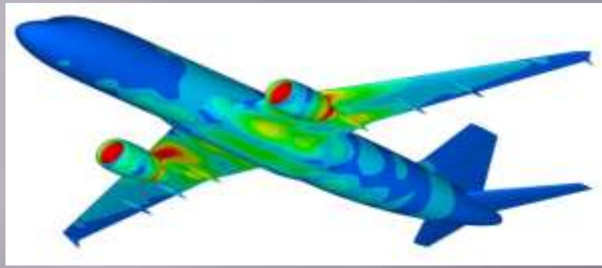
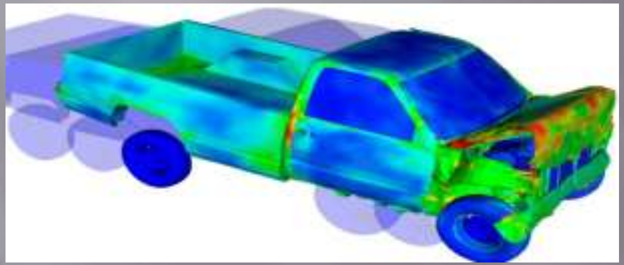
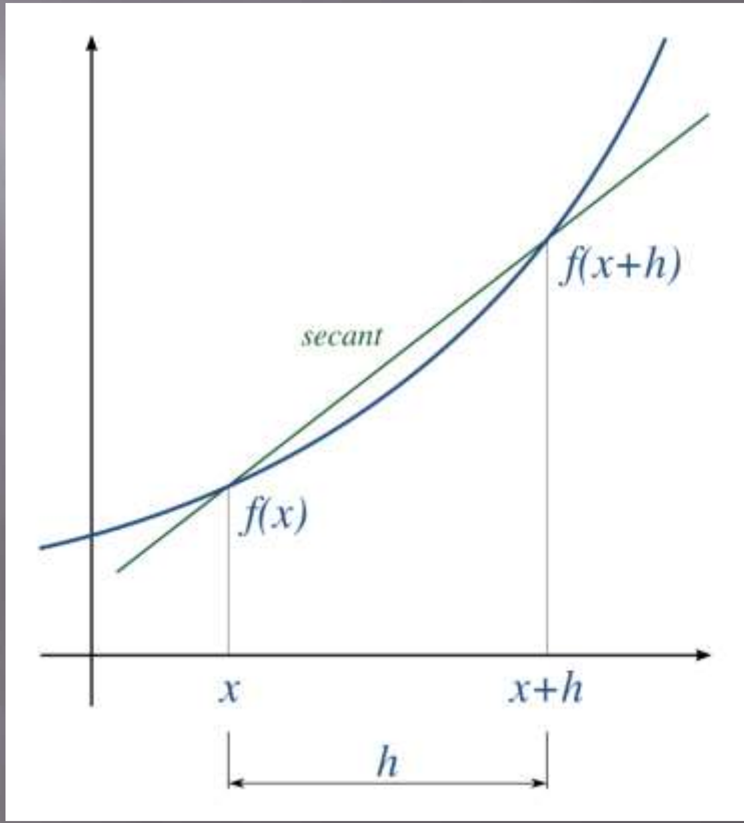
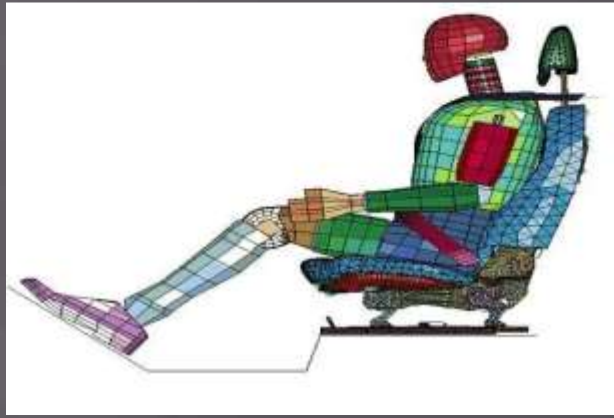
NUMERICAL DIFFERENTIATION









Dr. Himanshu Pathak

himanshu@iitmandi.ac.in

Introduction

- Calculus is the mathematics of change. Because engineers must continuously deal with systems and processes that change, calculus is an essential tool of engineering.
- Standing in the heart of calculus are the mathematical concepts of *differentiation* and *integration*:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

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

$$I = \int_a^b f(x)dx$$

Introduction

- Integration and differentiation are closely linked processes. They are, in fact, inversely related.

