\dfrac{x_{i+1}+x_{i-1}}{2}$, that is $x_{i+1}-x_i=x_i-x_{i-1}$.

$$I=\int_a^b f(x)\,dx=\int_{x_0}^{x_2} f(x)\,dx+\int_{x_2}^{x_4} f(x)\,dx+\int_{x_4}^{x_6} f(x)\,dx+\cdots+\int_{x_{N-2}}^{x_N} f(x)\,dx$$

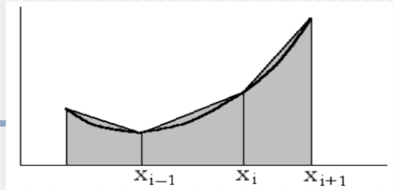
$$\approx f(x_1)(x_2-x_0)+f(x_3)(x_4-x_2)+\cdots+f(x_{N-1})(x_N-x_{N-2})$$

$$\approx\sum_{i=0}^{N/2-1} f(x_{2i+1})(x_{2i+2}-x_{2i})$$

$$\approx 2h\cdot\sum_{i=0}^{N/2-1} f(x_{2i+1})\quad\text{if}\quad(x_{2i+2}-x_{2i})=\text{constant}=2h$$

total truncation error ~ $O((b-a)\Delta x^2)$

- Trapezoidal rule



$$I=\int_a^b f(x)\,dx=\sum_{i=0}^{N-1}\left(\int_{x_i}^{x_{i+1}} f(x)\,dx\right)\approx\sum_{i=0}^{N-1}\left\{(x_{i+1}-x_i)\left(\frac{f(x_{i+1})+f(x_i)}{2}\right)\right\}$$

total truncation error ~ $O((b-a)\Delta x^2)$

for $x\in[x_i,x_{i+1}]$: $f(x)=f(\bar{x}_i)+(x-\bar{x}_i)f'(\bar{x}_i)+\dfrac{(x-\bar{x}_i)^2}{2}f''(\bar{x}_i)+O(\Delta x^3)$

$$f(x_i)=f(\bar{x}_i)-\frac{(x_{i+1}-x_i)}{2}f'(\bar{x}_i)+\frac{(x_{i+1}-x_i)^2}{8}f''(\bar{x}_i)+O(\Delta x^3)$$

$$f(x_{i+1})=f(\bar{x}_i)+\frac{(x_{i+1}-x_i)}{2}f'(\bar{x}_i)+\frac{(x_{i+1}-x_i)^2}{8}f''(\bar{x}_i)+O(\Delta x^3)$$

- Simpson rule Provided $x_i = \frac{x_{i+1}+x_{i-1}}{2}$ or $x_{i+1}-x_i = x_i - x_{i-1} \equiv h_i$.

$$\int_{x_{i-1}}^{x_{i+1}} f(x)dx = \frac{h_i}{3}\left(f_{i-1}+4f_i+f_{i-1}\right)+O\left(h_i^5\right)$$

total truncation error ~ $O\left((b-a)\Delta x^4\right)$

< show >

$$\int_{x_{i-1}}^{x_{i+1}} f(x)dx = \int_{x_{i-1}}^{x_{i+1}} \left\{ \begin{array}{l} f(x_i)+\cancel{(x-x_i)}f'(x_i)+\frac{(x-x_i)^2}{2}f''(x_i) \\ +\cancel{\frac{(x-x_i)^3}{6}}f'''(x_i)+\frac{(x-x_i)^4}{24}f^{(4)}(x_i)+O\left(\Delta x^5\right) \end{array} \right\} dx$$

$$= 2h_i f_i + \frac{1}{3}h_i^3 f_i'' + \frac{1}{60}h_i^5 f_i^{(4)} + O\left(h_i^7\right)$$

central difference method: $f_i'' = \frac{f_{i+1}-2f_i+f_{i-1}}{h_i^2}+O\left(h_i^2\right)$

$$\int_{x_{i-1}}^{x_{i+1}} f(x)dx = 2h_i f_i + \frac{1}{3}h_i^3 f_i'' + \frac{1}{60}h_i^5 f_i^{(4)} + O\left(h_i^7\right)$$

$$= 2h_i f_i + \frac{1}{3}h_i^3\left\{\frac{f_{i+1}-2f_i+f_{i-1}}{h_i^2}+O\left(h_i^2\right)\right\}+\frac{1}{60}h_i^5 f_i^{(4)}+O\left(h_i^7\right)$$

$$= 2h_i f_i + \frac{1}{3}h_i\left(f_{i+1}-2f_i+f_{i-1}\right)+O\left(h_i^5\right)$$

