CHAPTER 7a. DIFFERENTIATION AND INTEGRATION

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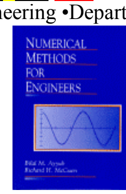

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ENCE 203 - Computation Methods in Civil Engineering II

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Differentiation and Integration

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- In calculus, differentiation is used to find the rate of change of the dependent variable $y = f(x)$.
- The rate of change of the dependent variable is needed because engineers is often deal with systems and processes that change.

Differentiation and Integration

- Also, in calculus, integration is used to find the area under the curve.
- In engineering applications, the area under the curve can have physical interpretation and implications.
- For example, it can mean finding the total energy or rate of flow Q through a cross section of a river.

Differentiation and Integration

- Therefore, calculus is the heart of differentiation and integration.
- Examples

$$y = f(x) = \sin x - x^2 \Rightarrow \frac{dy}{dx} = f'(x) = \cos x - 2x$$

$$y = f(x) = \frac{1}{x^2} + e^x + 3 \Rightarrow \frac{dy}{dx} = f'(x) = -\frac{1}{x} + e^x$$

Differentiation and Integration

■ Examples (cont'd)

$$y = f(x) = x^2 e^{2x} - \cos x + 2$$

$$\Rightarrow \frac{dy}{dx} = f'(x) = 2xe^{2x} + 2x^2 e^{2x} + \sin x$$

$$y = f(x) = x^3 - e^x + \sin x$$

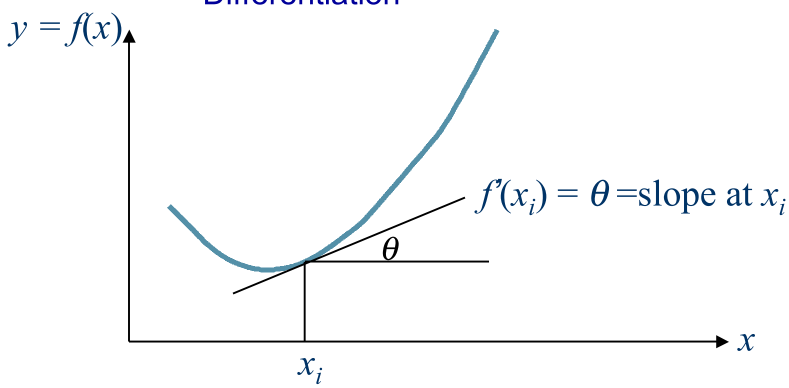
$$\Rightarrow \int y dx = \int f(x) dx = \int \left(x^3 - e^x + \sin x\right) dx$$

$$= \frac{x^4}{4} - e^x - \cos x$$

Differentiation and Integration

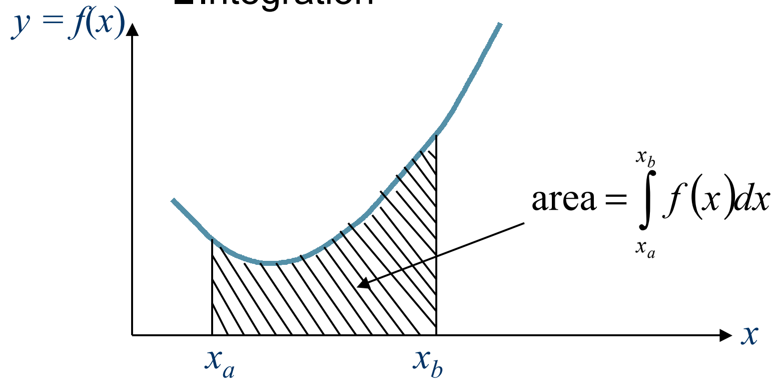
■ Examples (cont'd)

- Differentiation



Differentiation and Integration

- Examples (cont'd)
  - Integration



Differentiation

- Numerical Differentiation
  - A number of engineering problems require a numerically derived estimate of the derivative of a function $f(x)$.
  - There are two approaches:
    - The function is known, but the derivative cannot be computed analytically,
    - Fit a function to the data points, and differentiate the fitted interpolation function analytically.

