Numerical differentiation

Suppose the values of a function f are given at points $x_0, x_1, \cdots, x_n$, can we get ~~the~~ an estimate of $f'(x_i)$.

Forward difference Formula

$$D_+ f(x) = \frac{f(x+h) - f(x)}{h}$$

Backward difference formula

$$D_- f(x) = \frac{f(x) - f(x-h)}{h}$$

Central difference formula

$$D_0 f(x) = \frac{f(x+h) - f(x-h)}{2h}.$$

Suppose that f and f' are continuous on the closed interval $[x, x+h]$ and f'' exists on $(x, x+h)$. A Taylor formula shows that

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi) \qquad (*)$$

for some ξ between $x+h$ and x. This implies

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

Therefore

$$\left| D_+ f(x) - f'(x) \right| \leq \frac{h}{2} \| f'' \|_{L^\infty([x, x+h])}$$

Exc. Carry out the same exercise for $D_-^2 f(x)$.

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f^{(3)}(\xi_1) \quad ①$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f^{(3)}(\xi_2) \quad ②$$

② − ① ⇒

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{6}\left(f^{(3)}(\xi_2) + f^{(3)}(\xi_1)\right)$$

where $x-h < \xi_1 < x < \xi_2 < x+h$.

$$\Rightarrow \quad D_0 f(x) - f'(x) = \frac{h^2}{12}\left(f^{(3)}(\xi_2) + f^{(3)}(\xi_1)\right)$$

$$\Rightarrow \quad |D_0 f(x) - f'(x)| \le \frac{h^2}{6}\left(\|f^{(3)}\|_{L^\infty(x-h,x+h)}\right)$$

Second Order Derivative

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} h^{(3)}(x) + \frac{h^4}{24} h^{(4)}(\xi_1)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} h^{(3)}(x) + \frac{h^4}{24} h^{(4)}(\xi_2)$$

$$\Rightarrow \quad f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{24}\left(f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right)$$

$$\Rightarrow \quad \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \frac{h^2}{24}\left(f^{4}(\xi_1) + f^{(4)}(\xi_2)\right)$$

$$x-h < \xi_1 < x < \xi_2 < x+h$$

$$\Rightarrow \quad |D_2 f(x) - f''(x)| \le \frac{h^2}{12} \|f^{4}\|_{L^\infty(x-h,x+h)}$$

Differentiation via interpolation

Suppose that $n+1$ values of a function at points $x_0, x_1, \ldots, x_n$ are given. We can write a polynomial that interpolates f at the nodes x_i by

$$f(x) = \sum_{i=0}^{n} f(x_i)\, l_i(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x)\, \omega(x),$$

where $\omega(x) = \prod_{i=0}^{n} (x - x_i)$. This shows

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

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

Suppose that $x = x_\alpha$ is one of the nodes. Then $\omega(x_\alpha) = 0$. Thus:

$$f'(x_\alpha) = \sum_{i=0}^{n} f(x_i)\, l_i'(x_\alpha) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x)\, \omega'(x_\alpha).$$

Note that

$$\omega'(x) = \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j \neq i}}^{n} (x - x_j).$$

$$\Rightarrow \omega'(x_\alpha) = \prod_{\substack{j=0 \\ j \neq \alpha}}^{n} (x_\alpha - x_j) \quad \text{(verify)}$$

Thus the final differentiation formula is:

$$* \quad f'(x_\alpha) = \sum_{i=0}^{n} f(x_i)\, l_i'(x_\alpha) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_\alpha}) \prod_{\substack{j=0 \\ j \neq \alpha}}^{n} (x_\alpha - x_j)$$

Richardson Extrapolation

Example. Give the explicit form of $*$ with $n=2$ and $\alpha=1$.

The three Cardinal functions for Lagrange interpolation are

$$l_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad l_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)},$$

$$l_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}.$$

Their derivatives are given by,

$$l_0'(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)} \quad l_1'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$$

$$l_2'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

Evaluating at $x=x_1$, we obtain

$$l_0'(x_1) = \frac{x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

$$l_1'(x_1) = \frac{2x_1-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$$

$$l_2'(x_1) = \frac{x_1-x_0}{(x_2-x_0)(x_2-x_1)}$$

Therefore the numerical differentiation formula with the error term is given by

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

$$f(x_2)\frac{x_1-x_0}{(x_2-x_0)(x_2-x_1)} + \frac{1}{6}f'''(\xi_{x_1})(x_1-x_0)(x_1-x_2). \quad (\#)$$

Special case: $x_0 = x_1 - h$ and $x_2 = x_1 + h$. Then (#) implies

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

which is precisely the central difference formula.

