

## Lecture 3-I

### Curve fitting & interpolation

- Curve fitting
- linear regression
- general linear regression
- interpolation
  - Direct polynomial method
  - Newton's interpolation method
  - Lagrange's interpolation method
  - piecewise interpolation
- Integration
  - Trapezoidal rule (linear interpolation)
  - Simpson's  $\frac{1}{3}$ rd rule (quadratic interpolation)
  - Simpson's  $\frac{3}{8}$ th rule (cubic interpolation)
  - Integration using general order polynomial interpolation
  - Error in numerical integration
  - Integration of functions

### Error in numerical integration

Trapezoidal rule

$$E_T^i = \int_{x_i}^{x_{i+1}} f(x) dx - \int_{x_i}^{x_{i+1}} \hat{f}(x) dx$$



$$x_i \quad x_{i+1}$$

$\hat{f}$  linear interpolation using

$$(x_i, f(x_i)), (x_{i+1}, f(x_{i+1}))$$

we can show

$$E_t^i = -\frac{(x_{i+1}-x_i)^3}{12} f^{(2)}(z_i) \quad f^{(k)}(x) = \frac{d^k f}{dx^k}$$

$$\therefore E_t = \sum_{i=1}^n E_t^i$$

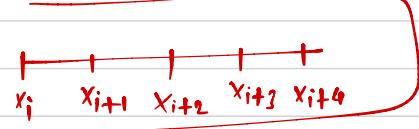
$$= -\frac{(b-a)^3}{12 n^3} \sum_{i=1}^n f^{(2)}(z_i)$$

$$= -\frac{(b-a)^3}{12 n^2} \overline{f}^{(2)}$$

- assuming

$$x_{i+1} - x_i = h = \frac{(b-a)}{n}$$

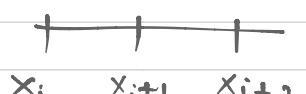
$$\overline{f}^{(k)} = \frac{1}{n} \sum_{i=1}^n f^{(k)}(z_i)$$



- Simpson's  $\frac{1}{3}$ rd rule (quadratic interpolation)

$$E_t^I = -\frac{1}{90} \left( \frac{x_{i+2}-x_i}{2} \right)^5 f^{(4)}(z_i)$$

$$= -\frac{h^5}{90} f^{(4)}(z_i)$$



- assuming

$$x_{i+1} - x_i = \frac{b-a}{n} = h$$

$$I = 1 \rightarrow (x_1, x_3)$$

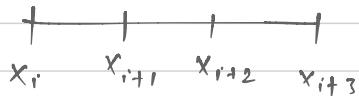
$$I = 2 \rightarrow (x_3, x_5)$$

.

$$I = m \rightarrow (x_{n-1}, x_{n+1})$$

} sum  $E_t^I$  to get total error

- Simpson's  $\frac{3}{8}$  th rule



$$E_t^I = -\frac{3}{80} \left( \frac{x_{i+3} - x_i}{3} \right)^5 f^{(4)}(x_i)$$

$$= -\frac{3}{80} h^5 f^{(4)}(x_i)$$

$$x_{i+1} - x_i = x_{i+2} - x_{i+1}$$

$$= \dots = \frac{b-a}{n}$$

$$= h$$

$$I = 1 \rightarrow (x_1, x_4)$$

$$I = 2 \rightarrow (x_4, x_7)$$

### Integration of function

$$f: [a, b] \rightarrow (-\infty, \infty)$$

We can compute  $f$  at discrete points  $(x_1, x_2, \dots, x_n)$

$$(y_1 = f(x_1), y_2 = f(x_2), \dots, y_n = f(x_n))$$

Idea is to choose discrete points  $(x_1, x_2, \dots, x_n)$  more wisely to further reduce errors.