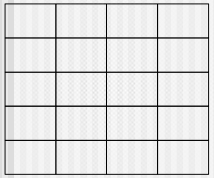
$$= \frac{h_i}{3}\left(f_{i-1}+4f_i+f_{i-1}\right)+O\left(h_i^5\right)$$

if h_i = constant $= h$:

$$\int_a^b f(x)dx \approx \sum_{i=0}^{N/2-1}\frac{h_i}{3}\left(f_{2i+2}+4f_{2i+1}+f_{2i}\right)+O\left((b-a)\Delta x^4\right)$$

§ Multiple Integrals

- regular domains



$$\int_a^b dx\int_c^d f(x,y)dy \approx \int_a^b dx\sum_{j=0}^{N}\beta_j f\left(x,y_j\right)$$

$$= \sum_{j=0}^{N}\beta_j\int_a^b f\left(x,y_j\right)dx$$

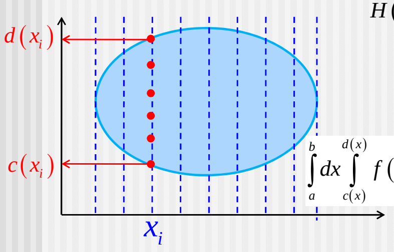
$$\approx \sum_{j=0}^{N}\beta_j\left(\sum_{i=0}^{M}\alpha_i f\left(x_i,y_j\right)\right)$$

$$= \sum_{j=0}^{N}\sum_{i=0}^{M}\alpha_i\beta_j f\left(x_i,y_j\right)$$

§ Multiple Integrals

- irregular domains

$$\int_a^b dx\int_{c(x)}^{d(x)} f(x,y)dy \equiv \int_a^b H(x)dx \approx \sum_{i=0}^{M}\alpha_i H(x_i)$$



$$H(x_i) = \int_{c(x_i)}^{d(x_i)} f(x_i,y)dy$$

$$\approx \sum_{j=0}^{N_i}\beta_{ij} f\left(x_i,y_{ij}\right)$$

$$\int_a^b dx\int_{c(x)}^{d(x)} f(x,y)dy \approx \sum_{i=0}^{M}\alpha_i\left\{\sum_{j=0}^{N_i}\beta_{ij} f\left(x_i,y_{ij}\right)\right\}$$

$$= \sum_{i=0}^{M}\sum_{j=0}^{N_i}\alpha_i\beta_{ij} f\left(x_i,y_{ij}\right)$$

§ Richardson's extrapolation

- construct a better answer based on some unsatisfactory answers.

Given a 1st-order formula $N_1(h)$ which approximates a quantity M, i.e.

$$M = N_1(h)+C_1h+C_2h^2+C_3h^3+\cdots$$

Want: an answer with a better accuracy

(1) $M = N_1(h)+C_1h+C_2h^2+C_3h^3+\cdots$

(2) $M = N_1\left(\frac{h}{2}\right)+C_1\frac{h}{2}+C_2\frac{h^2}{4}+C_3\frac{h^3}{8}+\cdots$

$2*(2)-(1)$=(3): $M = 2N_1\left(\frac{h}{2}\right)-N_1(h)-C_2\frac{h^2}{2}-C_3\frac{3h^3}{4}+\cdots$

$N_2(h)\equiv 2N_1\left(\frac{h}{2}\right)-N_1(h)$ ~ 2nd order accuracy

---

§ Richardson's extrapolation

(3) $M = N_2(h)-C_2\frac{h^2}{2}-C_3\frac{3h^3}{4}+\cdots$ $\quad N_2(h)=2N_1\left(\frac{h}{2}\right)-N_1(h)$

(4) $M = N_2\left(\frac{h}{2}\right)-C_2\frac{h^2}{8}-C_3\frac{3h^3}{32}+\cdots$ $\quad N_2\left(\frac{h}{2}\right)=2N_1\left(\frac{h}{4}\right)-N_1\left(\frac{h}{2}\right)$

$\frac{4*(4)-(3)}{3}$: $M = \frac{4N_2\left(\frac{h}{2}\right)-N_2(h)}{3}+C_3\frac{3h^3}{8}+\cdots$

$$N_3(h)=\frac{4}{3}N_2\left(\frac{h}{2}\right)-\frac{1}{3}N_2(h)$$

Conclusion:

$M = N_j(h)+O\left(h^j\right)$

$N_j(h)=N_{j-1}\left(\frac{h}{2}\right)+\frac{1}{2^{j-1}-1}\left(N_{j-1}\left(\frac{h}{2}\right)-N_{j-1}(h)\right)$ for $j\ge 2$

$N_1(h)$

$N_1\left(\frac{h}{2}\right)$ $\quad N_2(h)$

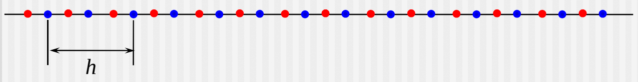
$N_1\left(\frac{h}{4}\right)$ $\quad N_2\left(\frac{h}{2}\right)$ $\quad N_3(h)$

