Lecture 7
Numerical Differentiation

- First order derivatives
- High order derivatives
- Richardson Extrapolation

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

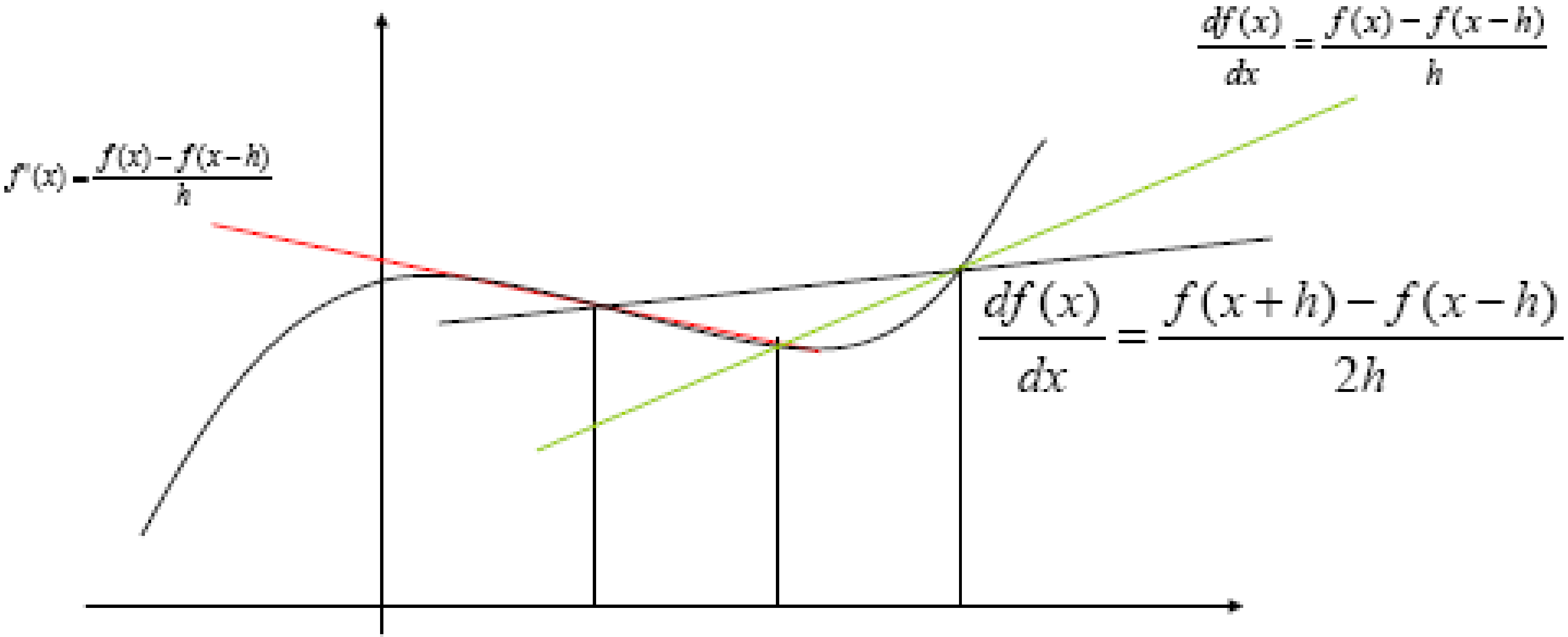
Forward Difference: $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x)}{h}$$

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?

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:

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

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

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

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

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 accuracy.
Central difference formula is expected to give a better answer.

Higher Order Formulas

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

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

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

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

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

Other Higher Order Formulas

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

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

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

Central Formulas with $Error = O(h^2)$

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

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

Example

- Use forward, backward and centered difference approximations to 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 step size h = 0.5 and h = 0.25
- Note that the derivative can be obtained directly:

  $f'(x) = -0.4x^3 - 0.45x^2 - 1.0x - 0.25$

  The true value of $f'(0.5) = -0.9125$
- In this example, the function and its derivative are known. However, in general, only tabulated data might be given.