Differentiation

■ Numerical Differentiation

– In the first approach, if the function is known and the derivative can not be evaluated analytically, the derivative can be estimated by computing the function for two values of the independent variables separated by Δx and dividing the difference by Δx as follows:

$$\frac{dy}{dx} = \frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x} \qquad (1)$$

Differentiation

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■ Numerical Differentiation

– In the second approach, we fit a function to the set of data points that describe the function and then differentiate the fitted function.

– Specifically, an interpolation polynomial of degree n could be fit to the data and the derivative of the polynomial is used to estimate the derivative of the function.

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Numerical Differentiation

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- Finite-difference Differentiation
  - Forward Difference

$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x)-f(x)}{\Delta x} \qquad (2)$$

Numerical Differentiation

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- Finite-difference Differentiation
  - Backward Difference

$$\frac{df(x)}{dx} \approx \frac{f(x)-f(x-\Delta x)}{\Delta x} \qquad (3)$$

Numerical Differentiation

■ Finite-difference Differentiation

– Two-Step Method

$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} \qquad (4)$$

Numerical Differentiation

■ Finite-difference Differentiation

– For many highly variable functions, the two-step method may give slightly more accurate estimates than either the forward or backward finite-difference approximations.

– The finite-difference approach can be used both when the data are given as tabular values or when a functional form is given.

Numerical Differentiation

■ Example 1

The data given in the following table gives the values of the cube of a number. For purposes of illustration, approximate the first derivative at x = 2 using the forward, backward, and two-step finite-difference schemes, and compare with the true value of derivative at x = 2.

x	0	1	2	3	4
$f(x)$	0	1	8	27	64

Numerical Differentiation

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■ Example 1 (cont'd)

– Forward Difference:

$$\frac{df(2)}{dx} = \frac{f(x+\Delta x) - f(x)}{\Delta x} = \frac{27-8}{3-2} = 19$$

– Backward Difference:

$$\frac{df(2)}{dx} = \frac{f(x) - f(x-\Delta x)}{\Delta x} = \frac{8-1}{2-1} = 7$$

Numerical Differentiation

- Example 1 (cont'd)
  - Two-Step Method:

$$\frac{df(2)}{dx} = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} = \frac{27-1}{3-1} = 13$$

  - True Value of the Derivative:

$$f(x) = x^3 \Rightarrow f'(x) = \frac{df(x)}{dx} = 3x^2$$

$$\frac{df(2)}{dx} = 3(2)^2 = 12$$

Numerical Differentiation

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- Example 1 (cont'd)
  - Comparison:

	Forward	Backward	Two-Step	True
$f'(2)$	19	7	13	12
|%error|	58.33	41.67	8.33	-

Numerical Differentiation

- Example 2

  Derive a second-degree interpolation polynomial to fit following data points, and then using the fitted polynomial to approximate the first derivative at x = 2. Compare your result with that of Example 1 and that of the exact derivative (i.e., $3x^2$).

x	1	2	3
$f(x)$	1	8	27

Numerical Differentiation

- Example 2 (cont'd)
  - The general form of the interpolation polynomial is given by

$$f(x) = b_0 + b_1 x + b_2 x^2 + b_3 x^3 + \cdots + b_n x^n$$

  - In our case it is

$$f(x) = b_0 + b_1 x + b_2 x^2$$

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- Example 2 (cont'd)
  - We need to find the coefficients b_0, b_1, and b_2.
  - We notice that have three unknowns, $n = 3$, that require solving 3 simultaneous linear equations using the pair, x_i and $f(x_i)$, of the given data as follows:

Numerical Differentiation

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- Example 2 (cont'd)

x	1	2	3
$f(x)$	1	8	27

$$f(x) = b_0 + b_1 x + b_2 x^2$$

$$1 = b_0 + b_1(1) + b_2(1)^2$$

$$8 = b_0 + b_1(2) + b_2(2)^2$$

$$27 = b_0 + b_1(3) + b_2(3)^2$$

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■ Example 2 (cont'd)

$$b_0 + b_1 + b_2 = 1$$
$$b_0 + 2b_1 + 4b_2 = 8$$
$$b_0 + 3b_1 + 9b_2 = 27$$

– OR

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 8 \\ 27 \end{bmatrix}$$

Numerical Differentiation

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■ Example 2 (cont'd)

– The solution of this set of equations yields

$$\begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 6 \\ -11 \\ 6 \end{bmatrix} \qquad f(x) = b_0 + b_1 x + b_2 x^2$$

– Therefore, the interpolation polynomial is

$$f(x) = 6 - 11x + 6x^2$$

– And its derivative is

$$f(x) = -11 + 12x$$

Numerical Differentiation

- Example 2 (cont'd)
  - The result is

$$\frac{df(2)}{dx} = f'(2) = -11 + 12(2) = 13$$

  - Comparison:

	Forward	Backward	Two-Step	2^{nd}-Poly	True
$f'(2)$	19	7	13	13	12
|%error|	58.33	41.67	8.33	8.33	-

Numerical Differentiation

- Differentiation Using a Finite-difference Table
  - The finite-difference table can also be used to approximate the derivatives of a function that is expressed in incremental form.
  - For example, in the following finite-difference table, the values of the Δf column can be used to make estimate of the first derivative.

Finite-difference Table

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	...	$\Delta^n f$
x	$f(x)$					
		$\Delta f(x)$				
$x + \Delta x$	$f(x + \Delta x)$		$\Delta^2 f(x)$			
		$\Delta f(x + \Delta x)$		$\Delta^3 f(x)$		
$x + 2\Delta x$	$f(x + 2\Delta x)$		$\Delta^2 f(x + \Delta x)$			
		$\Delta f(x + 2\Delta x)$		$\Delta^3 f(x + \Delta x)$		
$x + 3\Delta x$	$f(x + 3\Delta x)$		$\Delta^2 f(x + 2\Delta x)$			
		$\Delta f(x + 3\Delta x)$		$\Delta^3 f(x + 2\Delta x)$		
			$\Delta^2 f(x + 3\Delta x)$			
:	:	:	:	:	:::	$\Delta^n f(x)$
$x + (n-2)\Delta x$	$f[x + (n-2)\Delta x]$		$\Delta^2 f[x + (n-3)\Delta x]$			
		$\Delta f[x + (n-2)\Delta x]$		$\Delta^3 f[x + (n-3)\Delta x]$		
$x + (n-1)\Delta x$	$f[x + (n-1)\Delta x]$		$\Delta^2 f[x + (n-2)\Delta x]$			
		$\Delta f[x + (n-1)\Delta x]$				
$x + n\Delta x$	$f(x + n\Delta x)$					

Numerical Differentiation

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- Differentiation Using a Finite-difference Table
  - Also, the values in the $\Delta^i f$ column can be used to make estimate of the ith derivative.
  - For estimating the first derivative at any value of x, the Δf value in the diagonal row below the row for the value of x can be used to estimate the *forward difference*.

Numerical Differentiation

■ Differentiation Using a Finite-difference Table

- The Δf value in the diagonal row above the row for the value of x can be used to estimate the *backward difference*.
- The average of these two Δf values can be used to estimate the first derivative with the two-step method.

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■ Example 3

For the following data set, estimate the first derivative at x = 11 using a finite-difference table with forward, backward, and two-step methods. Also estimate the second derivative at x = 11.

x	10	11	12	13	14
$f(x)$	1000	1331	1728	2197	2744

Numerical Differentiation

■ Example 3 (cont'd)

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
10	1000				
		331			
11	1331		66		
		397		6	
12	1728		72		0
		469		6	
13	2197		78		
		547			
14	2744				

Numerical Differentiation

■ Example 3 (cont'd)

– By forward difference:

$$\frac{df(11)}{dx} = \frac{\Delta f_{i+1}}{\Delta x} = \frac{397}{11-10} = 397$$

