Numerical Differentiation

Recall the definition of first derivative $f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$

$$f'(x_i) \cong \frac{f(x_i + h) - f(x_i)}{h} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$ forward difference

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$ backward difference

averaging

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$ central difference

Truncation Error (formula order) using Taylor series (Theorem 1.16)

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + f''(x_0)\frac{(x-x_0)^2}{2!} + \dots + f^n(x_0)\frac{(x-x_0)^n}{n!} + f^{n+1}(c)\frac{(x-x_0)^{n+1}}{(n+1)!}$$

$x_0 < c < x$

Let $x = x_0 + h, \quad n = 1$

$$f(x_0 + h) = f(x_0) + f'(x_0)h + f''(c_1)\frac{h^2}{2!} \Rightarrow f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - f''(c_1)\frac{h}{2}$$

Forward difference with $O(h)$

Let $x = x_0 - h, \quad n = 1$

$$f(x_0 - h) = f(x_0) + f'(x_0)(-h) + f''(c_2)\frac{h^2}{2!} \Rightarrow f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h} + f''(c_2)\frac{h}{2}$$

Backward difference with $O(h)$

Centered Formula of Order $O(h^2)$

(5) $$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(c_1)h^3}{3!}$$

and

(6) $$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(c_2)h^3}{3!}.$$

After (6) is subtracted from (5), the result is

(7) $$f(x+h) - f(x-h) = 2f'(x)h + \frac{((f^{(3)}(c_1) + f^{(3)}(c_2))h^3}{3!}.$$

Since $f^{(3)}(x)$ is continuous, the intermediate value theorem can be used to find a value c so that

(8) $$\frac{f^{(3)}(c_1) + f^{(3)}(c_2)}{2} = f^{(3)}(c).$$

This can be substituted into (7) and the terms rearranged to yield

(9) $$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f^{(3)}(c)h^2}{3!}.$$

The first term on the right side of (9) is the central-difference formula (3), the second term is the truncation error, and the proof is complete. •

Error Analysis and Optimum Step Size

$$f(x_0 - h) = y_{-1} + e_{-1} \quad \text{and} \quad f(x_0 + h) = y_1 + e_1,$$

$$f'(x_0) \approx \frac{y_1 - y_{-1}}{2h}.$$

$$f'(x_0) = \frac{y_1 - y_{-1}}{2h} + E(f, h),$$

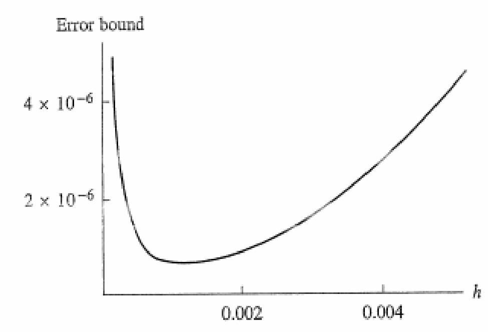
$$E(f,h) = E_{\text{round}}(f,h) + E_{\text{trunc}}(f,h)$$
$$= \frac{e_1 - e_{-1}}{2h} - \frac{h^2 f^{(3)}(c)}{6},$$

If $|e_{-1}| \le \epsilon$, $|e_1| \le \epsilon$, and $M = \max_{a \le x \le b}\{|f^{(3)}(x)|\}$,

$$|E(f,h)| \le \frac{\epsilon}{h} + \frac{Mh^2}{6}, \qquad h = \left(\frac{3\epsilon}{M}\right)^{1/3}.$$

Error Analysis and Optimum Step Size

$$h = \left(\frac{3\epsilon}{M}\right)^{1/3}.$$



Higher order derivatives

$f''(x)$ of order $O(h^2)$

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

and

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

Adding equations (1) and (2)

(3) $$f(x+h) + f(x-h) = 2f(x) + \frac{2h^2 f''(x)}{2} + \frac{2h^4 f^{(4)}(x)}{24} + \cdots.$$

Solving equation (3) for $f''(x)$ yields

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{2h^2 f^{(4)}(x)}{4!}$$

Table 6.3 Central-Difference Formulas of Order $O(h^2)$

$$f'(x_0) \approx \frac{f_1 - f_{-1}}{2h}$$

$$f''(x_0) \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}$$

$$f^{(3)}(x_0) \approx \frac{f_2 - 2f_1 + 2f_{-1} - f_{-2}}{2h^3}$$

$$f^{(4)}(x_0) \approx \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4}$$

