Rewrite Taylor series

① $f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(x) + \dots$

② $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f'''(x) + \dots$

Subtract: ② − ①

$$\star \quad f(x+h) - f(x-h) = 2hf'(x) + 2\frac{h^3}{3!} f'''(x) + \mathcal{O}(h^5)$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)$$

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

Centred difference or 3-point formula

add: ① + ②

$$f_{i+1} + f_{i-1} = 2f_i + h^2 f_i'' + \mathcal{O}(h^4)$$

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

Can generate higher order differences

E.g. $f(x+2h) - f(x-2h) = 4hf'(x) + 2\frac{(2h)^3}{3!} f'''(x) + \mathcal{O}(h^5)$

$$\frac{8h^3}{3} f'''(x) = f(x+2h) - 4hf'(x) - f(x-2h) + \mathcal{O}(h^5)$$

↳ plug into $\star$ to get

$$f'(x) = \frac{1}{12h}\left[f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)\right] + \mathcal{O}(h^4)$$

5-point formula

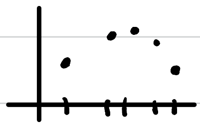
$$f_i' = \frac{1}{12h}\left(f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2} \right) + \mathcal{O}(h^4)$$

described as $\left\{ \begin{array}{l} \text{accurate to order } h^4 \\ 4^{th}\text{-order accurate} \\ \text{truncation error is } \mathcal{O}(h^4) \end{array} \right.$

As we have seen, subtraction reduces precision, so it is advantageous to reduce the number of subtractions

$$f_i' = \frac{1}{12h}\left[\left(f_{i-2} + 8f_{i+1} \right) - \left(f_{i+2} + 8f_{i-1} \right) \right]$$

Non-uniformly spaced data



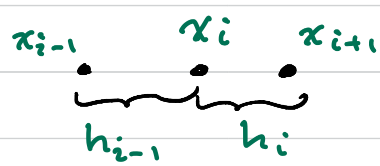
$\Delta x_i = x_{i+1} - x_i \neq \text{constant}$

one option: fit data to analytic function and then take derivative

- useful if there is theoretical motivation for the fit
- can introduce artefacts : extra peaks, rounded kinks

define $h_i = x_{i+1} - x_i$

$h_{i-1} = x_i - x_{i-1}$



$x_{i+1} = x_i + h_i$

$x_{i-1} = x_i - h_{i-1}$

Write Taylor series

$$f(x_{i\pm 1}) = f(x_i) + (x_{i\pm 1} - x_i) f'(x_i) + \frac{1}{2}(x_{i\pm 1} - x_i)^2 f''(x_i) + \ldots$$

or
$$f_{i+1} = f_i + h_i f_i' + \frac{1}{2} h_i^2 f_i'' + \mathcal{O}(h^3)$$

$$f_{i-1} = f_i - h_{i-1} f_i' + \frac{1}{2} h_{i-1}^2 f_i'' + \mathcal{O}(h^3)$$

algebra $\downarrow$ (eliminate f_i'')

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

3-point formula for non-uniform data

Richardson Extrapolation

Can construct algorithms to get derivatives to arbitrary order (but using higher order methods means assuming f^n is smooth)

For $f'(x)$: Let $\Delta_1(h) = \dfrac{f(x+h) - f(x-h)}{2h}$

$$\Delta_1(h) = f'(x) + \mathcal{O}(h^2)$$

can show that (5-pt formula)

$$\Delta_1(h) - 4\Delta_1(h/2) = -3f'(x) + \mathcal{O}(h^4)$$

and $\Delta_1(h) - 20\Delta_1\left(\frac{h}{2}\right) + 64\,\Delta_1\left(\frac{h}{4}\right) = 45\,f'(x) + \mathcal{O}(h^6)$

etc

Can determine the coefficients for higher orders systematically

write $\Delta_1(h) = \dfrac{f(x+h) - f(x-h)}{2h} = f'(x) + \sum_{k=1}^{\infty} C_{2k}\, h^{2k}$

call $\Gamma_{k0} = \Delta_1\left(\dfrac{h}{2^k}\right)$

can show

$$\Gamma_{k\ell} = \frac{4^\ell}{4^\ell - 1}\,\Gamma_{k\,\ell-1} - \frac{1}{4^\ell - 1}\,\Gamma_{k-1\,\ell-1}$$

for $0 \le \ell \le k$ leads to

$$f'(x) = \Gamma_{k\ell} - \sum_{m=\ell+1}^{\infty} B_{m\ell}\left(\frac{h}{2^k}\right)^{2m}$$

where $$B_{kl} = \frac{4^l + 4^k}{4^l - 1} B_{k\,l-1}$$

and
$$B_{kk} = 0$$

Example: $k = 1, \ l = 1$

$$f'(x) = \Gamma_{11} - \sum_{m=2}^{\infty} B_{m1} \left(\frac{h}{2}\right)^{2m}$$

