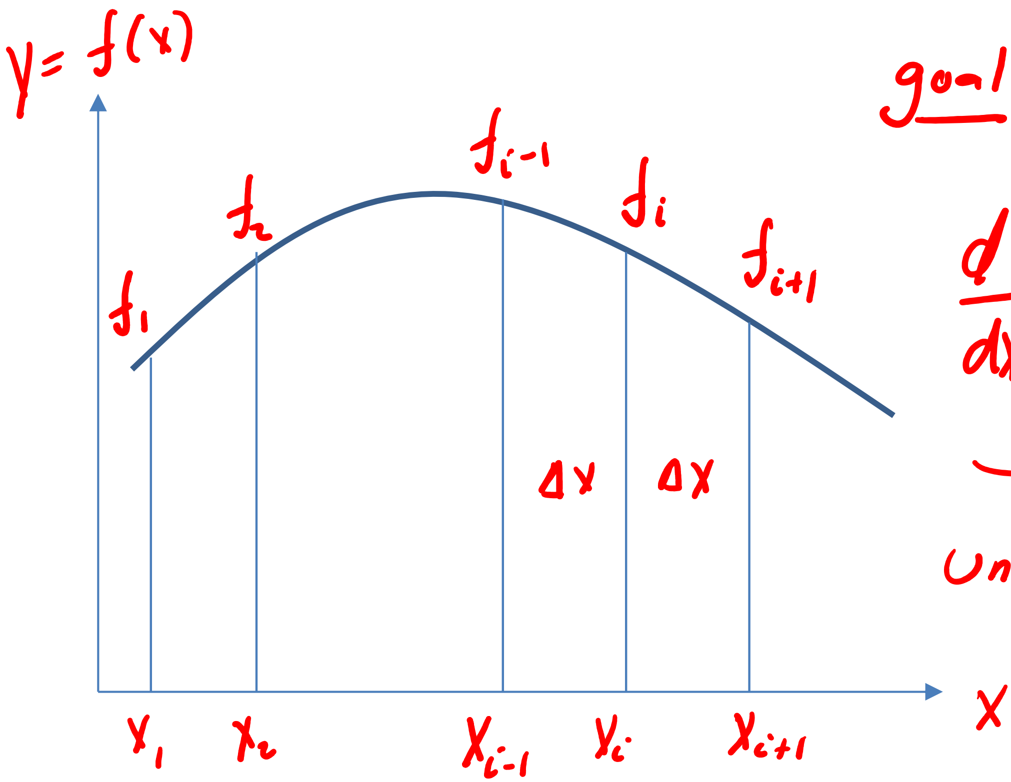
Numerical Differentiation

<u>Numerical differentiation</u> – approximating derivatives of functions

- uniform intervals Δx
- x_i: arbitrary location



<u>goal</u> relate derivatives

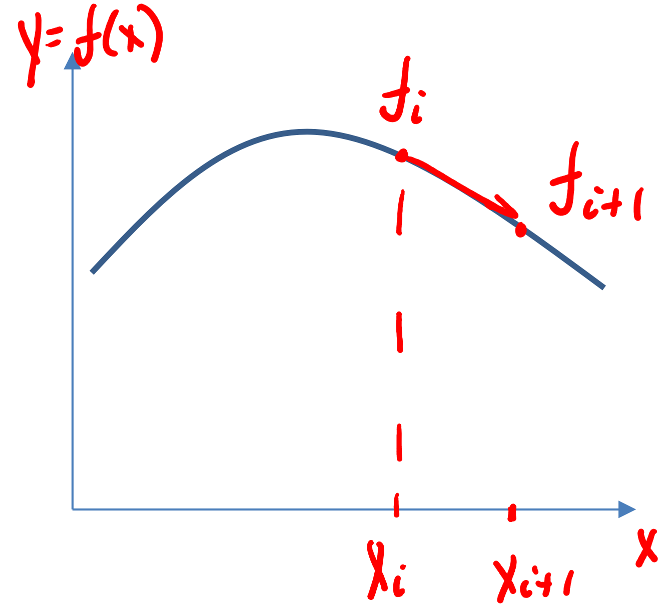
$$\underbrace{\frac{df}{dx},\ \frac{d^2f}{dx^2}}_{\text{unknown}} \text{ to } \underbrace{f \text{ values}}_{\text{known}}$$