Table 6.4 Central-Difference Formulas of Order $O(h^4)$

$$f'(x_0) \approx \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}$$

$$f''(x_0) \approx \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2}$$

$$f^{(3)}(x_0) \approx \frac{-f_3 + 8f_2 - 13f_1 + 13f_{-1} - 8f_{-2} + f_{-3}}{8h^3}$$

$$f^{(4)}(x_0) \approx \frac{-f_3 + 12f_2 - 39f_1 + 56f_0 - 39f_{-1} + 12f_{-2} - f_{-3}}{6h^4}$$

Table 6.7 Forward- and Backward-Difference Formulas of Order $O(h^2)$

$$f'(x_0) \approx \frac{-3f_0 + 4f_1 - f_2}{2h} \quad \text{(forward difference)}$$

$$f'(x_0) \approx \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} \quad \text{(backward difference)}$$

$$f''(x_0) \approx \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2} \quad \text{(forward difference)}$$

$$f''(x_0) \approx \frac{2f_0 - 5f_{-1} + 4f_{-2} - f_{-3}}{h^2} \quad \text{(backward difference)}$$

$$f^{(3)}(x_0) \approx \frac{-5f_0 + 18f_1 - 24f_2 + 14f_3 - 3f_4}{2h^3}$$

$$f^{(3)}(x_0) \approx \frac{5f_0 - 18f_{-1} + 24f_{-2} - 14f_{-3} + 3f_{-4}}{2h^3}$$

$$f^{(4)}(x_0) \approx \frac{3f_0 - 14f_1 + 26f_2 - 24f_3 + 11f_4 - 2f_5}{h^4}$$

$$f^{(4)}(x_0) \approx \frac{3f_0 - 14f_{-1} + 26f_{-2} - 24f_{-3} + 11f_{-4} - 2f_{-5}}{h^4}$$

Richardson's Extrapolation

(3) $$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

(10) $$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}.$$

Write (3) for step sizes h and $2h$

(27) $$f'(x_0) \approx D_0(h) + Ch^2$$

and

(28) $$f'(x_0) \approx D_0(2h) + 4Ch^2.$$

If we multiply relation (27) by 4 and subtract relation (28) from this product, then the terms involving C cancel and the result is

(29) $$3f'(x_0) \approx 4D_0(h) - D_0(2h) = \frac{4(f_1 - f_{-1})}{2h} - \frac{f_2 - f_{-2}}{4h}.$$

Next solve for $f'(x_0)$ in (29) and get

(30) $$f'(x_0) \approx \frac{4D_0(h) - D_0(2h)}{3} = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}.$$

The last expression in (30) is the central-difference formula (10).

Example 6.3. Let $f(x) = \cos(x)$

$$D_0(h) = \frac{(f_1 - f_{-1})}{2h} \qquad D_0(h) \approx \frac{f(0.81) - f(0.79)}{0.02}$$

$$D_0(2h) = \frac{f_2 - f_{-2}}{4h} \qquad D_0(2h) \approx \frac{f(0.82) - f(0.78)}{0.04}$$

$$f'(0.8) \approx \frac{4D_0(h) - D_0(2h)}{3} \approx -0.717356108.$$

$$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} \qquad h = 0.01$$

$$f'(0.8) \approx \frac{-f(0.82) + 8f(0.81) - 8f(0.79) + f(0.78)}{0.12} \approx -0.717356108.$$

Theorem 6.3 (Richardson's Extrapolation). Suppose that two approximations of order $O(h^{2k})$ for $f'(x_0)$ are $D_{k-1}(h)$ and $D_{k-1}(2h)$ and that they satisfy

(34) $$f'(x_0) = D_{k-1}(h) + c_1 h^{2k} + c_2 h^{2k+2} + \cdots$$

and

(35) $$f'(x_0) = D_{k-1}(2h) + 4^k c_1 h^{2k} + 4^{k+1} c_2 h^{2k+2} + \cdots .$$

Then an improved approximation has the form

(36) $$f'(x_0) = D_k(h) + O(h^{2k+2}) = \frac{4^k D_{k-1}(h) - D_{k-1}(2h)}{4^k - 1} + O(h^{2k+2}).$$