$$f'(x) = \frac{4^1}{4^1 - 1} \Gamma_{10} - \frac{1}{4^1 - 1} \Gamma_{00} + \mathcal{O}(h^4)$$

$$\Gamma_{00} = \Delta_1(h)$$
$$\Gamma_{10} = \Delta_1(h/2)$$

$$f'(x) = \frac{4}{3} \Delta_1\left(\frac{h}{2}\right) - \frac{1}{3} \Delta_1(h) + \mathcal{O}(h^4)$$

or $\Delta_1(h) - 4\Delta_1\left(\frac{h}{2}\right) = -3f'(x) + \mathcal{O}(h^4)$ as before

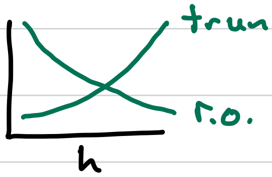
Can apply similar method for higher order derivatives

Let $$\Delta_2(h) = \frac{f(x+h) - 2f(x) + f(x+h)}{h^2}$$
$$= f''(x) + \mathcal{O}(h^2)$$

Can show
$$\Delta_2(h) - 4\Delta_2\left(\frac{h}{2}\right) = -3f''(x) + \mathcal{O}(h^4)$$
same form as with $f'(x)$ but with Δ_1 replaced with Δ_2

Error analysis

as h decreases truncation errors decrease but roundoff error from subtraction increases



error $\epsilon = \epsilon_{trunc} + \epsilon_{roundoff}$

ϵ is minimized when $\epsilon_{trunc} \simeq \epsilon_{ro}$

ϵ_{ro} from subtraction $\dfrac{f(x+h) - f(x)}{h}$ is $\epsilon_{ro} \sim \dfrac{\epsilon_M f(x)}{h}$

ϵ_{trunc}: forward difference $\mathcal{O}(h)$, $\simeq \dfrac{h}{2} f''(x)$ centred diff $\mathcal{O}(h^2)$, $\simeq \dfrac{h^2}{3} f'''(x)$

minimum error (best you can get) when $\epsilon_{ro} \simeq \epsilon_{tr}$

$$\frac{f\epsilon_M}{h_{FD}} \simeq \frac{h_{FD}}{2} f'' \qquad \frac{f\epsilon_M}{h_{CD}} \simeq \frac{h_{CD}^2}{3} f'''$$

Assume for simplicity $f \simeq f' \simeq f'' \simeq f''' \simeq 1$, $\epsilon_M \simeq 10^{-15}$ double prec.

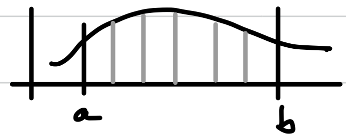
$$h_{FD} \simeq (2\epsilon_M)^{1/2} \simeq 4 \times 10^{-8} \qquad h_{CD} \simeq (3\epsilon_M)^{1/3} \simeq 2 \times 10^{-5}$$

$$\epsilon_{FD} \simeq \frac{\epsilon_M}{h_{FD}} \simeq 3 \times 10^{-8} \qquad \epsilon_{CD} \simeq \frac{\epsilon_M}{h_{CD}} \simeq 5 \times 10^{-11}$$

Centred diff. gives smaller optimal error with a larger step size.

Integration

$$I = \int_a^b f(x)\,dx \xrightarrow{\text{area}}_{\text{under curve}}$$



Before computers, approximated areas with quadrilaterals
- approach called numerical quadrature

Recall Riemann definition / rectangle rule

sum over rectangular areas, take limit as width $h = x_{i+1} - x_i \to 0$

$$I = \lim_{h \to 0} \sum_{i=1}^{\frac{b-a}{h}} h f(x_i)$$

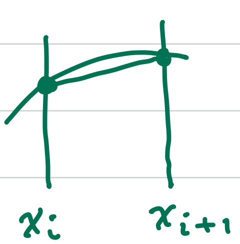
For finite h ($h \neq 0$), in general

$$\int_a^b f(x)\,dx \doteq \sum_{i=1}^{N} f(x_i)\,\omega_i \quad \text{for } N \text{ points in } [a,b]$$

- different algorithms yield different "weights" ω_i
  (for rectangles $\omega_i = h$)

Trapezoid rule

- use N points spaced evenly apart by h
  $$x_i = a + (i-1)h, \quad i = 1, \ldots N$$
- there are $N-1$ intervals $\quad h = \dfrac{b-a}{N-1}$
- over each interval, area is approximated by area of trapezoid



$$A_i = h\,\frac{1}{2}(f_i + f_{i+1}) = \frac{h}{2} f_i + \frac{h}{2} f_{i+1}$$