ME 310

Numerical Methods

Differentiation

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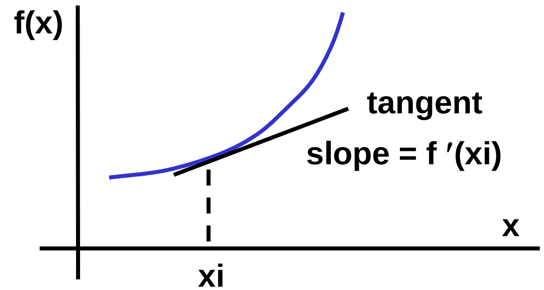
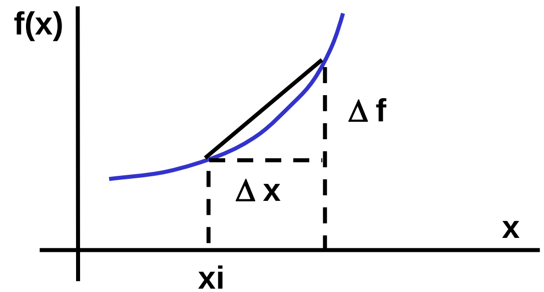
Derivative: Rate of change of a dependent variable with respect to an independent variable.

$$f = f(x) \quad \rightarrow \quad \left.\frac{df}{dx}\right|_{xi} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



which can be written approximately as a difference equation

$$\left.\frac{df}{dx}\right|_{xi} \approx \frac{\Delta f}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



- Numerical differentiation is considered if
    - the function can not be differentiated analytically
    - the function is known at discrete points only
    - the differentiation is to be automated in an algorithm.

Finite Divided Difference Formulas using TSE

Formulas for the first derivative

- **Forward differencing** (use 1st order TSE of $f(x_{i+1})$ around x_i. Call this TSE1)

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \qquad \text{where } h = x_{i+1} - x_i$$

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

- **Backward differencing** (use 1st order TSE of $f(x_{i-1})$ around x_i. Call this TSE2)

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \qquad \text{where } h = x_i - x_{i-1}$$

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

- **Centered differencing** (use TSE1 – TSE2. But consider 2nd order terms also.)

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

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

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

• Forward and centered difference formulas are first order, O(h), accurate. That is the error drops approximately by a factor of 2 as the step size h drops to h/2.

• Centered difference formula is second order, $O(h^2)$. Error drops by a factor of 4 as h drops to h/2.

• Centered difference formula uses the same number of arithmetic operations as forward and backward formulas, and it offers better accuracy. Therefore it is more efficient.

Example 33: Position of a body moving in a straight path is shown below. Find its velocity.

t	x	v
0.0	0.00	1.50
0.1	0.15	
0.2	0.47	2.35
0.3	0.62	
0.4	0.84	
0.5	0.98	1.40

• Use forward differencing at t = 0.0

$$\mathbf{v(0.0)} = \frac{\mathbf{x(0.1) - x(0.0)}}{\mathbf{h}} = \frac{\mathbf{0.15 - 0.00}}{\mathbf{0.1}} = \mathbf{1.50}$$

• Use centered differencing at t = 0.1, 0.2, 0.3 and 0.4

$$\mathbf{v(0.2)} = \frac{\mathbf{x(0.3) - x(0.1)}}{\mathbf{2\,h}} = \frac{\mathbf{0.62 - 0.15}}{\mathbf{0.2}} = \mathbf{2.35}$$

• Use backward differencing at t = 0.5

$$\mathbf{v(0.5)} = \frac{\mathbf{x(0.5) - x(0.4)}}{\mathbf{h}} = \frac{\mathbf{0.98 - 0.84}}{\mathbf{0.1}} = \mathbf{1.40}$$

Exercise 31: Complete the above table.

Higher order formulas for the first derivative

- To derive them use proper combinations of TSE of $f(x_{i+1})$, $f(x_{i-1})$, $f(x_{i+2})$, $f(x_{i-2})$

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

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

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

- See pages 633-634 for even more higher order formulas.

Exercise 32: Derive the above formulas.

Exercise 33: Solve the previous example using the above formulas. Note that for t=0.0 and 0.1 forward differencing must be used. For t=0.4 and 0.5 backward differencing is suitable. Centered differencing can be used only for t=0.2 and 0.3.

