October 17

<u>Last time</u>

Integrals $\quad P(v_x) = \sqrt{\frac{m}{2\pi kT}}\, e^{-mv_x^2/2kT}$

$\Rightarrow \int_{-a}^{a} P(v_x)\, dx$

$$\int_a^b f(x)\,dx \approx \sum_i^{n-1} c_i f(x_i)$$

$x_i \equiv$ abcissas (nodos)

$c_i \equiv$ weights

Newton-Cotes

$h = \frac{b-a}{n-1}$ $\quad$ N panels $(= n-1)$

rectangle rule $\quad \int_{x_i}^{x_{i+1}} f(x)\,dx \approx h f(x_i)$ $\quad$ Left hand side

$$\int_a^b f(x)\,dx \approx h\,[f(x_0) + f(x_1) + \ldots f(x_{n-2})]$$

$$\mathcal{E} = \frac{b-a}{2} h f'(\xi)$$

midpoint $\quad \int_{x_i}^{x_{i+1}} f(x)\,dx \approx h f(x_i + h/2)$

Midpoint rule

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx h\, f(x_i + h/2)$$

expand $f(x)$ about $x_i + h/2 \equiv \Delta_i$

$$f(x) \approx f(\Delta_i) + (x-\Delta_i) f'(\Delta_i) + \frac{1}{2}(x-\Delta_i)^2 f''(\xi_i)$$

let $u = \dfrac{x-\Delta_i}{h/2}$ follow same steps (HW problem)

$$\mathcal{E}_i = \frac{1}{24} h^3 f''(\xi_i) \Rightarrow \mathcal{E}_{TOTAL} = \frac{b-a}{24} h^2 f''(\xi)$$

Trapezoid rule

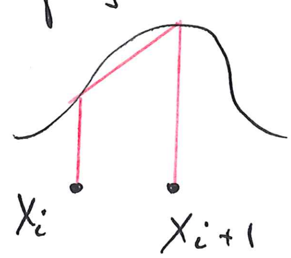
Use straight line instead of constant for function

1 panel w/ 2 abscissas determine line

We will use Lagrange interpolation

General: $q$ data points $x_{i+j}, f(x_{i+j})$ $j = 0, 1, \ldots q-1$

and we need interpolating polynomial

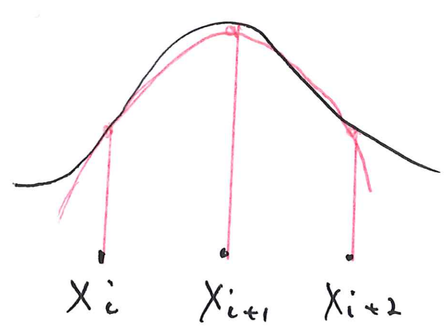



$q = 2 \Rightarrow$ line

$q = 3 \Rightarrow$ quadratic

In elementary interval

$\int_{x_i}^{x_{i+q-1}} f(x)\,dx$ needs to be approximated



approx $\int_{x_i}^{x_{i+q-1}} f(x)\,dx$ w/ $p(x) = \sum_{j=0}^{q-1} f(x_{i+j}) L_{i+j}(x)$

recall $L_k(x) = \dfrac{\prod_{j=0\ j\neq k}^{n-1} (x-x_j)}{\prod_{\text{same}} (x_k - x_j)}$ $\Rightarrow$ $L_{i+j}(x) = \dfrac{\prod_{k=0\ k\neq j}^{q-1} (x - x_{i+k})}{\prod (x_{i+j} - x_{i+k})}$

$k = 0, 1, \ldots n-1$ $\qquad$ $j = 0, 1, \cdot\, q-1$

$q = 3$ $\quad L_i(x), L_{i+1}(x), L_{i+2}(x)$ each is quadratic

to interpolate over $x_i, x_{i+1}, x_{i+2}$

$$\int_{x_i}^{x_{i+q-1}} f(x)\,dx \approx \int_{x_i}^{x_{i+q-1}} p(x)\,dx = \sum_{j=0}^{q-1} f(x_{i+j}) \int_{x_i}^{x_{i+q-1}} L_{i+j}(x)\,dx$$

$$= \sum_{j=0}^{q-1} \omega_{i+j} f(x_{i+j})$$

with $\omega_{i+j} \equiv \int_{x_i}^{x_{i+q-1}} L_{i+j}(x)\,dx$ $\Rightarrow$ do not depend on $f(x)$

We can find weights for a given $q$ $\underline{\underline{\text{once}}}$

Let $q = 2$ (trapezoid)

$L_i(x) = \dfrac{x - x_{i+1}}{\underbrace{x_i - x_{i+1}}_{-h}}$ $\qquad$ $L_{i+1}(x) = \dfrac{x - x_i}{\underbrace{x_{i+1} - x_i}_{h}}$

$j = 0$ $\qquad$ $j = 1$

$k = 1$ $\qquad$ $k = 0$

$$w_i = \int_{x_i}^{x_{i+1}} L_i(x)\,dx = -\frac{1}{h}\int_{x_i}^{x_i+h} (x - x_{i+1})\,dx$$

$$= -\frac{1}{h}\left[ \tfrac{1}{2}x^2 - x\,x_{i+1} \right]_{x_i}^{x_i+h}$$

$$= -\frac{1}{h}\left[ \frac{1}{2}(x_i+h)^2 - \frac{1}{2}x_i^2 - x_{i+1}h \right]$$

$$= -\frac{1}{h}\left[ x_i h + \frac{1}{2}h^2 - x_{i+1}h \right] = -\frac{1}{h}\left[ h(-h) + \tfrac{1}{2}h^2 \right]$$

$$= h/2$$

$$w_{i+1} = \int_{x_i}^{x_{i+1}} L_{i+1}(x)\,dx = \frac{1}{h}\int_{x_i}^{x_{i+1}} (x - x_i)\,dx = h/2$$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \sum_{j=0}^{q-1} w_{i+j}\, f(x_{i+j}) = \frac{h}{2}\left[ f(x_i) + f(x_{i+1}) \right]$$

