Numerical Methods in Engineering

NUMERICAL DIFFERENTIATION

Lecture 23

Read Chapter 23, Sections 1-2

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Lecture 23

NUMERICAL DIFFERENTIATION

- First order derivatives
- High order derivatives
- Richardson Extrapolation
- Examples

Motivation

- How do you evaluate the derivative of a tabulated function.
- How do we determine the velocity and acceleration from tabulated measurements.

Time (second)	Displacement (meters)
0	30.1
5	48.2
10	50.0
15	40.2

Recall

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

$$\text{Taylor Theorem:}$$

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(x)h^3}{3!} + O(h^4)$$

$$E = O(h^n) \Rightarrow \exists\, real,\ finite\ \ C,\ \ such\ that: \left|E\right| \le C\left|h\right|^n$$

$$\text{E is of order } h^n \Rightarrow E \text{ is approaching zero at rate similar to } h^n$$

Three Formulas

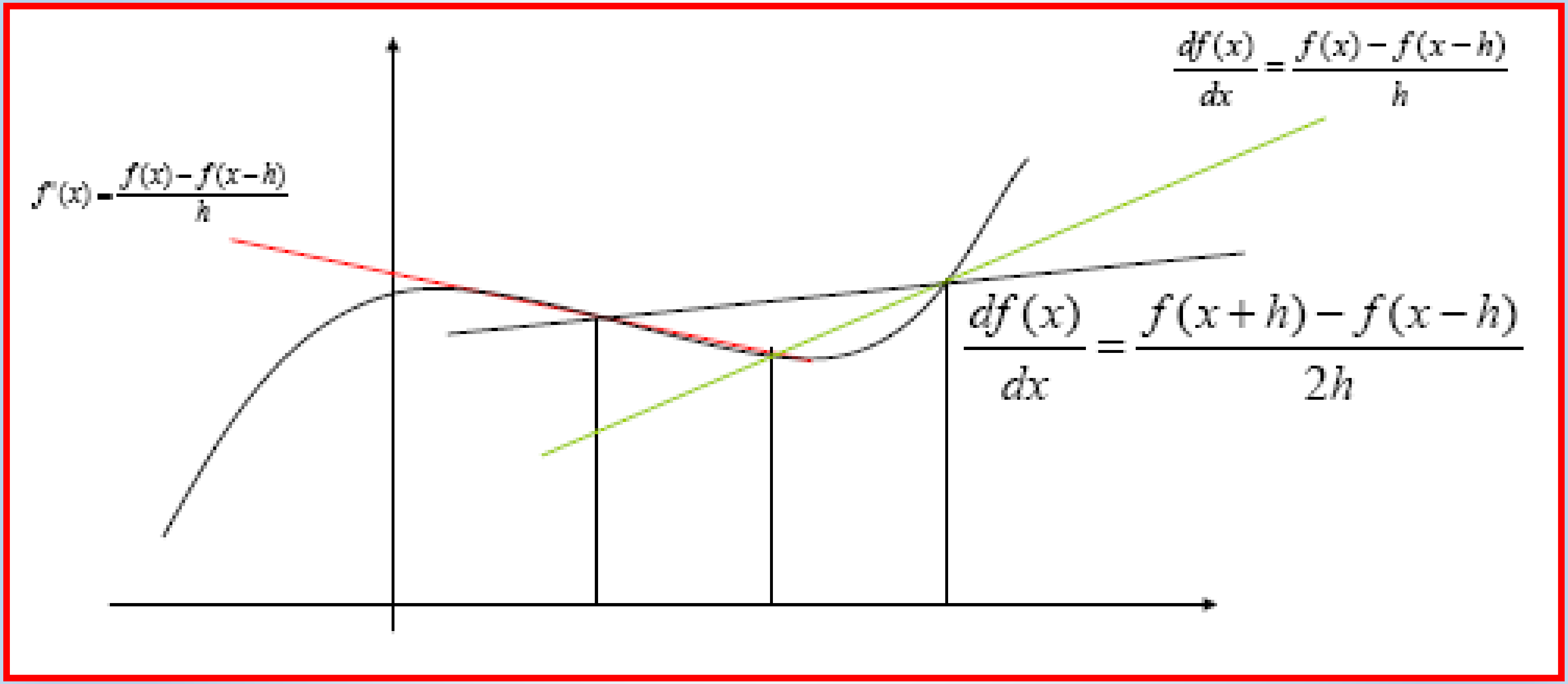
Forward Difference : $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x)}{h}$$

Backward Difference : $$\frac{df(x)}{dx} = \frac{f(x) - f(x-h)}{h}$$

Central Difference : $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x-h)}{2h}$$

Which method is better? How do we judge them?

