lecture 31

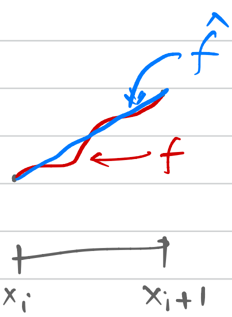
Curve fitting & interpolation

- 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 $1/3$ rd rule (quadratic interpolation)
  - Simpson's $3/8$ th rule (Cubic interpolation)
  - Integration using general order polynomial interpolation
  - Error in numerical integration
  - Integration of functions

- Error in numerical integration

Trapezoidal rule



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

$\hat{f}$ linear interpolation using

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

we can show

$$E_t^i = -\frac{(x_{i+1}-x_i)^3}{12} f^{(2)}(\xi_i)$$

— $f^{(k)}(x) = \dfrac{d^k f}{dx^k}$

— assuming

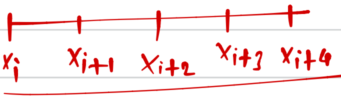
$x_{i+1} - x_i = h = \dfrac{(b-a)}{n}$

— $\bar{f}^{(k)} = \dfrac{1}{n}\sum_{i=1}^{n} f^{(k)}(\xi_i)$

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

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

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

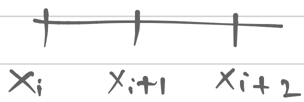


- Simpson's 1/3rd rule (quadratic interpolation)

even segment
— odd points
⇓
due to symmetry
higher accuracy

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

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



assuming

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

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

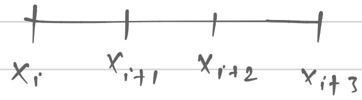
$I = 2 \longrightarrow (x_3, x_5)$

$\vdots$

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

sum E_t^I to get total error

- Simpson's $3/8^{th}$ rule



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

$$x_{i+1}-x_i = x_{i+2}-x_{i+1} = \cdots = \frac{b-a}{n} = h$$

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

→ Compare this with error in Simpson's $\frac{1}{3}$rd rule : Simpson's $\frac{1}{3}$rd rule accuracy is comparable while using one order lower interpolation!!

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

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

$\vdots$

- Integration of function

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

we can compute f at discrete points $(x_1, x_2, \ldots, x_n)$

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

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

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

• Gauss quadrature method

• Example of 2^{nd} order quadrature method

Usual interpolation method

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

• $I[1] = \hat{I}[1]$

$\Rightarrow \boxed{c_1 + c_2 = \int_a^b 1\, dx = b-a}$

• $I[x] = \hat{I}[x]$

$\Rightarrow \boxed{c_1 a + c_2 b = \int_a^b x\, dx = \frac{b^2-a^2}{2}}$

$f = \alpha + \beta x$

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

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

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

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

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

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

Solve for c_1 and c_2

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

Gauss Quadrature method

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

find c_1, c_2, x_1, x_2

• $I[1] = \hat{I}[1]$

• $I[x] = \hat{I}[x]$

• $I[x^2] = \hat{I}[x^2]$

• $I[x^3] = \hat{I}[x^3]$

Eq 1

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

Eq 2

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

$\checkmark \Rightarrow c\,(a+b) = \frac{b^2-a^2}{2}$

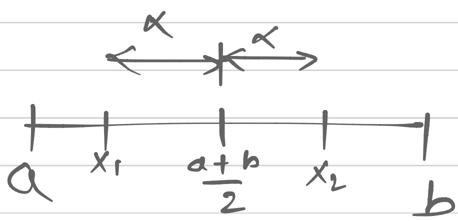
Eq 3

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

Eq 4

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

• $c_1 = c_2 = c$



• $x_1 = \frac{(a+b)}{2} - \alpha$

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

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

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

$$\Rightarrow \left(\frac{a+b}{2}\right)^2 + \alpha^2 - \cancel{(a+b)\alpha} + \left(\frac{a+b}{2}\right)^2 + \alpha^2 + \cancel{(a+b)\alpha}$$

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

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

$\Rightarrow$

Proof that 2^{nd} order Gauss quadrature is accurate upto cubic polynomials

$$f = \alpha_1 + \alpha_2 x + \alpha_3 x^2 + \alpha_4 x^3$$

$$I[f] = \alpha_1 I[f] + \alpha_2 I[x] + \alpha_3 I[x^2] + \alpha_4 I[x^3]$$

$$= \alpha_1 \hat{I}[1] + \alpha_2 \hat{I}[x] + \alpha_3 \hat{I}[x^2] + \alpha_4 \hat{I}[x^3]$$

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

Lecture 32

• Gauss Quadrature Method (Gauss – Legendre formulas)

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

find c_1, c_2, x_1, x_2 s.t

- $I[1] = \hat{I}[1]$
- $I[x] = \hat{I}[x]$
- $I[x^2] = \hat{I}[x^2]$
- $I[x^3] = \hat{I}[x^3]$

we found that

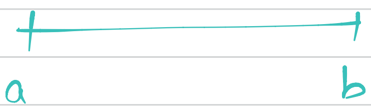
- $c_1 = c_2 = \dfrac{b-a}{2} = c$
- $x_1 = \dfrac{b+a}{2} - \alpha$, $\quad x_2 = \dfrac{b+a}{2} + \alpha$ where

