Derivatives

$$\underbrace{f(x_i+\Delta x)}_{=x} = f(x_i) + \underbrace{\Delta x}_{x-x_i=\Delta x} f'(x_i) + \frac{\Delta x^2}{2!} f^2(x_i) + \ldots \quad (1)$$

$$f(x_i-\Delta x) = f(x_i) - \Delta x\, f'(x_i) + \frac{\Delta x^2}{2!} f^2(x_i) + \ldots \quad (2)$$

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from (1)

$$\boxed{f'(x_i) = \frac{f(x_i+\Delta x) - f(x_i)}{\Delta x}} - \frac{\Delta x}{2!} f^2(x_i)$$

$$\boxed{f'(x_i) = \frac{f(x_i+\Delta x) - f(x_i)}{\Delta x}} + \underbrace{O(\Delta x)}_{\text{Indicates terms of order } \Delta x \text{ and more}}$$

Two-point Forward Difference approximation

Difference approximation

Using ②

$$\boxed{f'(x_i) = \frac{f(x_i) - f(x_i - \Delta x)}{\Delta x} + O(\Delta x)}$$

Two-point backward difference approximation.

① - ②

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

$$\boxed{f'(x_i) = \frac{f(x_i + \Delta x) - f(x_i - \Delta x)}{2\Delta x} + O(\Delta x^2)}$$

Two-point central difference approximation.

EXAMPLE: Compute the first derivative of $\cos(x)$ at $x = \frac{\pi}{6}$ using

(i) forward difference
(ii) backward difference
(iii) central difference

Use a step size of 1e-2 (=0.01) and 1e-4 (0.0001). Compare against the actual value.

Solution:

Actual value calculation.

$$y = \cos(x) \Rightarrow \frac{dy}{dx} = -\sin(x)$$

$$\left.\frac{dy}{dx}\right|_{x=\pi/6} = \frac{dy}{dx}\left(x = \pi/6\right) = -0.5$$

(i) Forward difference $\dfrac{f(x+\Delta x) - f(x)}{\Delta x}$

(ii) Backward difference $\dfrac{f(x) - f(x-\Delta x)}{\Delta x}$

(iii) Central difference $\dfrac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$

$\Delta x = 1e-2 = 0.01$

(i) Forward diff: $\dfrac{\cos(\pi/6 + 0.01) - \cos(\pi/6)}{0.01}$

$= -0.5042$

(ii) Backward diff: $\dfrac{\cos(\pi/6) - \cos(\pi/6 - 0.01)}{0.01}$

$= -0.4956$

(iii) Central diff: $\dfrac{\cos(\pi/6 + 0.01) - \cos(\pi/6 - 0.01)}{2(0.01)}$

$= -0.4999$

$= \quad -0.4999$

Using Octave for $\Delta x = 1e-4$ (see code)

Forward	-0.50004
Backward	-0.49995
Central	-0.49999

One can use the Taylor series to get $f^2(x)$, $f^3(x)$, ... so on.

Add (1) & (2) and solve for $f^2(x)$

$$\boxed{f^2(x) = \frac{f(x_i+\Delta x) + f(x_i-\Delta x) - 2f(x_i)}{\Delta x^2} + O(\Delta x^2)}$$

Three-point second difference approximation

Forward Difference

Forward Difference Approximations of $O(\Delta x)$

$$f_i' = \frac{f_{i+1} - f_i}{\Delta x}$$

$$f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{(\Delta x)^2} - 2$$

$$f_i''' = \frac{f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i}{(\Delta x)^3}$$

$$f_i'''' = \frac{f_{i+4} - 4f_{i+3} + 6f_{i+2} - 4f_{i+1} + f_i}{(\Delta x)^4}$$

Forward Difference Approximations of $O[(\Delta x)^2]$

$$f_i' = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x}$$

$$f_i'' = \frac{-f_{i+3} + 4f_{i+2} - 5f_{i+1} + 2f_i}{(\Delta x)^2}$$

$$f_i''' = \frac{-3f_{i+4} + 14f_{i+3} - 24f_{i+2} + 18f_{i+1} - 5f_i}{2(\Delta x)^3}$$

$$f_i'''' = \frac{-2f_{i+5} + 11f_{i+4} - 24f_{i+3} + 26f_{i+2} - 14f_{i+1} + 3f_i}{(\Delta x)^4}$$

$$f_i = f(x_i)$$

$$f_{i+1} = f(x_i + \Delta x)$$

$$f_{i-1} = f(x_i - \Delta x)$$

$$f_{i-2} = f(x_i - 2\Delta x)$$

Backward Difference

Backward Difference Approximations of $O(\Delta x)$

$$f_i' = \frac{f_i - f_{i-1}}{\Delta x}$$

$$f_i'' = \frac{f_i - 2f_{i-1} + f_{i-2}}{(\Delta x)^2}$$

$$f_i''' = \frac{f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3}}{(\Delta x)^3}$$

$$f_i'''' = \frac{f_i - 4f_{i-1} + 6f_{i-2} - 4f_{i-3} + f_{i-4}}{(\Delta x)^4}$$

Backward Difference Approximations of $O[(\Delta x)^2]$

$$f_i' = \frac{3f_i - 4f_{i-1} + f_{i-2}}{2\Delta x}$$

$$f_i'' = \frac{2f_i - 5f_{i-1} + 4f_{i-2} - f_{i-3}}{(\Delta x)^2}$$

$$f_i''' = \frac{5f_i - 18f_{i-1} + 24f_{i-2} - 14f_{i-3} + 3f_{i-4}}{2(\Delta x)^3}$$

$$f_i'''' = \frac{3f_i - 14f_{i-1} + 26f_{i-2} - 24f_{i-3} + 11f_{i-4} - 2f_{i-5}}{(\Delta x)^4}$$