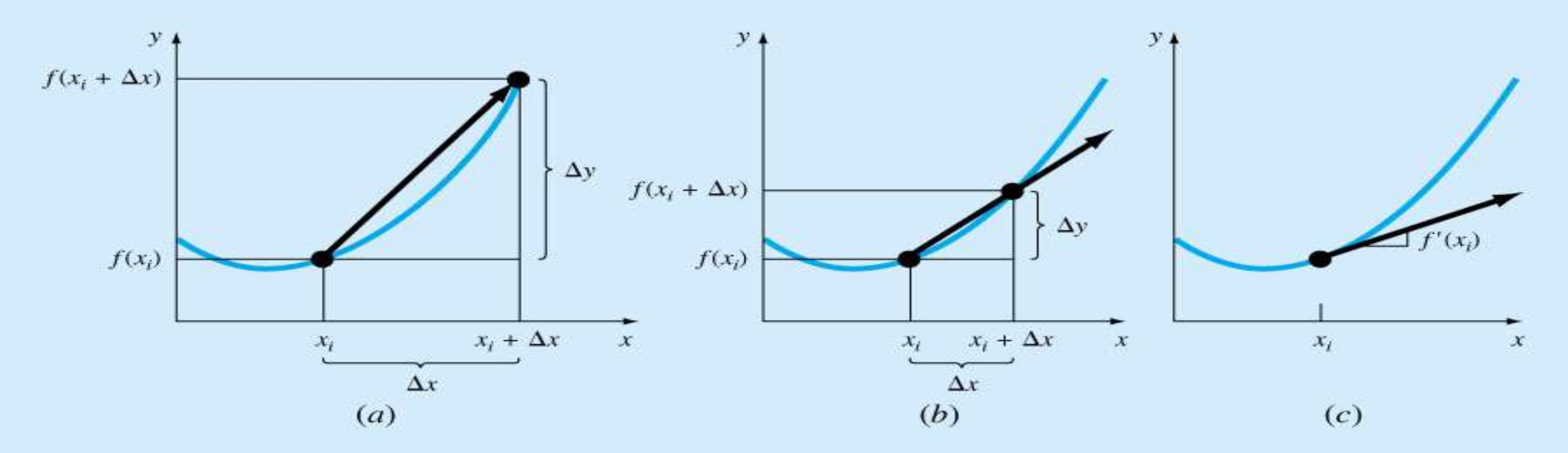
- Types of functions to be differentiated or integrated:
  1. Simple polynomial, exponential, trigonometric → analytically
  2. Complex function → numerically
  3. Tabulated function of experimental data → numerically

Applications

- Differentiation has so many engineering applications (heat transfer, fluid dynamics, chemical reaction kinetics, etc…)

- Integration is equally used in engineering (compute work in ME, nonuniform force in SE, cross-sectional area of a river, etc…)

Differentiation



$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

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

The finite difference becomes a derivative as Δx approaches zero.

Taylor Series Expansion

- Non-elementary functions such as trigonometric, exponential, and others are expressed in an approximate fashion using Taylor series when their values, derivatives, and integrals are computed.

- Any smooth function can be approximated as a polynomial. Taylor series provides a means to predict the value of a function at one point in terms of the function value and its derivatives at another point.

