(7.1) Numerical Differentiation & Integration

Question: Given (x_i, y_i), $i = 0, 1, \ldots, n$
can we estimate $f'(c)$ or $\int_a^b f(x)\,dx$?
If yes, then how?

Typically need to estimate derivatives in numerical solution of differential equations.

Examples: By Taylor's theorem

(I) $$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(\xi)$$
($\frac{h^2}{2} f''(\xi)$: error in Taylor's approx)

$$\Rightarrow f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi)$$

we can use this to approximate the derivative

and this to bound the error in our approx.

(II) $$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(\xi)$$
and
$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(\xi)$$

Subtracting:

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

$$\Rightarrow f'(x) = \underbrace{\frac{f(x+h) - f(x-h)}{2h}}_{\text{derivative approx.}} - \underbrace{\frac{h^2}{6} f'''(\eta)}_{\text{error}}$$

Observe: Approx (I) has error $O(h)$

Approx (II) has error $O(h^2)$

An approximation formula for second derivatives:

$$f''(x) = \underbrace{\frac{1}{h^2}\left[f(x+h) - 2f(x) + f(x-h)\right]}_{\text{approx}} - \underbrace{\frac{h^2}{12} f^{(4)}(\eta)}_{\text{error}}$$

These techniques are typically prone to numerical (roundoff) errors, see book.

Differentiation via polynomial Interpolation

Strategy: (1) Interpolate with a polynomial

(2) Differentiate the polynomial

(3) evaluate the derivative

Given $(x_i, f(x_i))$, $i = 0, \dots, n$

we can write:

$$f(x) = \underbrace{\sum_{i=0}^{n} f(x_i) \ell_i(x)}_{\text{Lagrange form of interp. poly.}} + \underbrace{\frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \overbrace{\prod_{i=0}^{n} (x - x_i)}^{\text{call this } w(x)}}_{\text{interpolation error}}$$

$$\Rightarrow f'(x) = \sum_{i=0}^{n} f(x_i) \ell_i'(x) + \left(\frac{1}{(n+1)!} f^{n+1}(\xi_x)\, w(x) \right)'$$

So $f'(x) = \sum_{i=0}^{n} f(x_i) \ell_i'(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w'(x)$

$$+ \frac{1}{(n+1)!} w(x) \frac{d}{dx} f^{(n+1)}(\xi_x)$$

ξ_x: function of x

at node x_j: $w(x_j) = 0 \Longrightarrow$

$$f'(x_j) = \sum_{i=0}^{n} f(x_i) \ell_i'(x_j) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_j}) w'(x_j)$$

have to compute this

$$w(x) = \prod_{i=0}^{n} (x - x_i) \xrightarrow{\text{prod. rule}} w'(x) = \sum_{i=0}^{n} \prod_{j \neq i} (x - x_j)$$

$$\Longrightarrow w'(x_j) = \prod_{\substack{i \neq j \\ 0}}^{n} (x_j - x_i)$$

So

$$f'(x_j) = \sum_{i=0}^{n} f(x_i) \ell_i'(x_j) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_j}) \prod_{i \neq j} (x_j - x_i)$$

error

Examples: When $n=2$, the above expression gives

$$f'(x_1) = f(x_0)\frac{x_1-x_2}{(x_0-x_1)(x_1-x_2)} + f(x_1)\frac{2x_1-x_0-x_2}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{x_1-x_0}{(x_2-x_0)(x_2-x_1)} + \frac{1}{6}f'''(\xi_{x_1})(x_1-x_0)(x_1-x_2)$$

(check this!)