Central Difference

Central Difference Approximations of $O[(\Delta x)^2]$

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2} \quad \Big\} \quad 1$$

$$f_i''' = \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2(\Delta x)^3}$$

$$f_i'''' = \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{(\Delta x)^4}$$

Central Difference Approximations of $O[(\Delta x)^4]$

$$f_i' = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x}$$

$$f_i'' = \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12(\Delta x)^2}$$

$$f_i''' = \frac{-f_{i+3} + 8f_{i+2} - 13f_{i+1} + 13f_{i-1} - 8f_{i-2} + f_{i-3}}{8(\Delta x)^3}$$

$$f_i'''' = \frac{-f_{i+3} + 12f_{i+2} - 39f_{i+1} + 56f_i - 39f_{i-1} + 12f_{i-2} - f_{i-3}}{6(\Delta x)^4}$$

EXAMPLE: Compute the 2^{nd} derivative of $\tan(x)$ at $x = \pi/6$ using

(i) 3-point central diff. $O(\Delta x^2)$

(ii) 3-point forward diff. $O(\Delta x)$

(iii) 3-point backward diff $O(\Delta x)$

Use step size 10^{-2} or 1e-2 and 10^{-4} or 1e-4.

Compare against actual value

Solution

Actual value $f(x) = \tan x$

$$f'(x) = \sec^2 x$$

$$f''(x) = (2\sec x)(\sec x \tan x)$$

$$= 2\sec^2 x \tan x$$

$$f''(\pi/6) = 1.5396$$

(i) Three-pt central: $\dfrac{f(x+\Delta x)+f(x-\Delta x)-2f(x)}{\Delta x^2}$

(ii) Three-pt. forward: $\dfrac{f(x+2\Delta x)-2f(x+\Delta x)+f(x)}{\Delta x^2}$

(iii) Three-pt. backward: $\dfrac{f(x)-2f(x-\Delta x)+f(x-2\Delta x)}{\Delta x^2}$

Using MATLAB

	$\Delta x = 1e^{-2}$	$\Delta x = 1e^{-4}$	True value
Three-pt central	1.5397 ✓	1.5396 ✓	1.5396
Three-pt. forward	1.5940	1.5401	
Three-pt backward	1.4873	1.5390	

Forward Difference

Forward Difference Approximations of $O(\Delta x)$

$$f_i' = \frac{f_{i+1} - f_i}{\Delta x}$$

$$f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{(\Delta x)^2}$$

$$f_i''' = \frac{f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i}{(\Delta x)^3}$$

$$f_i'''' = \frac{f_{i+4} - 4f_{i+3} + 6f_{i+2} - 4f_{i+1} + f_i}{(\Delta x)^4}$$

Forward Difference Approximations of $O[(\Delta x)^2]$

$$f_i' = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x}$$

$$f_i'' = \frac{-f_{i+3} + 4f_{i+2} - 5f_{i+1} + 2f_i}{(\Delta x)^2}$$

$$f_i''' = \frac{-3f_{i+4} + 14f_{i+3} - 24f_{i+2} + 18f_{i+1} - 5f_i}{2(\Delta x)^3}$$

$$f_i'''' = \frac{-2f_{i+5} + 11f_{i+4} - 24f_{i+3} + 26f_{i+2} - 14f_{i+1} + 3f_i}{(\Delta x)^4}$$

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Backward Difference

Backward Difference Approximations of $O(\Delta x)$

$$f_i' = \frac{f_i - f_{i-1}}{\Delta x}$$

$$f_i'' = \frac{f_i - 2f_{i-1} + f_{i-2}}{(\Delta x)^2}$$

$$f_i''' = \frac{f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3}}{(\Delta x)^3}$$

$$f_i'''' = \frac{f_i - 4f_{i-1} + 6f_{i-2} - 4f_{i-3} + f_{i-4}}{(\Delta x)^4}$$

Backward Difference Approximations of $O[(\Delta x)^2]$

$$f_i' = \frac{3f_i - 4f_{i-1} + f_{i-2}}{2\Delta x}$$

$$f_i'' = \frac{2f_i - 5f_{i-1} + 4f_{i-2} - f_{i-3}}{(\Delta x)^2}$$

$$f_i''' = \frac{5f_i - 18f_{i-1} + 24f_{i-2} - 14f_{i-3} + 3f_{i-4}}{2(\Delta x)^3}$$

$$f_i'''' = \frac{3f_i - 14f_{i-1} + 26f_{i-2} - 24f_{i-3} + 11f_{i-4} - 2f_{i-5}}{(\Delta x)^4}$$

Central Difference

Central Difference Approximations of $O[(\Delta x)^2]$

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2}$$

$$f_i''' = \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2(\Delta x)^3}$$

$$f_i'''' = \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{(\Delta x)^4}$$

Central Difference Approximations of $O[(\Delta x)^4]$

$$f_i' = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x}$$

$$f_i'' = \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12(\Delta x)^2}$$

$$f_i''' = \frac{-f_{i+3} + 8f_{i+2} - 13f_{i+1} + 13f_{i-1} - 8f_{i-2} + f_{i-3}}{8(\Delta x)^3}$$

$$f_i'''' = \frac{-f_{i+3} + 12f_{i+2} - 39f_{i+1} + 56f_i - 39f_{i-1} + 12f_{i-2} - f_{i-3}}{6(\Delta x)^4}$$