Solution with Step Size = 0.5

- $f(0.5) = 0.925$, $f(0) = 1.2$, $f(1.0) = 0.2$
- Forward Divided Difference:

  $f'(0.5) \approx (0.2 - 0.925)/0.5 = -1.45$

  $|\varepsilon_t| = |(-0.9125+1.45)/-0.9125| = 58.9\%$
- Backward Divided Difference:

  $f'(0.5) \approx (0.925 - 1.2)/0.5 = -0.55$

  $|\varepsilon_t| = |(-0.9125+0.55)/-0.9125| = 39.7\%$
- Centered Divided Difference:

  $f'(0.5) \approx (0.2 - 1.2)/1.0 = -1.0$

  $|\varepsilon_t| = |(-0.9125+1.0)/-0.9125| = 9.6\%$

Solution with Step Size = 0.25

- f(0.5)=0.925, f(0.25)=1.1035, f(0.75)=0.6363
- Forward Divided Difference:

  $f'(0.5) \approx (0.6363 - 0.925)/0.25 = -1.155$

  $|\varepsilon_t| = |(-0.9125+1.155)/-0.9125| = 26.5\%$
- Backward Divided Difference:

  $f'(0.5) \approx (0.925 - 1.1035)/0.25 = -0.714$

  $|\varepsilon_t| = |(-0.9125+0.714)/-0.9125| = 21.7\%$
- Centered Divided Difference:

  $f'(0.5) \approx (0.6363 - 1.1035)/0.5 = -0.934$

  $|\varepsilon_t| = |(-0.9125+0.934)/-0.9125| = 2.4\%$

Discussion

- For both the Forward and Backward difference, the error is O(h)
- Halving the step size h approximately halves the error of the Forward and Backward differences
- The Centered difference approximation is more accurate than the Forward and Backward differences because the error is $O(h^2)$
- Halving the step size h approximately quarters the error of the Centered difference.

Richardson Extrapolation

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

Can we get a better formula?

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

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

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

Richardson Extrapolation

To get a better formula:

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

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

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

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

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

$$\Rightarrow\ f'(x) = \frac{4}{3}\phi(h/2) - \frac{1}{3}\phi(h) + O(h^4)$$

Use two derivative estimates to compute a third, more accurate approximation

Richardson Extrapolation Example

- Use the function:

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

  Starting with $h_1 = 0.5$ and $h_2 = 0.25$, compute an improved estimate of $f'(0.5)$ using Richardson Extrapolation

- Recall the true value of $f'(0.5) = -0.9125$

Solution

- The first-derivative estimates can be computed with centered differences as:

$$\phi(h) = \frac{f(0.5+h) - f(0.5-h)}{2h} \text{ at } x = 0.5$$

$$\phi(0.5) = \frac{f(1) - f(0)}{1} = \frac{0.2 - 1.2}{1} = -1.0, \quad |\varepsilon_t| = 9.6\%$$

$$\phi(0.25) = \frac{f(0.75) - f(0.25)}{0.5} = -0.934375, \quad |\varepsilon_t| = 2.4\%$$

The improved estimate can be obtained by applying:

$$f'(0.5) \cong \frac{4}{3}\phi(h/2) - \frac{1}{3}\phi(h) = \frac{4}{3}(-0.934375) - \frac{1}{3}(-1) = -0.9125$$

which produces the exact result for this example

Higher Order

$$f'(x) = \frac{4}{3}\phi(h/2) - \frac{1}{3}\phi(h) + O(h^4) = \rho(h) + a_4 h^4 + a_6 h^6 + \ldots$$

where $\rho(h) = \frac{4}{3}\phi(h/2) - \frac{1}{3}\phi(h)$

$$= \frac{1}{12h}\left[8f(x+h/2) - 8f(x-h/2) - f(x+h) + f(x-h)\right]$$

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

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

$$\Rightarrow f'(x) = \frac{1}{15}\left[16\rho\left(\frac{h}{2}\right) - \rho(h)\right] + O(h^6)$$

Richardson Extrapolation Table

Repeating this operation, one can obtain the following 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)

Error Level $O(h^2)$ $O(h^4)$ $O(h^6)$ $O(h^8)$

Richardson Extrapolation Table

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

$$Others:$$

$$D(n,m) = \frac{4^m}{4^m - 1} D(n, m-1) - \frac{1}{4^m - 1} D(n-1, m-1)$$

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.

TRUE VALUE : 1.09157070928 8434

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

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

$$D(n,m) = \frac{4^m}{4^m - 1} D(n, m-1) - \frac{1}{4^m - 1} D(n-1, m-1)$$

$$D(1,1) = \frac{4}{3} D(1,0) - \frac{1}{3} D(0,0) = 1.09156$$

$$D(2,1) = \frac{4}{3} D(2,0) - \frac{1}{3} D(1,0) = 1.09157$$

$$D(2,2) = \frac{16}{15} D(2,1) - \frac{1}{15} D(1,1) = 1.09157$$

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 step size h.