Example: when the nodes above are equally spaced i.e., $x_1-x_0 = x_2-x_1 = h$

we get $f'(x) = \frac{f(x+h)-f(x-h)}{2h} - \frac{1}{6}f'''(\xi_x)h^2$

Richardson Extrapolation (Getting more accuracy)

When we can write the taylor series

$$f(x+h) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x)(h)^k}{k!}$$

$$\& \; f(x-h) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x)(-h)^k}{k!}$$

we can subtract to get (term at even values of k cancel)

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

$$\Rightarrow f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \left[\frac{h^2 f'''(x)}{3!} + \frac{h^4 f^{(5)}(x)}{5!} + \dots\right]$$

$$L = \varphi(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \dots$$

L does not depend on h

$$\Rightarrow 4L = 4\varphi(h/2) + 4a_2\frac{h^2}{4} + 4a_4\frac{h^4}{16} + \frac{4a_6 h^6}{64} + \dots$$

subtract & divide by 3 → estimate

$$\Rightarrow \frac{3L}{3} = \frac{4\varphi(h/2)}{3} - \frac{\varphi(h)}{3} - \frac{3a_4h^4}{3} - \frac{5a^6h^6/16}{3}$$

error is now $O(h^4)$! ←

So, now

$$L = \underbrace{\tfrac{4}{3}\varphi(h/2) - \tfrac{1}{3}\varphi(h)}_{\text{call this } \Psi(h)} - a^4h^4/4 - \tfrac{5}{3}a^6h^6/16$$

$F'(a)$

and we can repeat the procedure

$$L = \Psi(h) + b^4h^4 + b^6h^6 + \cdots$$

$$\Rightarrow \left(L = \Psi(h/2) + b^4\frac{h^4}{16} + \frac{b^6h^6}{64}\right) \times 16$$

subtracting & dividing by 15:

$$\frac{15}{15}L = \underbrace{\frac{16}{15}\Psi(h/2) - \frac{\Psi(h)}{15}}_{\text{estimate}} - \underbrace{\frac{3}{4\times 15}b^6h^6 - \cdots}_{\text{error: } O(h^6)}$$

So, now

$$L = \frac{16}{15}\Psi(h/2) - \frac{1}{15}\Psi(h) - \frac{b^6h^6}{20} - \cdots$$

$$\underbrace{\qquad\qquad}_{\text{call this } \Theta(h)}$$

$$\cdots \quad L = \frac{64}{63}\,\Theta(h/2) - \frac{1}{63}\,\Theta(h) - \frac{3c_8 h^8}{252} \cdots$$

We can keep doing this!

$\Rightarrow$ Richardson extrapolation algorithm with M steps:

(I) Select h & compute

$$D(n,0) = \varphi(h/2^n), \quad n = 0, \ldots, M$$

↳ recall $\varphi(h) = \frac{f(x+h) - f(x-h)}{2h}$

(II) Compute

$$D(n,k) = \frac{4^k}{4^k - 1} D(n, k-1) - \frac{1}{4^k - 1} D(n-1, k-1)$$

where $k = 1, \ldots, M$ & $n = k, k+1, \ldots, M$

So, we are computing

$\varphi(h) = L + O(h^2)$

$D(0,0)$

$D(1,0)$ $\quad D(1,1)$ $\quad \psi(h) = L + O(h^4)$

$\varphi(h/2)$ $\quad D(2,0)$ $\quad D(2,1)$ $\quad D(2,2)$ $\quad \sigma(h) = L + O(h^6)$

$\vdots$ $\quad \vdots$ $\quad \vdots$ $\quad \ddots$

$D(M,0)$ $\quad D(M,1)$ $\quad D(M,2)$ ... $D(M,M)$

Theorem: Suppose $L = \varphi(h) + \sum_{j=1}^{\infty} a_{2j} h^{2j}$

Then $D(n,k-1) = L + \underbrace{\sum_{j=k}^{\infty} A_{jk} \left(\frac{h}{2^n}\right)^{2j}}_{O(h^{2k})}$

Proof Sketch: Induction

Base case: Verify $\underbrace{D(n,0)}_{\varphi(h/2^n)} = L + \sum_{j=1}^{\infty} \underbrace{A_{jk}}_{a_{2j}} \left(\frac{h}{2^n}\right)^{2j}$

Induction: Assum valid for $D(n,k-1)$ & prove for $D(n,k)$ ▨

HW § 7.1 # 6, 7, 12, 15