Numerical Application of Taylor Series

- If $f(x)$ and its first n+1 derivatives are continuous on an interval containing x_{i+1} and x_i , then:

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \frac{f^{(3)}(x_i)}{3!}(x_{i+1} - x_i)^3 + \ldots + \frac{f^{(n)}(x_i)}{n!}(x_{i+1} - x_i)^n + R_n$$

Where the remainder R_n is defined as:

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x_{i+1} - x_i)^{n+1}$$

ξ is a value of x that lies somewhere between x_i and x_{i+1}.

Taylor Series ξ in the Remainder Term

- Limitations
  - ξ is not exactly known but lies somewhere between x_i and x_{i+1}
  - To evaluate R_n, the (n+1) derivative of *f* (x) has to be determined. To do this *f* (x) must be known

  → if *f* (x) was known there would be no need to perform the Taylor series expansion!!!

- Modification

  $R_n = O(h^{n+1})$ the truncation error is of the order of h^{n+1}. $(h = x_{i+1} - x_i)$
  - If the error is $O(h)$, halving the step size will halve the error.
  - If the error is $O(h^2)$, halving the step size will quarter the error.
  - In general, the truncation error is decreased by addition of more terms in the Taylor series.

Numerical Application of Taylor Series

- The series is built term by:

$$f(x_{i+1}) \cong f(x_i)$$ zero order approximation

- Continuing the addition of more terms to get better approximation we have:

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i)$$ 1st order approximation

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2$$ 2nd order approximation

Forward Difference Formulas- 1st derivative

- 2nd order Taylor series expansion of *f*(x) can be written as:

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

- Then, the first derivative can be expressed as:

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

- Given that *f*" (x) can be approximated by:

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

Forward Difference Formulas- 1st derivative

- Substituting equation (3) into equation (2):

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

- Collecting terms and simplifying, we have:

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

- Note that the inclusion of the second-derivative term has improved the accuracy to $O(h^2)$.

Forward Difference Formulas- 2nd derivative

- Start with Lagrange interpolation polynomial for *f*(x) based on the four points x_i, x_{i+1}, x_{i+2} and x_{i+3} .
- Differentiate the products in the numerators twice
- Substitute $x = x_i$ and consider the fact that $x_j - x_i = (j-i)h$
- The expression of the second derivative is then:

$$\boxed{f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} + O(h^2)}$$

Backward Difference Formulas- 1st derivative

- Using backward difference in the Taylor series expansion,

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

- And given that $f''(x)$ can be approximated by:

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

- The second-order estimate of $f'(x)$ can be obtained:

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

Backward Difference Formulas- 2nd derivative

- Start with Lagrange interpolation polynomial for *f*(x) based on the four points x_i, x_{i-1}, x_{i-2} and x_{i-3} .
- Differentiate the products in the numerators twice
- Substitute $x = x_i$ and consider the fact that $x_j - x_i = (j- i)h$
- The expression of the second derivative is then:

$$\boxed{f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2} + O(h^2)}$$

Centered Difference Formulas- 1st derivative $[O(h^2)]$

- Start with the 2nd degree Taylor expansions about x for *f*(x+h) and *f*(x-h):

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

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2}h^2 - O(h^3) \qquad (5)$$

- Subtract (5) from (4)

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

- Hence

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

Centered Difference Formulas- 1st derivative $[O(h^4)]$

- Start with the difference between the 4th degree Taylor expansions about x for *f*(x+h) and *f*(x-h):

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{2f'''(x_i)}{3!}h^3 + O(h^5) \qquad (6)$$

- Use the step size 2h, instead of h, in (6)

$$f(x_{i+2}) - f(x_{i-2}) = 4f'(x_i)h + \frac{16f'''(x_i)}{3!}h^3 + O(h^5) \qquad (7)$$

- Multiply equation (6) by 8, subtract (7) from it, and solve for *f*′(x)

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

Centered Difference Formulas- 2nd derivative [O(h^2)]

- Start with the 3rd degree Taylor expansions about x for *f*(x+h) and *f*(x-h):

