

$$\sin\left(\frac{\pi}{2} + h\right) = \sin\left(\frac{\pi}{2}\right) + \cos\left(\frac{\pi}{2}\right)h + \underbrace{\left(-\sin\left(\frac{\pi}{2}\right)\right)\frac{h^2}{2}} + \underbrace{\left(-\cos\left(\frac{\pi}{2}\right)\right)\frac{h^3}{3!}} + O(h^4)$$

Review: Numerical Differentiation

Formulas using Taylor Series

Given smooth function $f(x)$, we can approximate the derivative $f'(x)$

eg $\left. \frac{d \sin(x)}{dx} \right|_{x=\frac{\pi}{2}} = \sin'\left(\frac{\pi}{2}\right) : f = \sin(x), x_0 = \frac{\pi}{2}, f'(x) = \cos(x)$

$$f'(x_0) = \lim_{h \rightarrow 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

- Recall for small h , the Taylor series expansion of $f(x_0 + h)$ is given by:

eg?

$$\sum_{i=0}^{\infty} \frac{f^{(i)}(x_0)}{i!} h^i = f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(x_0) + O(h^4) \quad (1)$$

- The Big- O notation is used to describe the error term in the Taylor series expansion. And it means that the error term is bounded by a constant times h^4 !

- Therefore $D_h^+ f(x_0) \equiv \frac{f(x_0 + h) - f(x_0)}{h} \approx f'(x_0) + f''(x_0)\frac{h}{2}$. This is:

- Forward difference formula

$D_h^+ f(x_0) \approx f'(x_0) + f''(x_0)\frac{h}{2}$

First-order approximation of $f'(x_0)$

$$\frac{f(x_0 + h) - f(x_0)}{h} \approx f'(x_0) + f''(x_0)\frac{h}{2} + O(h^2)$$

Backward difference formula: $D_h^- f(x_0) \equiv \frac{f(x_0) - f(x_0 - h)}{h} \approx f'(x_0) - \frac{h}{2}f''(\xi)$, where $\xi \in [x_0 - h, x_0]$. We note this leads to

$$f'(x_0) = D_h^- f(x_0) + E_{\text{trunc}}(f, h), \quad E_{\text{trunc}}(f, h) = \frac{h}{2}f''(\xi_1) \quad (2)$$

$$f(x_0 + h) \approx f(x_0) + f'(x_0)h + f''(x_0)\frac{h^2}{2}$$

$$f(x_0 + h) \approx f(x_0) + f'(x_0)h + f''(\xi_1)\frac{h^2}{2}$$

Here $E_{\text{trunc}}(f, h)$ is the truncation error for using the backward difference formula $D_h^- f(x_0)$ to approximate $f'(x_0)$.

- **Definition:** Truncation errors are the errors that result from using an approximation $Df(x, h)$ in place of an exact mathematical procedure $f'(x_0)$:

$$E(h) = |f'(x_0) - Df(x_0, h)|, \quad (3)$$

\swarrow analytical \nwarrow value

where x_0 is fixed. The approximation is p -th order accurate, means

$$|E(h)| \leq Ch^p, \text{ for some } C > 0, h \geq 0 \text{ sufficiently small.} \quad (4)$$

We use the notation

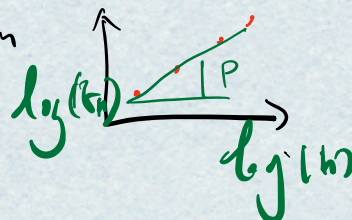
$$Df(x_0) = f'(x_0) + O(h^p) \quad (5)$$

- Plotting the error: assuming the error is $O(h^p)$, then the error should be proportional to h^p , i.e., $E(h) \approx Ch^p$, then

$$\log(|E(h)|) \approx \log(C) + p \log(h). \quad (*)$$

\nwarrow vertical \nwarrow horizontal

We can compute the error for different values of h and plot $\log(|E(h)|)$ versus $\log(h)$! and (*) show a line in



$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(x_0) + \mathcal{O}(h^4)$$

Central difference formula

- We note the Taylor series should give us:

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(x_0) + \mathcal{O}(h^4). \quad (6)$$

$$\frac{f(x_0 + h) - f(x_0 - h)}{2h} = f'(x_0) + \frac{h^2}{6}f'''(x_0) + \mathcal{O}(h^4)$$

- Then we have

$$D_0 f(x_0) \equiv \frac{1}{2}(D_h^+ f(x_0) + D_h^- f(x_0)) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} \approx f'(x_0) + \frac{h^2}{6}K$$

- This central difference *stencil* is second order accurate.

Example: A second-order one sided finite difference formula for derivative:

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h} + \frac{h^2}{3}f'''(\xi), \quad (7)$$

where $\xi \in [x_0, x_0 + h]$. How do we derive (7)? We want to set

$$D_2 f(x_0) \equiv af(x_0) + bf(x_0 + h) + cf(x_0 + 2h) = f'(x_0) + \mathcal{O}(h^2). \quad (8)$$

and note

$$f(x_0 + 2h) = f(x_0) + \frac{2h}{1}f'(x_0) + \frac{(2h)^2}{2}f''(x_0) + \frac{(2h)^3}{6}f'''(x_0) + \mathcal{O}(h^4) \quad (9)$$

So (8) is indeed

$$D_2f(x_0) = (a+b+c)f(x_0) + (b+2c)\frac{h}{1}f'(x_0) + (b+4c)\frac{h^2}{2}f''(x_0) + (b+8c)\frac{h^3}{6}f'''(x_0) + \mathcal{O}(h^4).$$

Now we can see this leads to

$$a + b + c = 0, \quad b + 2c = 1/h, \quad b + 4c = 0,$$

which gives $a = \frac{-3}{2h}$, $b = \frac{4}{2h}$, and $c = -\frac{1}{2h}$.

This method could be used to derive other finite difference formulas.

Example: A fourth-order central difference formula for derivative $f'(x_0)$:

$$f'(x_0) = \frac{-f(x_0 + 2h) + 8f(x_0 + h) - 8f(x_0 - h) + f(x_0 - 2h)}{12h} + \frac{h^4}{30}f^{(5)}(\xi),$$

where $\xi \in [x_0, x_0 + h]$.

Note: We can get higher order approximations by adding more neighboring points.

Centered formula for the second derivative: We note, the difference formula for the second derivative could be derived as $D_h^+(D_h^-f(x_0)) = \frac{1}{h}(D_h^-f(x_0+h) - D_h^-f(x_0))$,

$$D^2f(x_0) = D_h^+D_h^-f(x_0) = \frac{\frac{f(x_0+h)-f(x_0)}{h} - \frac{f(x_0)-f(x_0-h)}{h}}{h}$$