Forward difference

- uses "forward" values

f_i, f_{i+1}, f_{i+2}, etc. to approx. derivative at x_i

from calculus



$$\left.\frac{df}{dx}\right|_{x_i} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

$$= \text{slope of } f \text{ at } x_i$$

approx. using

$$\left.\frac{df}{dx}\right|_{x_i} \cong \frac{f_{i+1} - f_i}{\Delta x}$$

Accuracy of approximation based on Taylor series

$$f(x_{i+1}) = f(x_i) + \Delta x \underbrace{f'(x_i)}_{\text{to LHS}} + f''(x_i)\frac{\Delta x^2}{2!} + f'''(x_i)\frac{\Delta x^3}{3!} + \ldots$$

rearrange

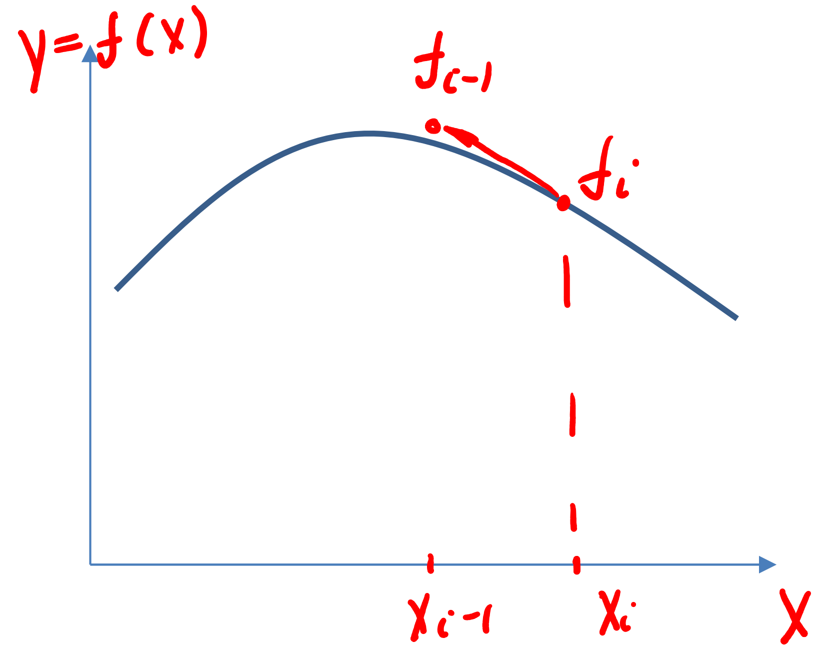
$$\left.\frac{df}{dx}\right|_{x_i} = \underbrace{\frac{f_{i+1} - f_i}{\Delta x}}_{\text{FD approx}} + \underbrace{\frac{\Delta x}{2!}\frac{d^2 f}{dx^2} + \frac{\Delta x^2}{3!}(\quad) + \cdots}_{\text{since } \Delta x < 1 \text{, neglect h.o.t.}}$$

error $E \propto \Delta x = O(\Delta x)$

$\therefore$ first order approximation

Backward difference

$$\left.\frac{df}{dx}\right|_{x_i} \cong \frac{f_i - f_{i-1}}{\Delta x} \quad , \quad E \propto \Delta x$$



Central difference

$$f(x_{i+1}) = f(x_i) + \Delta x\, f'(x_i) + f''(x_i)\frac{\Delta x^2}{2!} + f'''(x_i)\frac{\Delta x^3}{3!} + \ldots \leftarrow FD$$

$$-\left(f(x_{i-1}) = f(x_i) - \Delta x\, f'(x_i) + f''(x_i)\frac{\Delta x^2}{2!} - f'''(x_i)\frac{\Delta x^3}{3!} + \ldots\right) \leftarrow BD$$

$$f_{i+1} - f_{i-1} = 2\Delta x\, f'_i + 2\frac{\Delta x^3}{3!} f''' + \ldots \leftarrow \text{solve for } f'$$

$$\left.\frac{df}{dx}\right|_{x_i} \cong \frac{f_{i+1} - f_{i-1}}{2\Delta x} \quad , \quad E \propto \Delta x^2 \leftarrow \text{second order approx. method}$$

EXAMPLE $\frac{df(0.5)}{dx}$ for $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2\ x$