The Three Formulas



Forward/Backward Difference Formula

Forward Difference:

$$f(x+h) = f(x) + f'(x)h + O(h^2)$$

$$\Rightarrow f'(x)h = f(x+h) - f(x) + O(h^2)$$

$$\Rightarrow f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

Backward Difference:

$$f(x-h) = f(x) - f'(x)h + O(h^2)$$

$$\Rightarrow f'(x)h = f(x) - f(x-h) + O(h^2)$$

$$\Rightarrow f'(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

Central Difference Formula

Central Difference :

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \dots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \dots$$

$$f(x+h) - f(x-h) = 2f'(x)h + 2\frac{f^{(3)}(x)h^3}{3!} + \dots$$

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

The Three Formulas (Revisited)

Forward Difference : $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x)}{h} + O(h)$$

Backward Difference : $$\frac{df(x)}{dx} = \frac{f(x) - f(x-h)}{h} + O(h)$$

Central Difference : $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

Forward and backward difference formulas are comparable in accuracy.
Central difference formula is expected to give a better answer.

Higher Order Formulas

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \ldots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \ldots$$

$$f(x+h) + f(x-h) = 2f(x) + 2\frac{f^{(2)}(x)h^2}{2!} + 2\frac{f^{(4)}(x)h^4}{4!} + \ldots$$

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

$$\boxed{Error = -\frac{f^{(4)}(\xi)h^2}{12}}$$

Other Higher Order Formulas

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

$$f^{(3)}(x) = \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{2h^3}$$

$$f^{(4)}(x) = \frac{f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h)}{h^4}$$

Other formulas for $f^{(2)}(x), f^{(3)}(x)\ldots$ are also possible.

You can use Taylor Theorem to prove them and obtain the error order.

Richardson Extrapolation

$$\text{Central Difference}: \quad f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

Can we get a better formula?

$$\textit{Hold } f(x) \textit{ and } x \textit{ fixed}:$$

$$\phi(h) = \frac{f(x+h) - f(x-h)}{2h}$$

$$\phi(h) = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \ldots$$

Richardson Extrapolation

$$Hold\ \ f(x)\ and\ \ x\ \ fixed:$$

$$\phi(h) = \frac{f(x+h) - f(x-h)}{2h}$$

$$\phi(h) = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \ldots$$

$$\phi(\frac{h}{2}) = f'(x) - a_2\left(\frac{h}{2}\right)^2 - a_4\left(\frac{h}{2}\right)^4 - a_6\left(\frac{h}{2}\right)^6 - \ldots$$

$$\phi(h) - 4\phi(\frac{h}{2}) = -3f'(x) - \frac{3}{4}a_4 h^4 - \frac{15}{16}a_6 h^6 - \ldots$$

$$\Rightarrow\ f'(x) = \frac{\phi(h) - 4\phi(\frac{h}{2})}{-3} + O\left(h^4\right)$$

Richardson Extrapolation Table

D(0,0)=Φ(h)			
D(1,0)=Φ(h/2)	D(1,1)		
D(2,0)=Φ(h/4)	D(2,1)	D(2,2)	
D(3,0)=Φ(h/8)	D(3,1)	D(3,2)	D(3,3)

Richardson Extrapolation Table

$$First\ Column:\quad D(n,0)=\phi\left(\frac{h}{2^n}\right)$$

$$Others:$$

$$D(n,m)=D(n,m-1)+\frac{1}{4^m-1}\left[D(n,m-1)-D(n-1,m-1)\right]$$

Example

Evaluate numerically the derivative of :

$$f(x) = x^{\cos(x)} \qquad \text{at} \quad x = 0.6$$

Use Richardson Extrapolation with $h = 0.1$

Obtain D(2,2) as the estimate of the derivative.

Example
First Column

$$\Phi(h) = \frac{f(x+h) - f(x-h)}{2h}$$

$$\Phi(0.1) = \frac{f(0.7) - f(0.5)}{0.2} = 1.08483$$

$$\Phi(0.05) = \frac{f(0.65) - f(0.55)}{0.1} = 1.08988$$

$$\Phi(0.025) = \frac{f(0.625) - f(0.575)}{0.05} = 1.09115$$

Example
Richardson Table

$$D(0,0)=1.08483\,,\ \mathrm{D}(1,0)=\ 1.08988,\ \mathrm{D}(2,0)=1.09115$$

$$D(n,m)=D(n,m\text{-}1)+\frac{1}{4^m-1}\left[D(n,m\text{-}1)-D(n-1,m\text{-}1)\right]$$

$$D(1,1)=D(1,0)+\frac{1}{4-1}\left[D(1,0)-D(0,0)\right]=1.09156$$

$$D(2,1)=D(2,0)+\frac{1}{4-1}\left[D(2,0)-D(1,0)\right]=1.09157$$

$$D(2,2)=D(2,1)+\frac{1}{4^2-1}\left[D(2,1)-D(1,1)\right]=1.09157$$

Example
Richardson Table

1.08483		
1.08988	1.09156	
1.09115	1.09157	1.09157

This is the best estimate of the derivative of the function.

All entries of the Richardson table are estimates of the derivative of the function.

The first column are estimates using the central difference formula with different h.