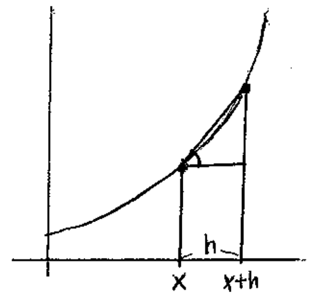
Numerical Differentiation

First-derivative (f') formula via Taylor series

forward: $f'(x) \cong \dfrac{f(x+h) - f(x)}{h}$



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

or $$f'(x) = \frac{f(x+h) - f(x)}{h} \underbrace{\boxed{- \tfrac{1}{2} h\, f''(\xi)}}_{\text{truncation error}} \quad : \quad O(h)$$

We want to have $O(h^2)$ or higher formula.

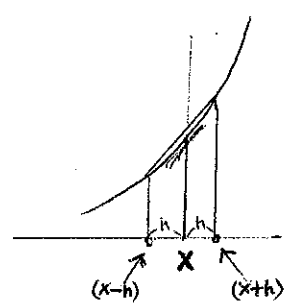
$$f(x+h) = f(x) + h\,f'(x) + \frac{1}{2} h^2 f''(x) + \frac{1}{3!} h^3 f'''(x) + \frac{1}{4!} h^4 f^{iv}(x) + \ldots$$

$$-)\; f(x-h) = f(x) - h\,f'(x) + \frac{1}{2} h^2 f''(x) - \frac{1}{3!} h^3 f'''(x) + \frac{1}{4!} h^4 f^{iv}(x) + \ldots$$

$$f(x+h) - f(x-h) = 2h\,\underline{f'(x)} + \frac{2}{3!} h^3 f'''(x) + \frac{2}{5!} h^5 f^{v}(x) + \ldots$$

$$\underline{f'(x)} = \frac{f(x+h) - f(x-h)}{2h} \underbrace{- \frac{h^2}{3!} f'''(x) + \frac{h^4}{5!} f^{v}(x) - \ldots}_{\text{truncate}}$$

centered $$\cong \underbrace{\boxed{\frac{1}{2h} [f(x+h) - f(x-h)]}}_{\phi(h)} + \underbrace{a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots}_{h_n}$$



Richardson Extrapolation

$$\phi(h) = \frac{f(x+h) - f(x-h)}{2h} \quad : \text{approximate of } f'(x) \text{ with error } O(h^2)$$

Choose h_n such that $\lim_{n\to\infty} h_n = 0$.

$$\phi(h) = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \ldots \qquad \text{(A)}$$
$$\phi(\tfrac{h}{2}) = f'(x) - a_2(\tfrac{h}{2})^2 - a_4(\tfrac{h}{2})^4 - a_6(\tfrac{h}{2})^6 - \ldots \qquad \text{(B)}$$

(A) – 4(B):

$$\phi(h) - 4\,\phi(\tfrac{h}{2}) = -3\, f'(x) - \tfrac{3}{4}\, a_4 h^4 - \tfrac{15}{16}\, a_6 h^6 - \ldots..$$

Divide by 3 and rearrange:

$$\boxed{\phi(\tfrac{h}{2}) + 1/3\, [\phi(\tfrac{h}{2}) - \phi(h)]} = f'(x) + \tfrac{1}{4}\, a_4 h^4 + \tfrac{5}{16}\, a_6 h^6 + \ldots \qquad : O(h^4)$$

Ex 19.2

$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$

Find $f'(0.5)$

Solution

Let $h = 0.5$

From centered difference,

$$D(0.5) = \frac{f(0.5+0.5) - f(0.5-0.5)}{2\cdot(0.5)} = \frac{0.2 - 1.2}{1} = -1.0 \quad (9.6\% \text{ error})$$

$$D(0.25) = \frac{f(0.5+0.25) - f(0.5-0.25)}{2\cdot(0.25)} = \frac{0.6363281 - 1.103516}{0.5} = -0.934375 \quad (2.4\% \text{ error})$$

Richardson extrapolation:

$$-0.934375 + \tfrac{1}{3}\left[-0.934375 - (-1.0)\right] = -0.934375 + \tfrac{1}{3}(0.065625)$$
$$= -0.934375 + 0.0328125$$
$$= -0.9125 \quad (0\% \text{ error})$$

Second-Derivatives (f'') Formulas via Taylor Series

$$
\begin{aligned}
& f(x+h) = f(x) + h\,f'(x) + \tfrac{1}{2} h^2 f''(x) + \tfrac{1}{3!} h^3 f'''(x) + \tfrac{1}{4!} h^4 f^{iv}(x) + \dots \\
+)\;& f(x-h) = f(x) - h\,f'(x) + \tfrac{1}{2} h\, f''(x) - \tfrac{1}{3!} h^3 f'''(x) + \tfrac{1}{4!} h^4 f^{iv}(x) + \dots \\
\hline
& f(x+h) + f(x-h) = 2\,f(x) + h^2 \underline{f''(x)} + 2\left[\tfrac{1}{4!} h^4 f^{iv}(x) + \dots\right]
\end{aligned}
$$

$$\boxed{f''(x) = \frac{1}{h^2}\left[\, f(x+h) - 2\,f(x) + f(x-h) \,\right]} + E \quad \text{where } E = O(h^2)$$

Fig. 19.5

Third-Derivative

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

Fourth-Derivative

$$\boxed{f^{iv}(x) = \frac{1}{h^4}\left[f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h) \right]}$$

Unequally Spaced Data

Idea.