$N_1\left(\frac{h}{8}\right)$ $\quad N_2\left(\frac{h}{4}\right)$ $\quad N_3\left(\frac{h}{2}\right)$ $\quad N_4(h)$

$N_2(h)=2N_1\left(\frac{h}{2}\right)-N_1(h)$

$N_2\left(\frac{h}{2}\right)=2N_1\left(\frac{h}{4}\right)-N_1\left(\frac{h}{2}\right)$

$N_3(h)=\frac{4}{3}N_2\left(\frac{h}{2}\right)-\frac{1}{3}N_2(h)$



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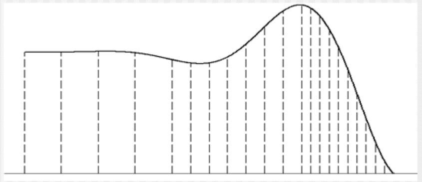
§ Adaptive Quadrature methods

Given: $f(x)$ and ε>0

Want: $I=\int_a^b f(x)dx$ within the sepcified tolerance ε

Idea: very dense grid points! ⇒ how dense?

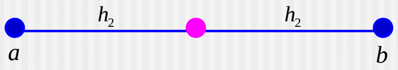
Efficiency desired: more points in regions where $f(x)$ has large variations.



Example: Simpson rule

$$\int_{x_{i-1}}^{x_{i+1}} f(x)dx = \frac{h_i}{3}\left(f_{i-1} + 4f_i + f_{i-1}\right) - \frac{h_i^5}{90} f^{(4)}(\mu) \quad \text{for some } \mu \in (x_i, x_{i+1})$$

Step1: 3 equally spaced nodes, $h_2 \equiv (b-a)/2$

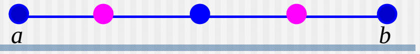


$$I = \int_a^b f(x)dx = \frac{h_2}{3}\left(f(a) + 4f(a+h_2) + f(b)\right) - \frac{h_2^5}{90} f^{(4)}(\mu)$$

$$\equiv S(a,b) - \frac{h_2^5}{90} f^{(4)}(\mu)$$

for some $\mu \in (a,b)$

Step 2: 5 equally spaced nodes



$$I = \int_a^{a+h_2} f(x)dx + \int_{a+h_2}^{b} f(x)dx$$

$$= \frac{h_2/2}{3}\left(f(a) + 4f\left(a + \frac{h_2}{2}\right) + f(a+h_2)\right)$$

$$+ \frac{h_2/2}{3}\left(f(a+h_2) + 4f\left(a + \frac{3h_2}{2}\right) + f(b)\right) - 2\times\left(\frac{h_2}{2}\right)^5 \frac{1}{90} f^{(4)}(\bar{\mu})$$

$$= S(a, a+h_2) + S(a+h_2, b) - \left(\frac{1}{16}\right)\frac{h_2^5}{90} f^{(4)}(\bar{\mu})$$

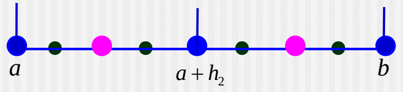
$$\begin{cases} I = S(a,b) - \dfrac{h_2^5}{90} f^{(4)}(\mu) \\ I = S(a,a+h_2) + S(a+h_2,b) - \left(\dfrac{1}{16}\right)\dfrac{h_2^5}{90} f^{(4)}(\bar{\mu}) \end{cases}$$

Assume $f^{(4)}(\mu) \approx f^{(4)}(\bar{\mu})$

$$\text{error} = \left(\frac{1}{16}\right)\frac{h_2^5}{90}\left|f^{(4)}(\bar{\mu})\right| \approx \frac{1}{15}\left|S(a,b) - S(a,a+h_2) - S(a+h_2,b)\right|$$

$< \varepsilon$? yes $\Rightarrow$ take the 5-point answer!

~ The error is estimated by using the 3-point and 5-point answer for any given range [*a*, *b*].



$$I = \int_a^{a+h_2} f(x)dx + \int_{a+h_2}^{b} f(x)dx = I_{1/2}^{(1)} + I_{1/2}^{(2)}$$