- Gauss Quadrature method
- Richardson's method
- Adaptive Quadrature

## Gauss quadrature method

### Accurate upto linear functions

$$\hat{I}[f] = c_1 f(a) + c_2 f(b)$$

$$\cdot I[1] = \hat{I}[1]$$

$$\rightarrow [c_1 + c_2 = \int_a^b 1 dx = b-a]$$

$$\cdot I[x] = \hat{I}[x]$$

$$\rightarrow [c_1 a + c_2 b = \int_a^b x dx = \frac{b^2 - a^2}{2}]$$

$$f = \alpha + \beta x$$

$$I[f] = \hat{I}[f]$$

$$I[f] = \int_a^b (\alpha + \beta x) dx$$

$$= \alpha \int_a^b dx + \beta \int_a^b x dx$$

$$= \alpha I[1] + \beta I[x]$$

$$= \alpha \hat{I}[1] + \beta \hat{I}[x]$$

$$= \hat{I}[\alpha + \beta x]$$

Solve for  $c_1$  and  $c_2$

$$c_1 = c_2 = \frac{b-a}{2}$$

$$\hat{I}[f] = c_1 f(x_1) + c_2 f(x_2)$$

$$\text{find } c_1, c_2, x_1, x_2$$

$$\cdot I[1] = \hat{I}[1]$$

$$\cdot I[x] = \hat{I}[x]$$

$$\cdot I[x^2] = \hat{I}[x^2]$$

$$\cdot I[x^3] = \hat{I}[x^3]$$

Eq 1

$$c_1 + c_2 = b-a \Rightarrow c = \frac{b-a}{2}$$

Eq 2

$$c_1 x_1 + c_2 x_2 = \frac{b^2 - a^2}{2} \Rightarrow c(x_1 + x_2) = \frac{b^2 - a^2}{2}$$

$$\sqrt{c}(a+b) = \frac{b^2 - a^2}{2}$$

$$\Rightarrow c = \frac{b-a}{2}$$

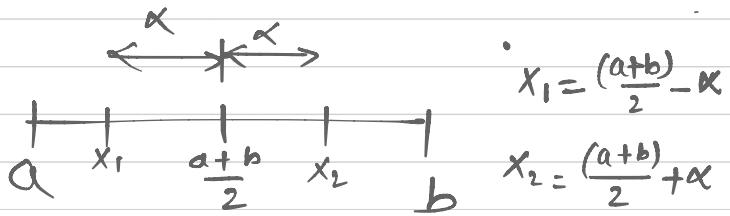
Eq 3

$$c_1 x_1^2 + c_2 x_2^2 = \frac{b^2 - a^2}{3} \Rightarrow$$

Eq 4

$$c_1 x_1^3 + c_2 x_2^3 = \frac{b^4 - a^4}{4}$$

$$\cdot c_1 = c_2 = c$$



$$\cdot x_1 = \frac{(a+b)}{2} - x$$

$$\cdot x_2 = \frac{(a+b)}{2} + x$$

$$C(x_1^2 + x_2^2) = \frac{b^3 - a^3}{3}$$

$$\Rightarrow C\left(\left(\frac{a+b}{2} - x\right)^2 + \left(\frac{a+b}{2} + x\right)^2\right) = \frac{b^3 - a^3}{3}$$

$$\begin{aligned}\Rightarrow \left(\frac{a+b}{2}\right)^2 + x^2 - \cancel{(a+b)x} + \left(\frac{a+b}{2}\right)^2 + x^2 + \cancel{(a+b)x} \\ = \frac{1}{c} \frac{(b^3 - a^3)}{3}\end{aligned}$$

$$\Rightarrow 2x^2 = \frac{1}{c} \frac{(b^3 - a^3)}{3} - \frac{(a+b)^2}{2}$$

∴

•  $x_1, x_2$  are quadrature points

•  $\hat{I}[f] = c_1 f(x_1) + c_2 f(x_2)$

$$c_1 = c_2 = \frac{b-a}{2}$$

$$x_1 = \frac{a+b}{2} - x, \quad x_2 = \frac{a+b}{2} + x$$

• Gauß-Legendre formula

$$\begin{aligned}f &= \alpha_1 + \alpha_2 x + \alpha_3 x^2 \\ &\quad + \alpha_4 x^3\end{aligned}$$

$$\begin{aligned}\hat{I}[f] &= \alpha_1 \hat{I}[f] + \alpha_2 \hat{I}[x] \\ &\quad + \alpha_3 \hat{I}[x^2] \\ &\quad + \alpha_4 \hat{I}[x^3]\end{aligned}$$

$$= \alpha_1 \hat{I}[1] + \alpha_2 \hat{I}[x]$$

$$+ \alpha_3 \hat{I}[x^2]$$

$$+ \alpha_4 \hat{I}[x^3]$$

$$= \hat{I}[\alpha_1 + \alpha_2 x + \alpha_3 x^2 + \alpha_4 x^3]$$

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- Gauss Quadrature Method (Gauss-Legendre formulas)

for  $\hat{I}[f] = c_1 f(x_1) + c_2 f(x_2)$   $f: [a, b] \rightarrow (-\infty, \infty)$

find  $c_1, c_2, x_1, x_2$  s.t.

