7.1 Numerical differentiation and Richardson extrapolation

Q: Given a func. f (usually by pt values)

approximate f'

$$f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$$

$$\rightsquigarrow f'(x) \approx \frac{f(x+h)-f(x)}{h} \quad \text{for small } h.$$

- One cannot take h to be arbitrarily small.
  - $f(x+h)-f(x)$ has round-off issue.
  - $f(x)$, $f(x+h)$ usually come from grid pts. When spacing h is small, # of grid pts $= O(\frac{1}{h})$. Expensive.

Error analysis

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(\xi)h^2$$

$$\frac{f(x+h)-f(x)}{h} = f'(x) + \underbrace{\frac{1}{2}f''(\xi)h}_{\text{truncation error}} \rightsquigarrow \text{first order accuracy.}$$

- When the truncation error is $O(h^p)$, the numerical method has p-th order accuracy.
- A better method:

$$f'(x) \approx \frac{f(x+h)-f(x-h)}{2h} \quad \text{(centered difference)}$$

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

$$f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(\xi_2)h^3$$

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{1}{12}\left(f'''(\xi_1) + f'''(\xi_2)\right)h^2$$

(second order accurate)

Differentiation via poly. interp.

Suppose $f(x_0), \dots, f(x_n)$ are available

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

$$\omega(x) := \prod_{j=0}^{n} (x - x_j)$$

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

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

Suppose $x = x_\alpha$ is a node.

$$f'(x_\alpha) = \underbrace{\sum_{i=0}^{n} f(x_i)\, l_i'(x_\alpha)}_{\text{approximation}} + \underbrace{\frac{1}{(n+1)!} f^{(n+1)}(\xi) \prod_{\substack{j=0 \\ j \neq \alpha}}^{n} (x_\alpha - x_j)}_{\text{error.}}$$

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

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

- Suppose $x_0, \dots, x_n$ have pairwise distance $O(h)$ then error $= O(h^n)$
- Case $n=2$ w/ $x_0 = x-h$, $x_1 = x$, $x_2 = x+h$

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

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

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

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

To approximate $f'(x_1)$,

$$l_0'(x_1) = \frac{-h}{2h^2} = -\frac{1}{2h}$$

$$l_1'(x_1) = 0$$

$$l_2'(x_1) = \frac{1}{2h}$$

$$f'(x_1) = -\frac{1}{2h} f(x_0) + 0 \cdot f(x_1) + \frac{1}{2h} f(x_2) + \frac{1}{6} f'''(\xi)(-h^2)$$

(centered diff.)

To approximate $f'(x_2)$,

$$l_0'(x_2) = \frac{1}{2h}$$

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

$$l_2'(x_2) = \frac{3}{2h}$$

$$f'(x_2) = \frac{1}{2h} f(x_0) - \frac{2}{h} f(x_1) + \frac{3}{2h} f(x_2) + \frac{1}{6} f'''(\xi) \cdot 2h^2$$

(backward difference formula)

- Application to higher order derivatives

One expects $f^{(m)}(x_\alpha) \approx \sum_{i=0}^{n} f(x_i)\, l_i^{(m)}(x)$

at least for $m \le n$

Example $n=2$, $x-h, x, x+h$. want $f''(x_1)$

$x_0 = x-h$, $x_1 = x$, $x_2 = x+h$

$l_0''(x) = \frac{1}{h^2}$ $\quad l_1''(x) = -\frac{2}{h^2}$ $\quad l_2''(x) = \frac{1}{h^2}$

$$f''(x_1) \approx \frac{1}{h^2} f(x_0) - \frac{2}{h^2} f(x_1) + \frac{1}{h^2} f(x_2)$$

(centered diff)

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

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \frac{1}{24}f''''(\xi_1)h^4$$

$$f(x) = f(x)$$

$$f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(x)h^3 + \frac{1}{24}f''''(\xi_2)h^4$$

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

$$= f''(x) + \frac{1}{24}\left(f''''(\xi_1) + f''''(\xi_2)\right)h^2$$

(second order accurate).