For first drivative (f') formula,

Step 1. Find $P \cong f$ (Lagrange interpolation)

Step 2. $f' \simeq P'$ (divided difference)

n = 2:

$$P_1(x) = f(x_1) + f[x_1,x_2]\,(x - x_1)$$

$$f'(x) \simeq P_1'(x) = f[x_1,x_2] = \frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

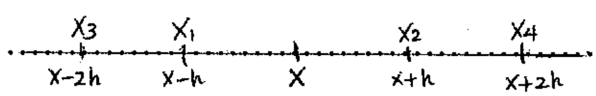
Note. if $x_1 = x$, $x_2 = x + h$, then $f'(x) \cong \frac{f(x+h) - f(x)}{h}$: forward

if $x_1 = x - h$, $x_2 = x + h$, then $f'(x) \cong \frac{f(x+h) - f(x-h)}{2h}$: centered

n = 3: $P_2(x) = f(x_1) + f[x_1,x_2]\,(x - x_1) + f[x_1,x_2,x_3]\,(x - x_1)(x - x_2)$

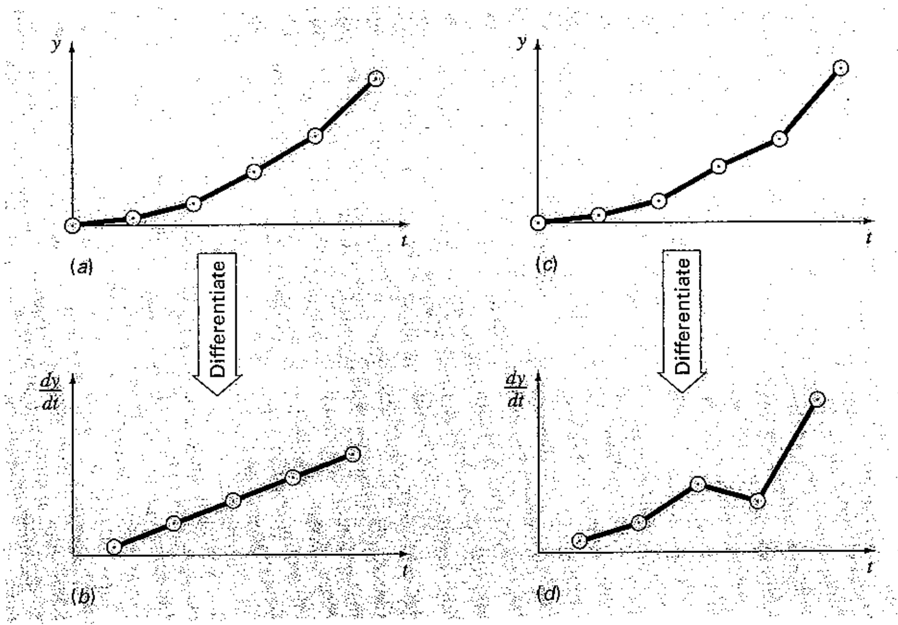
$$P_2'(x) = f[x_1,x_2] + f[x_1,x_2,x_3]\,(2x - x_1 - x_2)$$

n = 4:



$$f'(x) \cong \frac{f(x+h) - f(x-h)}{2h} - \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{12h}$$

Data with errors

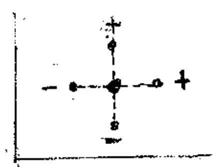


PARTIAL DERIVATIVES

First:

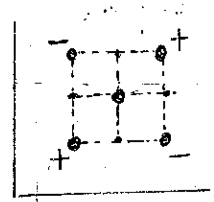
$$\frac{\partial f}{\partial x} = \frac{f(x+\Delta x, y) - f(x-\Delta x, y)}{2\Delta x}$$

$$\frac{\partial f}{\partial y} = \frac{f(x, y+\Delta y) - f(x, y-\Delta y)}{2\Delta y}$$



Second:

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)$$



$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\frac{\partial f}{\partial y}(x+\Delta x, y) - \frac{\partial f}{\partial y}(x-\Delta x, y)}{2\Delta x}$$

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\frac{f(x+\Delta x, y+\Delta y) - f(x+\Delta x, y-\Delta y)}{2\Delta y} - \frac{f(x-\Delta x, y+\Delta y) - f(x-\Delta x, y-\Delta y)}{2\Delta y}}{2\Delta x}$$

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{f(x+\Delta x, y+\Delta y) - f(x+\Delta x, y-\Delta y) - f(x-\Delta x, y+\Delta y) + f(x-\Delta x, y-\Delta y)}{4\Delta x \Delta y}$$