# Numerical Differentiation & Integration

**Question:** Given $(x_i, y_i)$, $i = 0, 1, \dots, n$
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) $f(x+h) = f(x) + h f'(x) + \underbrace{\frac{h^2}{2} f''(\xi)}_{\text{error in Taylor's approx}}$

$$\Rightarrow f'(x) = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{we can use this to approximate the derivative}} - \underbrace{\frac{h}{2} f''(\xi)}_{\text{and this to bound the error in our approx.}}$$

(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:

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

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

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

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

(which is better when $h$ is small)

An approximation formula for second derivatives:

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

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

## Differentiation via polynomial Interpolation

Strategy: (1) Interpolate with a polynomial

(2) Differentiate the polynomial

(3) evaluate the derivative

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

we can write:

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

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

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

function of $x$

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

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

have to compute this

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

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

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

## 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)

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

$$\Rightarrow \underbrace{f'(x)}_{L} = \underbrace{\frac{f(x+h) - f(x-h)}{2h}}_{\varphi(h)} - \underbrace{\left[ \frac{h^2 f'''(x)}{3!} + \frac{h^4 f^{(5)}(x)}{5!} + \cdots \right]}_{a_2 h^2 + a_4 h^4 + a_6 h^6 + \cdots}$$

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

$L$ doesnot depend on $h$

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

subtract & divide by 3

$$\Rightarrow \frac{3L}{3} = \overbrace{\frac{4\varphi(h/2)}{3} - \frac{\varphi(h)}{3}}^{\text{estimate}} \underbrace{- \frac{3}{3}a_4 h^4/4 - \frac{5a^6h^6/16}{3}}$$

error is now $O(h^4)$!

So, now

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

$f'(x)$

and we can repeat the procedure

$$L = \psi(h) + b^4h^4 + b^6h^6 + \dots$$

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

subtracting:
& dividing by 15

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

So, now

$$L = \underbrace{\frac{16}{15}\psi(h/2) - \frac{1}{15}\psi(h)}_{\text{call this } \theta(h)} - \frac{b^6h^6}{20} - \dots$$

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

We can keep doing this!

$\Longrightarrow$ Richardson extrapolation algorithm with $M$ steps:

(I) Select $h$ & compute

$$D(n,0) = \underbrace{\varphi(h/2^n)}\,, \quad n = 0, \dots, M$$

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

(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 $k = 1, \dots, M$ & $n = k, k+1, \dots, M$

So, we are computing

$$\begin{array}{llll} D(0,0) \to \varphi(h) = L + O(h^2) & & & \\ \varphi(h/2) \leftarrow D(1,0) & D(1,1) \to \psi(h) = L + O(h^4) & & \\ D(2,0) & D(2,1) & D(2,2) \to \theta(h) = L + O(h^6) & \\ \vdots & \vdots & \vdots & \ddots \\ D(M,0) & D(M,1) & D(M,2) & \cdots \; D(M,M) \end{array}$$

**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 $D(n,k)$ ∎