Richardson extrapolation

We assume that $f(x+h)$ and $f(x-h)$ are represented by the Taylor series':

$$f(x+h) = \sum_{k=0}^{\infty}\frac{1}{k!}h^k f^{(k)}(x) \quad \text{and} \quad f(x-h) = \sum_{k=0}^{\infty}\frac{1}{k!}(-1)^k h^k f^{(k)}(x)$$

Subtraction will show that

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

A rearrangement yields:

$$f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] - \left[\frac{1}{3!}h^2 f^{(3)}(x) + \frac{1}{5!}h^4 f^{(5)}(x) + \frac{1}{7!}h^{(6)} f^{(7)}(x) + \cdots\right]$$

This is of the form

(1) $$L = \varphi(h) + a_2h^2 + a_4h^4 + a_6h^6 + \cdots$$

where L stands for $f'(x)$ and $\varphi(h)$ stands for the numerical differentiation formula. ie.

$$\varphi(h) = \frac{1}{2h}\left(f(x+h) - f(x-h)\right)$$

For sufficiently small values of h, the dominant term is always $a_2 h^2$. Therefore we will seek a way to eliminate this term. Write equation ① with h replacing $h/2$.

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

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

$$② - ① \quad \Rightarrow \quad 3L = 4\varphi(h/2) - \varphi(h) - 3a_4 h^4/4 - 15 a_6 h^6/16$$

$$\Rightarrow \quad L = \frac{4}{3}\varphi(h/2) - \frac{1}{3}\varphi(h) - a_4 \frac{h^4}{4} - 5a_6 \frac{h^6}{16} - \cdots \quad ⓑ$$

This shows that

$$\psi(h) = \frac{4}{3}\varphi(h/2) - \frac{1}{3}\varphi(h)$$

is a better approximation to L with an error of the ~~form~~ order h^4. We can further extend the process:

$$\cancel{L = \frac{4}{3}} \quad L = \psi(h) + b_4 h^4 + b_6 h^6 + \cdots \quad ③$$

$$\Rightarrow \quad L = \psi(h/2) + b_4 h^4/16 + b_6 h^6/64 + \cdots$$

$$\Rightarrow \quad 16L = 16\psi(h/2) + b_4 h^4 + b_6 h^6/4 + \cdots \quad ④$$

$$④ - ③ \Rightarrow 15L = 16\psi(h/2) - \psi(h) - 3b_6 h^6/4 - \cdots$$

$$\Rightarrow \quad L = \frac{16}{15}\psi(h/2) - \frac{1}{15}\psi(h) - b_6 h^6/20 - \cdots$$

Thus $\theta(h) = \frac{16}{15}\psi(h/2) - \frac{1}{15}\psi(h)$ is an even better approximation.

Repeat the process again to arrive at

$$L = \frac{64}{63}\,\varphi(h/2) - 1/63\,\varphi(h) - 3c_8 h^8/52 - \cdots$$

as a better approximation. This suggests the following algorithm.

Richardson extrapolation algorithm.

- Select a convinient h. and compute M+1 numbers

$$D(n,0) = \varphi(h/2^n) \qquad 0 \leq n \leq M$$

- Compute additional quantities by the formula

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

for $k = 1,2,\cdots,M$ and $n = k, k+1, \cdots, M.$}

Then observe that $D(0,0) = \varphi(h)$, $D(1,0) = \varphi(h/2)$, $D(1,1) = \psi(h)$ (Verify). The quantities $D(n,1)$ conform to ⊙ with h repeatedly replaced by $h/2$. Similarly $D(n,2)$ corresponds to ⊙. ~~with~~ Verify that

$$D(n,0) = L + O(h^2)$$
$$D(n,1) = L + O(h^4)$$
$$D(n,2) = L + O(h^6).$$
~~$D(n,k-1) =$~~

Theorem. The quantities $D(n,k)$ defined in Richardson extrapolation algorithm obey an equation of the form

$$D(n,k-1) = L + \sum_{j=k}^{\infty} A_{jk} (h/2^n)^{2j}.$$

Proof. When $k=1$, the formula

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

that

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

$$= L - \sum_{j=1}^{\infty} a_{2j} (h/2^n)^{2j}.$$

Therefore, we can let $A_{j1} = -a_{2j}$. Now we proceed by induction. We assume that the formula is valid for some $k-1$. From the formulae

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

$$D(n,k-1) = L + \sum_{j=k}^{\infty} A_{jk} (h/2^n)^{2j}$$ it follows that

$$D(n,k) = \frac{4^k}{4^k-1}\left[L + \sum_{j=k}^{\infty} A_{jk} (h/2^n)^{2j}\right]$$

$$- \frac{1}{4^k-1}\left[L + \sum_{j=k}^{\infty} A_{jk} (h/2^{n-1})^{2j}\right].$$

A simplification leads to

$$D(n,k) = L + \sum_{j=k}^{\infty} A_{jk} \left[\frac{4^k - 4^j}{4^k-1}\right] (h/2^n)^{2j}$$

Thus $A_{j,k+1}$ should be defined by $A_{jk+1} = A_{jk}\left[\frac{4^k-4^j}{4^k-1}\right]$.

Note that $A_{k,k+1} = 0 \Rightarrow$

$$D(n,k) = L + \sum_{j=k+1}^{\infty} A_{j,k+1} (h/2^n)^{2j}.$$

$\boxtimes$