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \frac{f'''(x_i)}{3!}h^3 + O(h^4) \qquad (8)$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2}h^2 - \frac{f'''(x_i)}{3!}h^3 + O(h^4) \qquad (9)$$

- Add equations (8) and (9), and solve for *f*′′(x)

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

Centered Difference Formulas- 2nd derivative [O(h^4)]

- Start with the addition between the 5th degree Taylor expansions about x for *f*(x+h) and *f*(x-h):

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + \frac{2f''(x_i)}{2!}h^2 + \frac{2f^{(4)}(x_i)}{4!}h^4 + O(h^6) \qquad (10)$$

- Use the step size 2h, instead of h, in (10)

$$f(x_{i+2}) + f(x_{i-2}) = 2f(x_i) + \frac{8f''(x_i)}{2!}h^2 + \frac{32f^{(4)}(x_i)}{4!}h^4 + O(h^6) \qquad (11)$$

- Multiply equation (10) by 16, subtract (11) from it, and solve for *f'*(x)

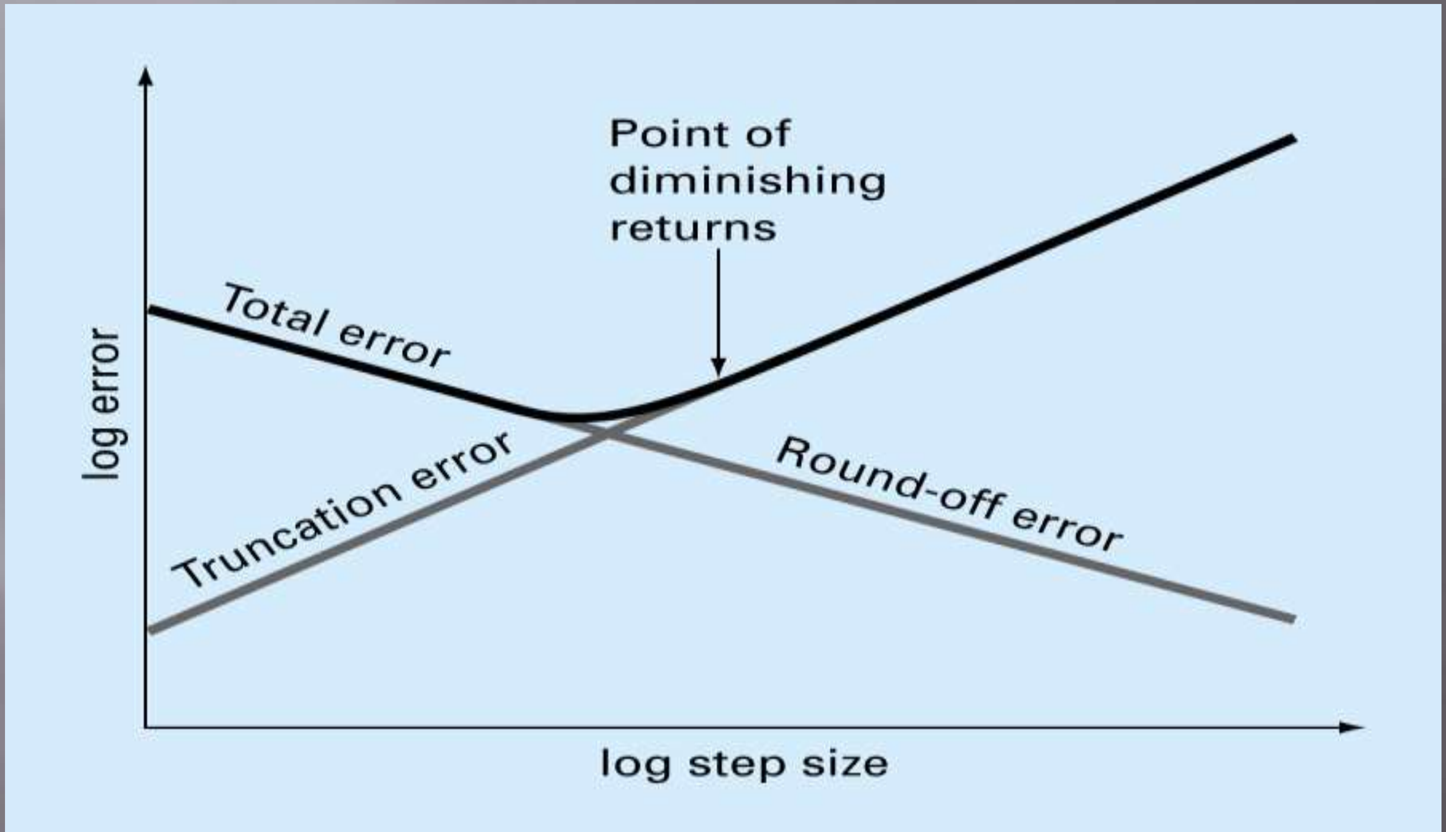
$$\boxed{f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} + O(h^4)}$$