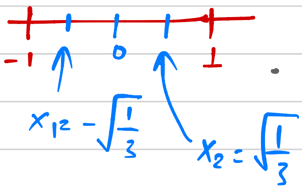
$$2\alpha^2 = \frac{1}{c}\,\frac{(b^3-a^3)}{3} - \frac{(a+b)^2}{2}$$

Take $a=-1$, $b=1$ then • $\boxed{c_1 = c_2 = 1 = c}$ ← weights

• $2\alpha^2 = \dfrac{1}{1}\dfrac{(1+1)}{3} - \dfrac{0^2}{2} = \dfrac{2}{3}$

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





• $$\boxed{\begin{aligned} x_1 &= \frac{b+a}{2} - \alpha = -\sqrt{\frac{1}{3}} \\ x_2 &= \frac{b+a}{2} + \alpha = \sqrt{\frac{1}{3}} \end{aligned}}$$ ← quadrature points

$\therefore$ $\hat{I}[f] = f\left(-\dfrac{1}{\sqrt{3}}\right) + f\left(\dfrac{1}{\sqrt{3}}\right)$ for $f:[-1,1] \to (-\infty,\infty)$

Change of variable to approximate integration over any interval $[a,b]$

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

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

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

$\Rightarrow x = \dfrac{z-\alpha}{\beta}$, $dx = \dfrac{dz}{\beta}$ $\qquad$ • $z = -1$ at $x = a$

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

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

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

use quadrature formula that we obtained for $f: [-1, 1] \to (-\infty, \infty)$.

- $z = 1$ at $x = b$

so $\left\{\begin{array}{l} \alpha + \beta a = -1 \\ \alpha + \beta b = 1 \end{array}\right.$

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

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

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

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

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

Check

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

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

$$= -1$$

when $x = b$, $z = 1$.

$\hat{I}[g]$ $g(-\frac{1}{\sqrt{3}}) + g(\frac{1}{\sqrt{3}})$ $\Rightarrow$

$$\boxed{I[f] \approx \frac{1}{\beta} \hat{I}[g] = \frac{1}{\beta}\left(g\left(-\frac{1}{\sqrt{3}}\right) + g\left(\frac{1}{\sqrt{3}}\right)\right) = \frac{1}{\beta} f\left(\frac{\frac{-1}{\sqrt{3}} - \alpha}{\beta}\right) + \frac{1}{\beta} f\left(\frac{\frac{1}{\sqrt{3}} - \alpha}{\beta}\right)}$$

Higher order formula

we can consider $\hat{I}[f] = c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n)$

which has $2n$ unknowns so we can exactly integrate upto $(2n-1)^{th}$ order polynomial

- $I[1] = \hat{I}[1]$
- $I[x] = \hat{I}[x]$

$$\vdots$$

$$\left.I[x^{2n-1}] = \hat{I}[x^{2n-1}]\right\} \longrightarrow 2n \text{ equations}$$

$\boxed{\text{Table 20.1 provides values of unknowns upto } n = 6}$

• Richardson's Extrapolation

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

h_1, $x_1 = a$, $x_2 = x_1 + h_1$, $x_3 = x_2 + h_1$, ..., $x_{n_1} = b$

h_2, $x_1 = a$, $x_2 = x_1 + h_2$, $x_3 = x_2 + h_2$, ..., $x_{n_2} = b$

$$I[f] = \int_a^b f(x)dx \approx \hat{I}[f] = \frac{h_1}{2}\Big[f(x_1) + f(x_{n_1}) + 2\big(f(x_2) + \cdots + f(x_{n_1-1})\big)\Big]$$

$$I[f] \approx \hat{I}[f] = \frac{h_2}{2}\big[f(x_1) + \quad - \quad \big]$$

<u>lets</u> $\hat{I}[h_1]$ is approximation of $I[f]$ using h_1

$\hat{I}[h_2]$ is ——— " ——— $I[f]$ using h_2

I is exact integral of f

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

Here $E[h_1]$, $E[h_2]$ are errors due to approximation of integral $I[f]$

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

$$E[h_1] = -\frac{(b-a)^2}{12} h_1^2 \, \bar{f}^{(2)}[h_1] \,, \qquad \bar{f}^{(2)}[h_1] = \frac{1}{n_1} \sum_{i=1}^{n_1} f^{(2)}(\eta_i)$$

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

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

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

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

$$\hat{I}[h_1] + \frac{h_1^2}{h_2^2} E[h_2] = \hat{I}[h_2] + E[h_2]$$

$$\rightarrow \boxed{E[h_2] = \frac{\hat{I}[h_1] - \hat{I}[h_2]}{1 - \frac{h_1^2}{h_2^2}}}$$

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

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

I assume $h_2 < h_1$

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

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

$$= \hat{I}[h/2] - \frac{1}{3}\left(\hat{I}[h] - \hat{I}[h/2]\right)$$

$$\boxed{I \approx \frac{4}{3}\hat{I}[h/2] - \frac{1}{3}\hat{I}[h]}$$

We have effectively built more accurate approximation of $I[f]$ using two Trapezoidal approximations

Idea can be used to similarly combine two simpson's $\frac{1}{3}$rd rule approximation to get higher order approximation !!!

• Adaptive Quadrature Method

$\Downarrow$

Choose more points in parts where function varies a lot and use fewer points elsewhere !!