SE031Numerical Methods
Topic 6
Numerical Differentiation

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(Term 053)
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Read chapter 23.1 and 23.2

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

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

$$Taylor\ Theorem:$$

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

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

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

Three formula

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?

Forward 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:

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

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

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

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 formula (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 accurcy
Central difference formula is expected to give better answer

Higher Order Formulas

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

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

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

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

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

High Accuracy Differentiation Formulas (1)

- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.
- Consider the forward finite-divided difference

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2)$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

High Accuracy Differentiation Formulas (2)

- Consider the backward finite-divided difference

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$$

$$f'(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 3f(x_i)}{2h} + O(h^2)$$

- Consider the central finite-divided difference

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + O(h^4)$$

Example

Estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

At $x = 0.5$ using finitite divided - difference and a step size of $h = 0.25$.

Find the true error for each case : Forward, Backward and Central

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

Central Difference

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!} f'''(x) - \frac{h^4}{5!} f^{v}(x) - \ldots$$

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

Constants $a_2, a_4, \ldots$ depend on f and x

Richardson Extrapolation

$$\textit{Hold} \quad f(x) \ \textit{and} \quad x \quad \textit{fixed}, \text{ define}$$

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

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

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

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

divide by -3 and rearrange, we get

$$\Rightarrow \quad f'(x) = \frac{-1}{3}\left[\phi(h) - 4\phi\left(\frac{h}{2}\right)\right] + O\left(h^4\right)$$

Richardson Extrapolation Table

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

others

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

Richardson Extrapolation Table

$D(0,0)=\Phi(h)$			
$D(1,0)=\Phi(h/2)$	$D(1,1)$		
$D(2,0)=\Phi(h/4)$	$D(2,1)$	$D(2,2)$	
$D(3,0)=\Phi(h/8)$	$D(3,1)$	$D(3,2)$	$D(3,3)$

Example

Evaluate numerically the derivative of

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

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

$$D(0,0)=1.08483\text{, D(1,0)}=\ 0.10988\text{, D(2,1)}=1.09115$$

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

$$D(1,1)=D(1,0)+\frac{1}{4-1}\left[D(1,0)-D(0,0)\right]=1.09114$$

$$D(2,1)=D(2,0)+\frac{1}{4-1}\left[D(2,0)-D(1,0)\right]=1.09146$$

$$D(2,2)=D(2,1)+\frac{1}{4^2-1}\left[D(2,1)-D(1,1)\right]=1.09148$$

Example

Richardson Table

1.08483		
1.08988	1.09114	
1.09115	1.09146	1.09148

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.

Summary