Error Analysis

- Generally, if numerical differentiation is performed, only about half the accuracy of which the computer is capable is obtained unless we are fortunate to find an optimal step size.
- The total error has part due to round-off error plus a part due to truncation error.

Total Numerical Error

Total numerical error = truncation error + round-off error.



Trade-off between truncation and round-off errors

Example 1

Estimate the first and second derivatives of:

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

at x = 0.5 and h = 0.25 using

a) forward finite-divided difference

b) Centered finite-divided difference

c) backward finite-divided difference?

Example 1 - Solution

a) **Forward difference**

- 1^{st} derivative computation

The data needed is:

$$x_i = 0.5 \qquad f(x_i) = 0.925$$
$$x_{i+1} = 0.75 \qquad f(x_{i+1}) = 0.636328$$
$$x_{i+2} = 1 \qquad f(x_{i+2}) = 0.2$$

First derivative:

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

$$f'(0.5) = \frac{-f(1) + 4f(0.75) - 3f(0.5)}{2(0.25)} = -0.859375$$

εt = 5.82%

True value=-0.9125

Example 1 - Solution

- Second derivative computation

The data needed is:

$$x_i = 0.5 \qquad f(x_i) = 0.925$$
$$x_{i+1} = 0.75 \qquad f(x_{i+1}) = 0.636328$$
$$x_{i+2} = 1 \qquad f(x_{i+2}) = 0.2$$
$$x_{i+3} = 1.25 \qquad f(x_{i+3}) = 1.94336$$

Second derivative:

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$$

$$f''(0.5) = \frac{-(1.94336) + 4(0.2) - 5(0.636328) + 2(0.925)}{(0.25)^2} = -39.6$$

Example 1 - Solution

b) **Centered finite-divided difference**

- The data needed is:

$$x_{i-2} = 0 \qquad f(x_{i-2}) = 1.2$$
$$x_{i-1} = 0.25 \qquad f(x_{i-1}) = 1.103516$$
$$x_{i+1} = 0.75 \qquad f(x_{i-1}) = 0.636328$$
$$x_{i+2} = 1 \qquad f(x_{i-2}) = 0.2$$

- First derivative:

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

$$f'(x_i) = \frac{-(0.2) + 8(0.636328) - 8(1.103516) + (1.2)}{12(0.25)}$$

$$f'(x_i) = -0.9125$$

εt = 0%

True value=-0.9125

Example 1 - Solution

c) **Backward finite-divided difference**

- The data needed is:

$$x_{i-2} = 0 \qquad f(x_{i-2}) = 1.2$$
$$x_{i-1} = 0.25 \qquad f(x_{i-1}) = 1.103516$$
$$x_i = 0.5 \qquad f(x_i) = 0.925$$

- First derivative :

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

$$f'(x_i) = \frac{3(0.925) - 4(1.103516) + (1.2)}{2(0.25)} = -0.878125$$

εt = 3.77%

True value=-0.9125

Richardson Extrapolation

- Numerical derivation can be accurate by (a) Increasing turncation order and (b) Decreasing step size.
- Richardson extrapolation uses two derivative estimates to compute a third, more accurate approximation

Richardson extrapolation

$$D \cong \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)$$

For centered difference approximations with ***O(h²)***, the application of this formula will yield a new derivative estimate of ***O(h⁴)***.