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-2} \int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$\approx \frac{h}{2}\left[ f(x_0) + f(x_1) + f(x_1) + f(x_2) + f(x_2) + f(x_3) + \dots + f(x_{n-2}) + f(x_{n-1}) \right]$$

$$\approx \frac{h}{2} f(x_0) + h\, f(x_1) + h\, f(x_2) + \dots\, h\, f(x_{n-2}) + \frac{h}{2} f(x_{n-1})$$

Cummalitive set of weights $\left[ \int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} c_i f(x_i) \right]$

$$c_i = h\left\{ \tfrac{1}{2}, 1, 1, \dots 1, \tfrac{1}{2} \right\}$$

Simpson's rule : $q = 3$ , quadratic
(2 panels)

$$L_i(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} \qquad L_{i+1}(x) = \frac{(x - x_i)(x - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}$$

$$L_{i+2}(x) = \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}$$

define $u = \frac{1}{h}(x - x_{i+1})$

$$w_i = \int_{x_i}^{x_{i+2}} L_i(x)\,dx = \frac{h}{2}\int_{-1}^{1} du\,(u-1)u = h/3$$

$$w_{i+1} = -h\int_{-1}^{1} du\,(u+1)(u-1) = 4h/3$$

$$w_{i+2} = \frac{h}{2}\int_{-1}^{1} du\,(u+1)u = h/3$$

$$\int_{x_i}^{x_{i+2}} f(x)\,dx \approx \frac{h}{3}\left[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})\right]$$

$$\int_a^b f(x)\,dx = \sum_{i=0,2,4}^{n-3} \int_{x_i}^{x_{i+2}} f(x)\,dx$$

$x_0$ $x_1$ $x_2$ $x_3$ $x_4$ . . .

$\underbrace{1/3 \quad 4/3 \quad 1/3}$

$\underbrace{1/3 \quad 4/3 \quad 1/3}$

$\underbrace{1/3 \quad 4/3 \quad 1/3}$

$$C_i = \frac{h}{3}\{1, 4, 2, 4, 2, 4, 2, \ldots, 2, 4, 1\}$$

[See code]

Error in Simpsons

Taylor expand $f(x)$ around $x_{i+1}$

$$f(x) = f(x_{i+1}) + \Delta x f'(x_{i+1}) + \frac{1}{2}\Delta x^2 f''(x_{i+1}) + \frac{1}{6}\Delta x^3 f'''(x_{i+1}) + \frac{1}{24}\Delta x^4 f^{(4)}(\xi_i) \qquad \Delta x = x - x_{i+1}$$

integrate and substitute $u = \frac{x - x_{i+1}}{h}$

$$\int_{x_i}^{x_{i+2}} f(x)\,dx = h\int_{-1}^{1} du\left[ f(x_{i+1}) + \cancel{h u f'(x_{i+1})} + \frac{1}{2}h^2u^2 f''(x_{i+1}) + \cancel{\frac{1}{6}h^3u^3 f'''(x_{i+1})} + \frac{1}{24}h^4u^4 f^{(4)}(\xi_i)\right]$$

$$= 2hf(x_{i+1}) + \frac{1}{3}h^3 f''(x_{i+1}) + \frac{1}{60}h^5 f^{(4)}(\xi_i)$$

We found a finite diff formula for $f''$ in Chap 3

$$f''(x_{i+1}) = \frac{f(x_{i+2}) + f(x_i) - 2f(x_{i+1})}{h^2} - \frac{h^2}{12}f^{(4)}(\xi_i)$$

$$= 2hf(x_{i+1}) + \frac{1}{3}h^3\left[\frac{f(x_{i+2}) + f(x_i) - 2f(x_{i+1})}{h^2} - \frac{h^2}{12}f^{(4)}(\xi_i)\right] + \frac{1}{60}h^5 f^{(4)}(\xi_i)$$

$$= \frac{h}{3}\left[f(x_{i+2}) + f(x_i) + 4f(x_{i+1})\right] - \frac{1}{90}h^5 f^{(4)}(\xi_i)$$

Compare to Simpson's

$$\int_{x_i}^{x_{i+2}} f(x)\,dx \approx \frac{h}{3}\left[ f(x_i) + 4f(x_{i+1}) + f(x_{i+2}) \right]$$

$$\Rightarrow \mathcal{E}_i = -\frac{1}{90} h^5 f^{(4)}(\xi_i)$$

$$\mathcal{E} = \sum_{i=0,2,4,\ldots}^{n-3} \mathcal{E}_i \Rightarrow \mathcal{E} = -\frac{b-a}{180} h^4 f^{4}(\xi_i)$$

For polynomials up to third degree Simpson gives exact answer (even though we used quadratic)

→ use this method typically

## Gaussian Quadrature

No longer use equally spaced $x_i$

We ignore panels now and consider full integral from $[a,b]$ at the start

For ease we will choose $a=-1$ $b=1$ but we can scale to any other interval $t = \frac{b+a}{2} + \frac{b-a}{2}x$

$x \in [-1,1] \Rightarrow t \in [a,b]$

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{k=0}^{n-1} c_k f(x_k) \quad \left(\begin{array}{c}\text{open method so} \\ x_k \text{ is not } -1 \text{ or } 1\end{array}\right)$$

We can integrate polynomials up to degree $2n-1$ exactly with this method