Numerical Differentiation

$x_0, \; x_1, \; x_2, \; - - \; x_n$

$f(x_0), \; f(x_1), \; f(x_2), \; - - \; x_n$

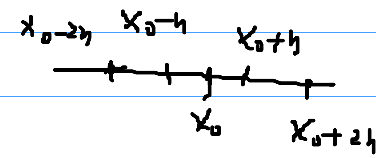
Three-point Endpoint Formula $\qquad h = x_{i+1} - x_i$

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0)$$

Three-point Midpoint Formula

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f^{(3)}(\xi_0)$$

So if we consider five points in Lagrange polynomial, we have Five-Point Midpoint formula and Five-Point Endpoint formula

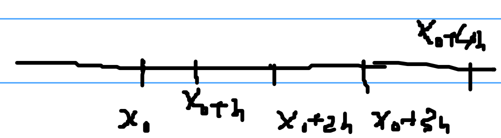


Five-point Midpoint

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30} f^{(5)}(\xi)$$

$$x_0 - 2h < \xi < x_0 + 2h$$

Five-point Endpoint formula



$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] + \frac{h^4}{5} f^{(5)}(\xi)$$

$$x_0 < \xi < x_0 + 4h$$

By replacing h by $-h$ the above formula can be used for x_0-4h, x_0-3h, x_0-2h, x_0-h, x_0

$f(x_0-2h)$ $f(x_0-h)$ $f(x_0+h)$ $f(x_0+2h)$

Example x_0 $h=0.1$ $h=0.2$

x :	1.8,	1.9,	2.0,	2.1,	2.2
$f(x)$:	10.889,	12.703,	14.778,	17.148	19.855

$f(x) = xe^{x}$ $f'(0.2) =$

Use all possible Mid-point and End-point formulas to find $f'(2.0)$.

Here $x_0 = 2.0$

(1) Five-point Mid-point formula, $h = 0.1$

x_0-2h	x_0-h	x_0	x_0+h	x_0+2h
1.8	1.9	2	2.1	2.2

(2) Three-point Endpoint

(i) $h = 0.1$, x_0, x_0+h, x_0+2h

2   2.1   2.2

(ii) $h = 0.1$ $x_0 = 2$ $x_0 - h = 1.9$ $x_0 - 2h = 1.8$

(3) Three-point Midpoint formula

$h = 0.1$ 1.9, 2, 2.1

$h = 0.2$ 1.8, 2 2.2

Round off error instability

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f^{(3)}(\xi_0) \quad \text{— (A)}$$

round off error

$$f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h) \quad \text{— (a)}$$

approximate function value after round off

$$f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h) \quad \text{—— (b)}$$

Substitute these (a) and (b) in (A)

$$f'(x_0) = \frac{1}{2h}\left[\left(\tilde{f}(x_0+h) + e(x_0+h)\right) - \left(\tilde{f}(x_0-h) - e(x_0-h)\right)\right] - \frac{h^2}{6} f^{(3)}(\xi_0)$$

$$f'(x_0) - \frac{1}{2}\left[\tilde{f}(x_0+h) - \tilde{f}(x_0-h)\right] = \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_0)$$

$$\text{Total Error} = \underbrace{\frac{e(x_0+h) - e(x_0-h)}{2h}}_{\text{Round off error}} - \underbrace{\frac{h^2}{6} f^{(3)}(\xi_0)}_{\text{Truncation Error}}$$

$$\left| \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_0) \right| \leq \frac{1}{2h}\left|e(x_0+h)\right| + \frac{1}{2h}\left|e(x_0-h)\right| + \frac{h^2}{6}\left|f^{(3)}(\xi_0)\right|$$

Assume that round off error is bounded by ε

$|e(x_0+h)| \leq \varepsilon$,

$|e(x_0-h)| \leq \varepsilon$, $\quad \varepsilon$ is machine precision,

and the maximum value of $f^{(3)}(x)$ is bounded by $M > 0$

ie, $|f^{(3)}(\xi_0)| \leq M$

$$\left| \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_0) \right| \leq \frac{\varepsilon}{2h} + \frac{\varepsilon}{2h} + \frac{h^2}{6} M = \frac{\varepsilon}{h} + \frac{h^2}{6} M$$

$$E(h) = \frac{\varepsilon}{h} + \frac{h^2}{6} M$$

$$E'(h) = -\frac{\varepsilon}{h^2} + \frac{2h}{6} M$$

$$= -\varepsilon/h^2 + \frac{h}{3} M, \qquad E'(h) = 0,$$

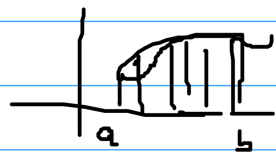
$$-\frac{\varepsilon}{h^2} + h/3\, M = 0, \qquad \frac{\varepsilon}{h^2} = \frac{h}{3} M$$

$$\frac{3\varepsilon}{M} = h^3 , \quad h = \left(\frac{3\varepsilon}{M}\right)^{1/3}$$

$E(h)$ is minimum for $h = \left(\frac{3\varepsilon}{m}\right)^{1/3}$

Numerical integration (4.3)

$$\int_0^1 e^{x^2}\,dx$$



$$\int f(x)\,dx = F(x) + C$$

$$F' = f$$