$$\cdot I[1] = \hat{I}[1]$$

$$\cdot I[x] = \hat{I}[x]$$

$$\cdot I[x^2] = \hat{I}[x^2]$$

$$\cdot I[x^3] = \hat{I}[x^3]$$

we found that

$$\cdot c_1 = c_2 = \frac{b-a}{2} = c$$

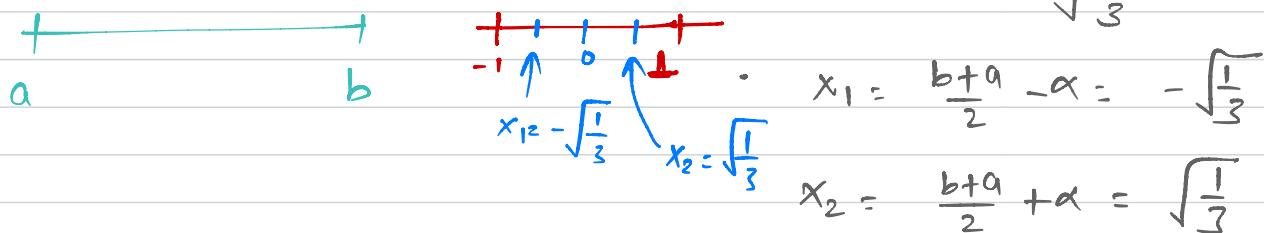
$$\cdot x_1 = \frac{b+a}{2} - \alpha, \quad x_2 = \frac{b+a}{2} + \alpha \quad \text{where}$$

$$2\alpha^2 = \frac{1}{c} \frac{(b^3 - a^3)}{3} - \frac{(a+b)^2}{2}$$

$$\text{Take } a = -1, b = 1 \quad \text{then} \quad \cdot c = c_2 = 1 = c$$

$$\cdot 2\alpha^2 = \frac{1}{1} \frac{(1+1)}{3} - \frac{0^2}{2} = \frac{2}{3}$$

$$\Rightarrow \alpha = \sqrt{\frac{1}{3}}$$



$$\cdot x_1 = \frac{b+a}{2} - \alpha = -\sqrt{\frac{1}{3}}$$

$$x_2 = \frac{b+a}{2} + \alpha = \sqrt{\frac{1}{3}}$$

$$\stackrel{d}{=} \hat{I}[f] = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \quad \text{for } f: [-1, 1] \rightarrow (-\infty, \infty)$$

## Change of variable

Let  $f: [a, b] \rightarrow (-\infty, \infty)$

$$I[f] = \int_a^b f(x) dx,$$

Consider  $z = \alpha + \beta x$  choose  $\alpha, \beta$  s.t

$$\Rightarrow x = \frac{z-\alpha}{\beta}, \quad dx = \frac{dz}{\beta} \quad \cdot z = -1 \text{ at } x = a$$

•  $z = 1$  at  $x = b$

then

$$I[f] = \int_{-1}^1 f\left(\frac{z-\alpha}{\beta}\right) \frac{dz}{\beta}$$

$$= \frac{1}{\beta} \int_{-1}^1 f\left(\frac{z-\alpha}{\beta}\right) dz$$

define

$$g(z) = f\left(\frac{z-\alpha}{\beta}\right)$$

Then

$$g: [-1, 1] \rightarrow (-\infty, \infty)$$

$$\therefore I[f] = \frac{1}{\beta} I[g]$$

$$= \frac{1}{\beta} \left( \int_{-1}^1 g(x) dx \right)$$

use quadrature formula that we obtained for

$$f: [-1, 1] \rightarrow (-\infty, \infty).$$

$$I[g] = g(-\frac{1}{\sqrt{2}}) + g(\frac{1}{\sqrt{2}})$$

Higher order formula

we can consider

$$\hat{I}[f] = c_1 f(x_1) + c_2 f(x_2) + \dots + c_n f(x_n)$$

which has  $2n$  unknowns so we can exactly

integrate upto  $(2n-1)^{\text{th}}$  order polynomial

$$\cdot I[1] = \hat{I}[1]$$

$$\cdot I[x] = \hat{I}[x]$$

$$\begin{cases} \frac{b-a}{2} \\ \alpha + \beta a = -1 \\ \alpha + \beta b = 1 \end{cases}$$

$$\beta(a-b) = -1 - 1$$

$$\therefore \beta = \frac{2}{b-a}$$

$$\therefore \alpha = 1 - \frac{2}{(b-a)} b$$

$$\therefore z = \frac{b-a-2b}{(b-a)} + \frac{2}{(b-a)} x$$

$$\therefore z = -\frac{(a+b)}{(b-a)} + \frac{2}{(b-a)} x$$

check

$$\text{when } x=a, z = -\frac{(a+b)}{(b-a)} + \frac{2}{(b-a)} a$$

$$= \frac{1}{(b-a)} (2a - a - b)$$

$$= -1$$

$$\text{when } x=b, z = 1.$$

$$\cdot I[x^{2n-1}] = \sum [x^{2n-1}]$$

}  $\rightarrow 2n$  equations

Table 20.1 provides values of unknowns upto  $n=6$

### Richardson's Extrapolation

$$f: [a, b] \rightarrow (-\infty, \infty)$$

$$h_1 = \frac{b-a}{n_1-1}, \quad x_1 = a, \quad x_2 = x_1 + h_1, \quad x_3 = x_2 + h_1, \dots, \quad x_{n_1} = b$$