$f'_{exact} = -0.9125$

select $\Delta x = 0.5$

$x_{i-1} = 0$ $\quad f_{i-1} = 1.2$

$x_i = 0.5$ $\quad f_i = 0.925$

$x_{i+1} = 1$ $\quad f_{i+1} = 0.2$

$$f'_{FD} = \frac{0.2 - 0.925}{0.5} = -1.45 \qquad E = 0.5375\ (59\%)$$

$$f'_{BD} = \frac{0.925 - 1.2}{0.5} = -0.55 \qquad E = 0.3625\ (40\%)$$

$$f'_{CD} = \frac{0.2 - 1.2}{2(0.5)} = -1.0 \qquad E = 0.0875\ (10\%)$$

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

x	*f(x)*	*f'(x)*	*E*
$x_{i-1} = 0.25$	1.104	$f'_{FD} = -1.155$	27%
$x_i = 0.5$	0.925	$f'_{BD} = -0.714$	22%
$x_{i+1} = 0.75$	0.636	$f'_{CD} = -0.934$	2.4%

reduce Δx by factor of 2

FD, BD: first order, $E \propto \Delta x$

59% → 27%, 40% → 22%

CD second order, $E \propto \Delta x^2$

reduced by $2^2 = 4$

10% → 2.4%

2^{nd} derivatives - requires 3 points

Forward difference → eliminate f'

$$f(x_{i+2})=f(x_i) + 2\Delta x\, f'(x_i)+ f''(x_i)\,\frac{(2\Delta x)^2}{2!} + f'''(x_i)\,\frac{(2\Delta x)^3}{3!}+\ldots$$

$$(-2)\times\left(f(x_{i+1})=f(x_i) + \Delta x\, f'(x_i) + f''(x_i)\,\frac{\Delta x^2}{2!} + f'''(x_i)\,\frac{\Delta x^3}{3!}+\ldots \right)$$

$$f_{i+2} - 2f_{i+1} = -f_i + f_i''\,\Delta x^2 + \qquad f'''\,\Delta x^3 (\qquad) + \ldots$$

$$f''_{i,FD} = \frac{f_{i+2} - 2f_{i+1} + f_i}{\Delta x^2}, \quad E \propto \Delta x$$

first order approx.

Higher accuracy approximations by including more points

Forward difference , first derivative , eliminate f''

$$f(x_{i+2})=f(x_i) + 2\Delta x\, f'(x_i) + f''(x_i)\frac{(2\Delta x)^2}{\cancel{2!}}{}^{2} + f'''(x_i)\frac{(2\Delta x)^3}{3!} + \ldots$$

$$4\times\left(f(x_{i+1})=f(x_i) + \Delta x\, f'(x_i) + f''(x_i)\frac{\Delta x^2}{\cancel{2!}}{}^{1/2} + f'''(x_i)\frac{\Delta x^3}{3!} + \ldots\right)$$

$$f_{i+2} - 4f_{i+1} = -3f_i - 2\Delta x\, f_i' + \Delta x^3 f_i'''(\quad) + \ldots$$

$$f'_{i,FD} = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x}, \quad E \propto \Delta x^2$$

Forward difference equation summary (Fig. 23.1)

First Derivative | Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} \qquad O(h)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} \qquad O(h^2)$$

Second Derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} \qquad O(h)$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} \qquad O(h^2)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3} \qquad O(h)$$

$$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3} \qquad O(h^2)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4} \qquad O(h)$$

$$f''''(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4} \qquad O(h^2)$$

Backward difference equation summary (Fig. 23.2)

First Derivative	**Error**
$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$	$O(h^2)$

Central difference equation summary (Fig. 23.3)

First Derivative | Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \qquad O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} \qquad O(h^4)$$

Second Derivative

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} \qquad O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} \qquad O(h^4)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3} \qquad O(h^2)$$

$$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3} \qquad O(h^4)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4} \qquad O(h^2)$$

$$f''''(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4} \qquad O(h^4)$$

EXAMPLE $\frac{df(0.5)}{dx}$ for $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2\ x$

$\Delta x = 0.25$

x	$f(x)$
$x_{i-2} = 0$	1.2
$x_{i-1} = 0.25$	1.104
$x_i = 0.5$	0.925
$x_{i+1} = 0.75$	0.636
$x_{i+2} = 1.0$	0.2

$$f'_{FD} = \frac{\left(-0.2 + 4(0.636) - 3(0.925)\right)}{2(0.25)}$$

$$= -0.859 \quad (5.8\%)$$

$$f'_{CD} = \frac{\left(-0.2 + 8(0.636) - 8(1.104) + 1.2\right)}{12(0.25)}$$

$$= 0.9125 \quad (\approx 0\% \text{ error})$$