Example 2

Estimate the first and second derivatives of:

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

at x = 0.5 and h_1 = 0.5; h_2 = 0.25 using

a) Centered finite-divided difference and Richardson extrapolation

Example 2 - Solution

- Centered finite-divided difference

$$D(0.5) = \frac{0.2 - 1.2}{1} = -1.0 \qquad \varepsilon_t = -9.6\%$$

$$D(0.25) = \frac{0.6363281 - 1.1035156}{0.5} = -0.934375 \qquad \varepsilon_t = -2.4\%$$

- Richardson extrapolation :

$$D = \frac{4}{3}(-0.934375) - \frac{1}{3}(-1) = -0.9125$$

εt = 0%

True value=-0.9125

Finite Divided Difference Method

- Divided differences is a recursive division process. The method can be used to calculate the coefficients in the interpolation polynomial in the Newton form.
- The Taylor series used to approximate divided differences.

Taylor Series

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

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

First Forward Difference

Δf_i is referred to as the first forward difference and h is called the step size

Finite Divided Difference Table

i	x_i	$f[x_i]$	First order differences	Second order differences	Third order differences	Fourth order differences	Fifth order differences
0	x_0	$f[x_0]$					
			$f[x_0, x_1]$				
1	x_1	$f[x_1]$		$f[x_0,x_1,x_2]$			
			$f[x_1,x_2]$		$f[x_0,x_1,x_2,x_3]$		
2	x_2	$f[x_2]$		$f[x_1,x_2,x_3]$		$f[x_0,x_1,x_2,x_3,x_4]$	
			$f[x_2,x_3]$		$f[x_1,x_2,x_3,x_4]$		$f[x_0,x_1,x_2,x_3,x_4,x_5]$
3	x_3	$f[x_3]$		$f[x_2,x_3,x_4]$		$f[x_1,x_2,x_3,x_4,x_5]$	
			$f[x_3,x_4]$		$f[x_2,x_3,x_4,x_5]$		
4	x_4	$f[x_4]$		$f[x_3,x_4,x_5]$			
			$f[x_4,x_5]$				
5	x_5	$f[x_5]$					

i	x_i	$f[x_i]$	1st order differences	2nd order differences	3rd order differences	4th order differences
0	0	0				
			$\frac{1-0}{1-0} = 1$			
1	1	1		$\frac{7-1}{2-0} = 3$		
			$\frac{8-1}{2-1} = 7$		$\frac{6-3}{3-0} = 1$	
2	2	8		$\frac{19-7}{3-1} = 6$		$\frac{1-1}{4-0} = 0$
			$\frac{27-8}{3-2} = 19$		$\frac{9-6}{4-1} = 1$	
3	3	27		$\frac{37-19}{4-2} = 9$		
			$\frac{64-27}{4-3} = 37$			
4	4	64				

Example 3

Example: Compute f(0.3) for the data using Newton's divided difference formula.

x	0	1	3	4	7
f	1	3	49	129	813

Divided difference table

x_i	f_i			
0	1			
		2		
1	3		7	
		23		3
3	49		19	
		80		3
4	129		37	
		228		
7	813			

$$f(x) = f[x_0] + (x - x_0)\, f[x_0, x_1] + (x - x_0)(x - x_1)\, f[x_0, x_1, x_2] + (x - x_0)(x - x_1)(x - x_2)\, f[x_0, x_1, x_2, x_3]$$

$$f(0.3) = 1 + (0.3 - 0)\, 2 + (0.3)(0.3 - 1)\, 7 + (0.3)(0.3 - 1)(0.3 - 3)\, 3$$
$$= 1.831$$

THANK YOU

Questions??