$$f(x_1), f(x_2), \dots, f(x_3), \dots, f(x_{n_1})$$

$$I[f] = \int_a^b f(x) dx \approx \frac{h_1}{2} [f(x_1) + 2f(x_2) + \dots + f(x_{n_1})]$$

$\hat{I}[h_1]$

$$h_2 = \frac{b-a}{n_2-1}, \quad x_1 = a, \quad x_2 = x_1 + h_2, \quad x_3 = x_2 + h_2, \dots, \quad x_{n_2} = b$$

$$I[f] = \int_a^b f(x) dx \approx \frac{h_2}{2} [f(x_1) + 2f(x_2) + \dots + 2f(x_{n_2-1}) + f(x_{n_2})]$$

$\hat{I}[h_2]$

In general I can write

$$I[f] = \hat{I}[h_1] + E[h_1], \quad I[f] = \hat{I}[h_2] + E[h_2]$$

$$\hat{I}[h_1] + E[h_1] = \hat{I}[h_2] + E[h_2]$$

for Trapezoidal rule,

$$E[h] = -\frac{(b-a)^2}{12} h^2 \bar{f}^{(2)}[h]$$

$$\begin{aligned}\bar{f}^{(k)}[h] &= \frac{1}{n} \sum_{i=1}^n f^{(k)}(z_i) \\ \cdot f^{(k)} &= \frac{d^k f}{dx^k} \\ \cdot h &= \frac{b-a}{n-1}\end{aligned}$$

Assume that  $\bar{f}^{(2)}[h]$  is almost constant for different  $h$ .

$$E[h_1] = -\frac{(b-a)^2}{12} h_1^2 \bar{f}^{(2)}[h_1]$$

$$E[h_2] = -\frac{(b-a)^2}{12} h_2^2 \bar{f}^{(2)}[h_2]$$

divide

$$\frac{E[h_1]}{E[h_2]} = \frac{h_1^2}{h_2^2} \frac{\bar{f}^{(2)}[h_1]}{\bar{f}^{(2)}[h_2]}$$

$$\Rightarrow \frac{E[h_1]}{E[h_2]} \approx \frac{h_1^2}{h_2^2}$$

$$\text{Combine with } \hat{I}[h_1] + E[h_1] = \hat{I}[h_2] + E[h_2]$$

$$\Rightarrow \hat{I}[h_1] + E[h_2] \frac{h_1^2}{h_2^2} (\Rightarrow) \hat{I}[h_2] + E[h_2]$$

$$\therefore E[h_2] \approx \frac{\hat{I}[h_1] - \hat{I}[h_2]}{1 - \frac{h_1^2}{h_2^2}}$$

$$I \approx \hat{I}[h_1] + \frac{\hat{I}[h_2] - \hat{I}[h_1]}{1 - \frac{h_1^2}{h_2^2}}$$

from

$$I = \hat{I}[h_2] + E[h_2]$$

$$I \approx \hat{I}[h_2] + \frac{\hat{I}[h_1] - \hat{I}[h_2]}{1 - \frac{h_1^2}{h_2^2}}$$

Richardson's Extrapolation

$$\hat{I}[h] \rightarrow O(h^2)$$

$$E[h] = -\frac{(b-a)^2}{12} h^2 f''(h)$$

$$\hat{I}[h_2] + \frac{\hat{I}[h_1] - \hat{I}[h_2]}{1 - \frac{h_1^2}{h_2^2}} \rightarrow O(h_2^4)$$

Specific  $h_1 = h, \quad h_2 = \frac{h}{2}$

$$I \approx \hat{I}[h_2] + \frac{\hat{I}[h] - \hat{I}[h_2]}{1 - \frac{h^2}{h^2/4}} \rightarrow 1 - 4$$

$$= \hat{I}[h_2] - \frac{1}{3} (\hat{I}[h] - \hat{I}[h_2])$$

$$= \hat{I}[h_2] \left(1 + \frac{1}{3}\right) - \frac{1}{3} \hat{I}[h]$$

↗

$$I \approx \frac{4}{3} \hat{I}[h_2] - \frac{1}{3} \hat{I}[h]$$