Numerical Approximation of Derivatives

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Key Questions

- Explain how a 1st derivative is approximated numerically when you know only function values
- Explain how a 2nd derivative is approximated numerically when you know only function values

Forward Approximation of 1st Derivative

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

Backward Approximation of 1st Derivative

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

Central Approximation of 1st Derivative

- $f(x+\Delta x) = f(x) + f'(x)\Delta x + \frac{f''(x)}{2!}\Delta x^2 + \cdots$
- $f(x-\Delta x) = f(x) - f'(x)\Delta x + \frac{f''(x)}{2!}\Delta x^2 + \cdots$
- $f(x+\Delta x) - f(x-\Delta x) = 2f'(x)\Delta x + O(\Delta x^3)$
- $f'(x) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + O(\Delta x^2)$

Approximation of 2nd Derivative

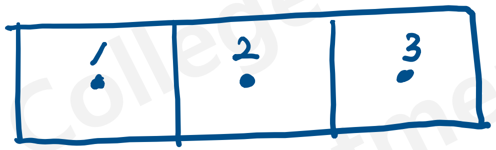
- $f(x+\Delta x) = f(x) + f'(x)\Delta x + \frac{f''(x)}{2!}\Delta x^2 + \cdots$
- $f(x-\Delta x) = f(x) - f'(x)\Delta x + \frac{f''(x)}{2!}\Delta x^2 + \cdots$
- $f(x+\Delta x) + f(x-\Delta x) = 2f(x) + f''(x)\Delta x^2 + O(\Delta x^4)$
- $f''(x) = \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta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

Smaller Δx is Better?

- No
- Smaller Δx makes $\partial f / \partial x$ more accurate, but if Δx is too small, $f(x + \Delta x) - f(x)$ may be zero
- How to decide Δx?
  - ✓Not too large, not too small
  - ✓1%, 0.1%, 0.01%, … of x
  - ✓Depends on your problem
  - ✓Central approximation is less sensitive to a perturbation size (Δx) than forward and backward approximations

Central Approximation is Always Better?

- No
- Higher computation cost
- Not appropriate in some cases



x_1, x_2, x_3: locations

u_1, u_2, u_3: x-directional velocity

$$\left.\frac{\partial u}{\partial x}\right|_{x_2} = \frac{u_3 - u_1}{2\delta x} \quad \text{central}$$

$$\frac{u_3 - u_2}{\delta x} \quad \text{forward}$$

유동방향이 2 → 3 으로 흐른다면 forward 가 더 적절할 수 있음.