– By backward difference:

$$\frac{df(11)}{dx} = \frac{\Delta f_{i}}{\Delta x} = \frac{331}{11-10} = 331$$

Numerical Differentiation

- Example 3 (cont'd)
  - By two-step method:

$$\frac{df(11)}{dx} = \frac{\Delta f_i + \Delta f_{i+1}}{2\Delta x} = \frac{331+397}{2} = 364$$

  - The second derivative can be estimated as follows:

$$\frac{d^2 f(11)}{dx^2} = \frac{\Delta^2 f}{(\Delta x)^2} = \frac{66}{1} = 66$$

Numerical Differentiation

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- Differentiating an Interpolating Polynomial
  - For any set of data points, an interpolating polynomial can be developed as a function of the independent variable x.
  - This polynomial can be differentiated analytically to estimate the nth derivative of the function.

Numerical Differentiation

- Differentiating an Interpolating Polynomial

  The *n*th Degree Polynomial

$$f(x) = b_n x^n + b_{n-1} x^{n-1} + b_{n-2} x^{n-2} + \cdots + b_1 x + b_0$$

$$\frac{df(x)}{dx} = n b_n x^{n-1} + (n-1) b_{n-1} x_{n-2} + (n-2) b_{n-2} x^{n-3} + \cdots + b_1$$

Numerical Differentiation

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- Differentiating an Interpolating Polynomial

  – Gregory-Newton Interpolation Formula

$$f(x) = a_1 + a_2(x - x_1) + a_3(x - x_1)(x - x_2) + a_4(x - x_1)(x - x_2)(x - x_3)$$
$$+ a_n(x - x_1)(x - x_2)\ldots(x - x_{n-1}) + a_{n+1}(x - x_1)(x - x_2)\ldots(x - x_n)$$

  - For the first four terms:

$$\frac{df(x)}{dx} = a_2 + a_3[(x - x_2) + (x - x_1)] + a_4[(x - x_2)(x - x_3)$$
$$+ (x - x_1)(x - x_3) + (x - x_1)(x - x_2)]$$

Numerical Differentiation

■ Example 4

The vapor pressure of water at various temperatures is provided in the following table. Derive a Gregory-Newton polynomial for set of data, and differentiate this polynomial analytically to estimate the slope of the vapor pressure at $T = 60^0$C.

T (C^0)	40	48	56	64
P(mm Hg)	55.3	83.7	123.8	179.2

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■ Example 4 (cont'd)

The general form the Gregory-Newton formula is given by

$$f(x) = a_1 + a_2(x - x_1) + a_3(x - x_1)(x - x_2) + a_4(x - x_1)(x - x_2)(x - x_3)$$

and

$$\frac{df(x)}{dx} = a_2 + a_3[(x - x_2) + (x - x_1)] + a_4[(x - x_2)(x - x_3) + (x - x_1)(x - x_3) + (x - x_1)(x - x_2)]$$

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■ Example 4 (cont'd)

i	T (^{0C})	P (mm Hg)	Process	a_i
1	40	55.3	$55.3 = a_1$	55.3
2	48	83.7	$83.7 = a_1 + a_2(48-40)$	3.55
3	56	123.8	$123.8 = a_1 + a_2(56-40) + a_3(56-40)(56-48)$	0.09141
4	64	179.2	$179.2 = a_1 + a_2(64-40) + a_3(64-40)(64-48) + a_4(64-40)(64-48)(64-56)$	0.00117

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■ Example 4 (cont'd)

$$\frac{dP(T)}{dT} = 3.55 + 0.09141[(T-48)+(T-40)] + 0.00117[(T-48)(T-56) + (T-40)(T-56) + (T-40)(T-48)]$$

$$\frac{dP(60)}{dT} = 3.55 + 0.09141[(60-48)+(60-40)] + 0.00117[(60-48)(60-56) + (60-40)(60-56) + (60-40)(60-48)]$$

$$= 6.91 \frac{\text{mm Hg}}{{}^0\text{C}}$$