Physics 77

Introduction to Computational Techniques in Physics

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Numerical Differentiation

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See also Python workbook Lecture08a.ipynb

Numerical Differentiation

Definition :

$$\frac{df(x)}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Approximation :

$$\frac{df(x)}{dx} = \frac{\Delta f(x)}{\Delta x}$$

$$\Delta^n f(x) = \Delta[\Delta^{n-1} f(x)]$$

Numerical Differentiation

- *The nth difference of a polynomial of degree n is a constant ($a_n n! h^n$), and the (n+1)th difference is zero.*

A Typical Finite Difference Table for $f(x) = x^2$

x_i	$f(x_i)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$
2	$f(2)=4$			
		$\Delta f(2)=5$		
3	$f(3)=9$		$\Delta^2 f(2)=2$	
		$\Delta f(3)=7$		$\Delta^3 f(2)=0$
4	$f(4)=16$		$\Delta^2 f(3)=2$	
		$\Delta f(4)=9$		$\Delta^3 f(3)=0$
5	$f(5)=25$		$\Delta^2 f(4)=2$	
		$\Delta f(5)=11$		
6	$f(6)=36$			

Taylor Series

$$f(x_0+kh) = f(x_0) + khf'(x_0) + \frac{(kh)^2 f''(x_0)}{2!} +$$

$$\frac{(kh)^3 f'''(x_0)}{3!} + \cdots + \frac{(kh)^n f^n(x_0)}{n!}$$

Solve for $f'(x)$

$$\frac{f(x_0+kh) - f(x_0)}{kh} = f'(x_0) + \frac{(kh) f''(x_0)}{2!} +$$

$$\frac{(kh)^2 f'''(x_0)}{3!} + \cdots + \frac{(kh)^{n-1} f^n(x_0)}{n!}$$

For $k = -1$,

$$\frac{f(x_0) - f(x_0-h)}{h} = f'(x_0) + O(h) \text{ (backward difference)}$$

Taylor Series

$$f(x_0 + kh) = f(x_0) + khf'(x_0) + \frac{(kh)^2 f''(x_0)}{2!} +$$

$$\frac{(kh)^3 f'''(x_0)}{3!} + \cdots + \frac{(kh)^n f^n(x_0)}{n!}$$

Solve for $f'(x)$

$$\frac{f(x_0 + kh) - f(x_0)}{kh} = f'(x_0) + \frac{(kh) f''(x_0)}{2!} +$$

$$\frac{(kh)^2 f'''(x_0)}{3!} + \cdots + \frac{(kh)^{n-1} f^n(x_0)}{n!}$$

For $k = 1$,

$$\frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0) + O(h) \text{ (forward difference)}$$

Taylor Series

$$f(x_0+kh)=f(x_0)+khf'(x_0)+\frac{(kh)^2 f''(x_0)}{2!}+$$

$$\frac{(kh)^3 f'''(x_0)}{3!}+\cdots+\frac{(kh)^n f^n(x_0)}{n!}$$

$$f(x_0-kh)=f(x_0)-khf'(x_0)+\frac{(kh)^2 f''(x_0)}{2!}-$$

$$\frac{(kh)^3 f'''(x_0)}{3!}+\cdots(-1)^n\frac{(kh)^n f^n(x_0)}{n!}$$

Subtract the two above equations, and set $k=1$:

$$\frac{f(x_0+h)-f(x_0-h)}{2h}=f'(x_0)+O(h^2)\ (\text{central difference})$$

Taylor Series

$$f(x_0 + kh) = f(x_0) + khf'(x_0) + \frac{(kh)^2 f''(x_0)}{2!} +$$

$$\frac{(kh)^3 f'''(x_0)}{3!} + \cdots + \frac{(kh)^n f^n(x_0)}{n!}$$

$$f(x_0 - kh) = f(x_0) - khf'(x_0) + \frac{(kh)^2 f''(x_0)}{2!} -$$

$$\frac{(kh)^3 f'''(x_0)}{3!} + \cdots (-1)^n \frac{(kh)^n f^n(x_0)}{n!}$$

add the two above equations :

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

Higher Order Approximations

$$\text{1st order } f'(x) = \frac{f(x_0 + h) - f(x_0)}{h}$$

$$\text{2nd order } f'(x) = \frac{f(x_0 + h) - f(x_0 - h)}{2h}$$

$$\text{1st order } f''(x) = \frac{f(x_0 + h) + f(x_0 - h) - 2f(x)}{(2h)^2}$$

$$\text{2nd order } f''(x) = \frac{-f(x+3h) + 4f(x+2h) - 5f(x+h) + 2f(x)}{(h)^2}$$

Example: Evaporation Rates

Table: Saturation Vapor Pressure (e_s) in mm Hg as a Function of Temperature (T) in $^{\circ}$C

T($^{\circ}$C)	e_s(mm Hg)
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

The slope of the saturation vapor pressure curve at 22°C (3 methods) :

$$\text{forward} \quad \frac{de_s}{dT} = \frac{e_s(23) - e_s(22)}{23 - 22} = \frac{21.05 - 19.82}{1} = 1.23 \text{ mm Hg/°C}$$

$$\text{backward} \quad \frac{de_s}{dT} = \frac{e_s(22) - e_s(21)}{22 - 21} = \frac{19.82 - 18.65}{1} = 1.17 \text{ mm Hg/°C}$$

$$\text{two-step} \quad \frac{de_s}{dT} = \frac{e_s(23) - e_s(21)}{23 - 21} = \frac{21.05 - 18.65}{2} = 1.20 \text{ mm Hg/°C}$$

The true value is 1.20 mm Hg/°C, so the two-step method provides the most accurate estimate.

See also examples in Python workbook Lecture07a.ipynb