

Numerical Derivatives:

$$\frac{df}{dx} = f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} \quad (\text{forward difference})$$

truncation error:

$$f(x+h) = \underline{f(x)} + \underline{h} f'(x) + \frac{h^2}{2} f''(x) + \mathcal{O}(h^3)$$

$$f'(x) \Rightarrow \frac{f(x+h) - f(x)}{h} = \underline{f'(x)} + \underbrace{\frac{h}{2} f''(x) + \frac{h^2}{6} f'''(x) + \dots}_{\text{truncation error}}$$

truncation error increases w/ h
roundoff error decreases w/ h

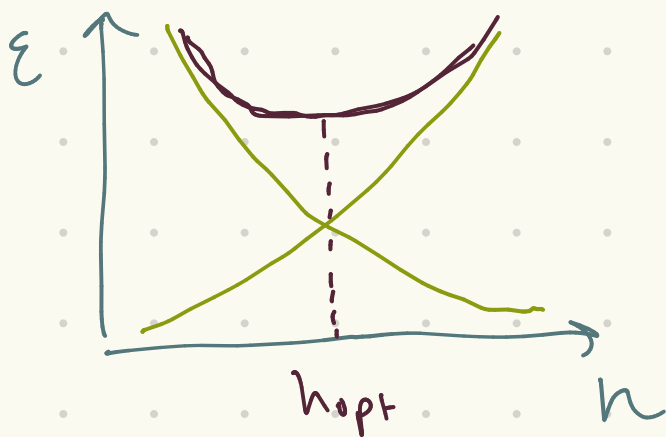
optimizing h :

$$\text{roundoff error} \sim \epsilon_r \sim \epsilon_f \frac{|f|}{h}$$

→ single precision 10^{-7}
double precision 10^{-16}

total error:

$$\epsilon = \epsilon_t + \epsilon_r \sim h f'' + \epsilon_f \frac{|f|}{h}$$



$$\frac{d\epsilon}{dh} = 0 = f'' - \epsilon_f \frac{f}{h^2}$$

$$\Rightarrow h_{\text{opt}} = \sqrt{\frac{\epsilon_f f}{f''}}$$

centered difference method:

$$\frac{df}{dx} = f'(x) = \frac{f(x+h/2) - f(x-h/2)}{h}$$

... Taylor series ... $= f'(x) + \frac{h^2}{24} f'''(x) + \mathcal{O}(h^3)$

↑
no second derivative term

$$e \sim h^2 f''' + \epsilon_f f/h$$

optimal h : $\frac{de}{dh} = 0 = 2hf''' - \epsilon_f f/h^2$

$$h_{opt} \sim \sqrt[3]{\epsilon_f (f/f''')}$$

 larger h_{opt} , smaller ϵ

a more precise method:

$$f'(x) = \frac{f(x+h/4) - f(x-h/4)}{h/2} = f' + \frac{h^2}{96} f''' + \mathcal{O}(h^4)$$

$$\Rightarrow h_{opt} \sim \epsilon_f^{1/5} \sqrt[5]{f/f'''}$$