Formulas for the second derivative

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

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

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

- See pages 633-634 for formulas for the 3rd and 4th derivatives.

Exercise 34: Derive the above formulas. Use proper combinations of TSE of $f(x_{i+1})$, $f(x_{i-1})$, $f(x_{i+2})$ and $f(x_{i-2})$.

Exercise 35: Use the table given for the first example to calculate the acceleration of the particle. Use the above formulas to take the second derivative of time. You can also take the first derivative of the previously calculated velocities. Compare and comment on the results.

How can we improve the derivative estimates?

- Use small h values.
- Use higher order approximations.

Exercise 36: The following two tables are for the function $f(x) = e^x$. They use step sizes of 0.2 and 0.1. Calculate the first derivative of the function using $O(h^2)$ estimates. Calculate true errors. Compare the results.

x	f(x)	f′(x)	ε_t
0.4	1.4918247		
0.6	1.8221188		
0.8	2.2255409		
1.0	2.7182818		

x	f(x)	f′(x)	ε_t
0.4	1.4918247		
0.5	1.6487213		
0.6	1.8221188		
0.7	2.0137527		
0.8	2.2255409		
0.9	2.4596031		
1.0	2.7182818		

- Another alternative to improve derivative estimates is to use Richardson Extrapolation. It combines two estimates obtained with different h values to get a better estimate.
- Later we will use Richardson Extrapolation for integration too.

Richardson's Extrapolation

D: Exact derivative (usually not known)

D_1: Estimated derivative using $h=h_1$. E_1: Error of the estimation D_1. $\rightarrow$ $D = D_1 + E_1$

D_2: Estimated derivative using $h=h_2$. E_2: Error of the estimation D_2. $\rightarrow$ $D = D_2 + E_2$

$$\mathbf{D_1 + E_1 = D_2 + E_2}$$

If we used second-order differentiation to get D_1 and D_2, than $E_1 = O(h_1^2)$, $E_2 = O(h_2^2)$

$$\frac{E_1}{E_2} \approx \frac{h_1^2}{h_2^2} \rightarrow E_1 \approx E_2\left(\frac{h_1}{h_2}\right)^2$$

Substitute this into the first equation $\quad D_1 + E_2\left(\frac{h_1}{h_2}\right)^2 \approx D_2 + E_2$

Solve for E_2 $\quad E_2 \approx \dfrac{D_2 - D_1}{(h_1/h_2)^2 - 1}$

Combine this with D_2 $\quad \boxed{D \approx D_2 + \dfrac{D_2 - D_1}{(h_1/h_2)^2 - 1}}$

This estimate is or order $O(h^4)$, obtained by two $O(h^2)$ estimates.

A special case of $h_2 = h_1/2$ results in $\quad D \approx D_2 + \dfrac{D_2 - D_1}{3} = \dfrac{4}{3}D_2 - \dfrac{1}{3}D_1$

Example 34:

Use Richardson Extrapolation to estimate the first derivative of sin(x) at $x=\pi/4$ using step sizes of $h_1=\pi/3$ and $h_2=\pi/6$. Use centered differences of $O(h^2)$.

Using $h_1=\pi/3$ $$D_1 = f'(\pi/4) \approx \frac{\sin(\pi/4 + \pi/3) - \sin(\pi/4 - \pi/3)}{2(\pi/3)} = 0.584772601$$

$|\varepsilon_t| = 17.3\ \%$

Using $h_2=\pi/6$ $$D_2 = f'(\pi/4) \approx \frac{\sin(\pi/4 + \pi/6) - \sin(\pi/4 - \pi/6)}{2(\pi/6)} = 0.675237237$$

$|\varepsilon_t| = 4.5\ \%$

Apply Richardson Extrapolation $$f'(\pi/4) \approx \frac{4}{3}\,0.675237237 - \frac{1}{3}\,0.584772601 = 0.70539215$$

$|\varepsilon_t| = 0.24\ \%$

Romberg Algorithm

Apply multiple Richardson Extrapolation one after the other until the error falls below a specified tolerance.

Exercise 37: In the above example use $h_3=\pi/12$ to calculate D_3. Combine D_1 with D_2, and D_2 with D_3 to get two $O(h^4)$ estimates. Than combine these two estimates to get an estimate of order $O(h^6)$.