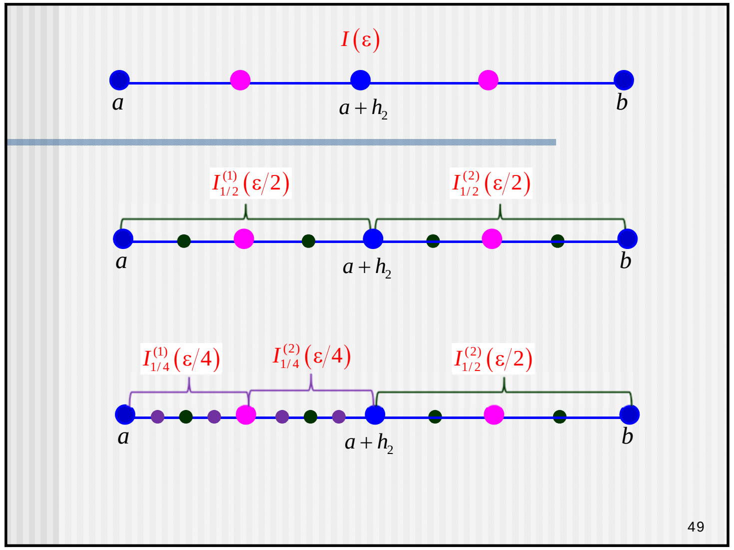
I within ε $\Rightarrow$ $I_{1/2}^{(1)}$ within $\varepsilon/2$ and $I_{1/2}^{(2)}$ within $\varepsilon/2$

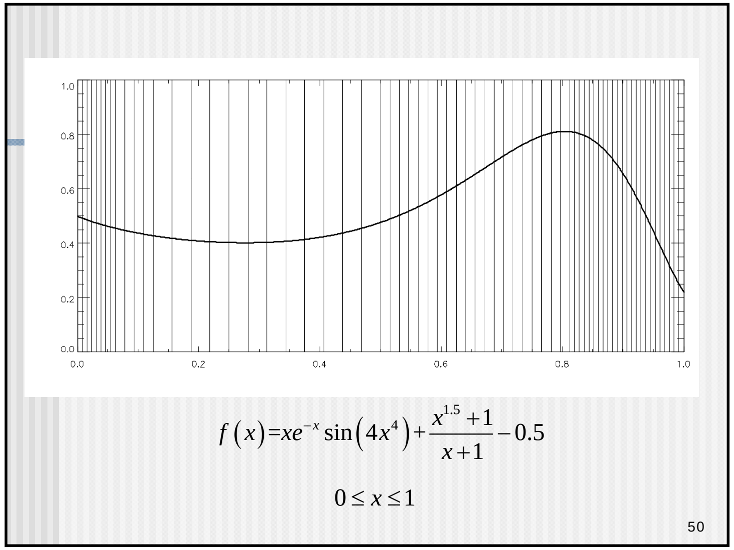
$$I_{1/2}^{(1)} = S\left(a, a+\frac{h_2}{2}\right) + S\left(a+\frac{h_2}{2}, a+h_2\right) + error_1$$

$$error_1 \approx \frac{1}{15}\left|S(a,a+h_2) - S\left(a,a+\frac{h_2}{2}\right) - S\left(a+\frac{h_2}{2}, a+h_2\right)\right| < \frac{\varepsilon}{2}?$$

$$I_{1/2}^{(2)} = S\left(a+h_2, a+\frac{3h_2}{2}\right) + S\left(a+\frac{3h_2}{2}, b\right) + error_2$$

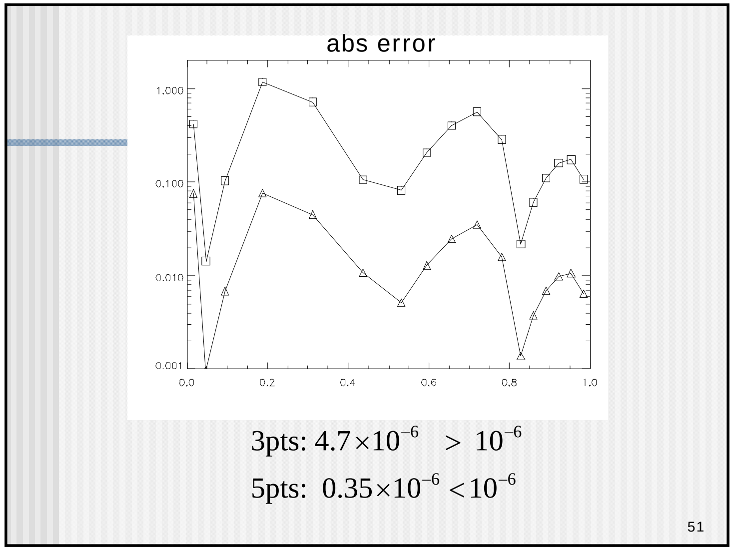
$$error_2 \approx \frac{1}{15}\left|S(a+h_2,b) - S\left(a+h_2,a+\frac{3h_2}{2}\right) - S\left(a+\frac{3h_2}{2}, b\right)\right| < \frac{\varepsilon}{2}?$$





$$f(x)=xe^{-x}\sin\left(4x^4\right)+\frac{x^{1.5}+1}{x+1}-0.5$$

$$0\le x\le 1$$



3pts: $4.7\times10^{-6} > 10^{-6}$

5pts: $0.35\times10^{-6} < 10^{-6}$