CHAPTER 7b. DIFFERENTIATION AND INTEGRATION

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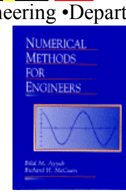

by

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ENCE 203 - Computation Methods in Civil Engineering II

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Numerical Differentiation

- Recall the forward, backward, and two-step finite-difference formulas for numerical differentiation:
  - Forward Difference

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

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– Backward Difference

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

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– Two-Step

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

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■ Example 5 – Specific Heat Capacity

The specific heat capacity is an important element in thermodynamics processes. For a process in which the pressure is constant, the specific heat capacity, c_p, equals the slope of the relationship between the specific enthalpy, h, and the temperature, T, as follows:

$$c_p = \frac{dh}{dT}$$

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■ Example 5 – Specific Heat Capacity

T (^{0}F)	H (Btu/lb)	Δh	$\Delta^2 h$	$\Delta^3 h$	$\Delta^4 h$
800	1305				
		155			
1000	1460		-30		
		125		25	
1200	1585		-5		-20
		120		5	
1400	1705		0		
		120			
1600	1825				

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■ Example 5 (cont'd) – Specific Heat Capacity

At a temperature of $T = 1200^0$ F, the forward finite-difference will give

$$c_p = \frac{dh}{dT} \approx \frac{\Delta h}{\Delta T} = \frac{1705 - 1585}{1400 - 1200}$$

$$= \frac{120}{200} = 0.6 \ \text{Btu/lb/}^0\text{F}$$

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■ Example 5 (cont'd) – Specific Heat Capacity

At a temperature of $T = 1200^0$ F, the backward finite-difference will give

$$c_p = \frac{dh}{dT} \approx \frac{\Delta h}{\Delta T}$$

$$= \frac{125}{200} = 0.625 \ \text{Btu/lb/}^0\text{F}$$

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- Example 5 (cont'd) – Specific Heat Capacity

  At a temperature of $T = 1200^0$ F, the two-step finite-difference will give

$$c_p = \frac{dh}{dT} \approx \frac{\Delta h}{\Delta T} = \frac{125+120}{2\Delta T}$$

$$= \frac{245}{400} = 0.6125 \text{ Btu/lb/}^0\text{F}$$

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- Example 5 (cont'd) – Specific Heat Capacity

  At a temperature of $T = 1200^0$ F, the rate of change of c_p can be approximated by the second derivative as follows:

$$\frac{d^2h}{dT^2} \approx \frac{\Delta^2 h}{(\Delta T)^2} = \frac{-5}{(200)^2} = -0.000125 \text{ Btu/lb/}\left({}^0\text{F}\right)^2$$

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- Taylor Series Expansion and Numerical Differentiation
  - The basic finite-difference equations, i.,e., forward and backward difference, for differentiation result from the Taylor series expansion:

$$f(x_0+h)=f(x_0)+hf^{(1)}(x_0)+\frac{h^2}{2!}f^{(2)}(x_0)+\frac{h^3}{3!}f^{(3)}(x_0)+\ldots+\frac{h^n}{n!}f^{(n)}(x_0)+R_{n+1} \quad (5)$$

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- Taylor Series Expansion and Numerical Differentiation

  Where $x = x_0 + h, \quad h = x - x_0 = \Delta x$

  Taylor series can be rewritten with new symbols as

$$f(x+\Delta x)=f(x)+\frac{df(x)}{dx}\Delta x+\frac{d^2 f(x)}{dx^2}\frac{(\Delta x)^2}{2!}+\frac{d^3 f(x)}{dx^3}\frac{(\Delta x)^3}{3!}+\cdots \quad (6)$$

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- Taylor Series Expansion and Numerical Differentiation
  - If we truncate Taylor series (Eq. 6) at the second term, the forward finite-difference formula for differentiation can be derived from Taylor series expansion as follows:

$$f(x+\Delta x) = f(x) + \frac{df(x)}{dx}\Delta x \qquad (7)$$

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- Taylor Series Expansion and Numerical Differentiation

$$\frac{df(x)}{dx}\Delta x = f(x+\Delta x) - f(x) \qquad (8)$$

Or

$$\frac{df(x)}{dx} = \frac{f(x+\Delta x) - f(x)}{\Delta x} \qquad (9)$$

Eq. 9 is indeed the first approximation forward finite-difference formula of the first derivative.

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■ Second-Order Approximation for the First Derivative

If we truncate the Taylor series (Eq. 6) at the third term (at the second derivative), the result will be as follows:

$$f(x+\Delta x)=f(x)+\frac{df(x)}{dx}\Delta x+\frac{d^2 f(x)}{dx^2}\frac{(\Delta x)^2}{2!} \qquad (10)$$

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■ Second-Order Approximation for the First Derivative

Equation 10 can be rearrange as

$$\frac{df(x)}{dx}\Delta x=f(x+\Delta x)-f(x)-\frac{d^2 f(x)}{dx^2}\frac{(\Delta x)^2}{2!}$$

or

$$\frac{df(x)}{dx}=\frac{f(x+\Delta x)-f(x)}{\Delta x}-\frac{d^2 f(x)}{dx^2}\frac{(\Delta x)^2}{2!\Delta x}$$

or

$$\frac{df(x)}{dx}=\frac{f(x+\Delta x)-f(x)}{\Delta x}-\frac{d^2 f(x)}{dx^2}\frac{\Delta x}{2} \qquad (11)$$

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Numerical Differentiation

- Second-Order Approximation for the First Derivative
  - Equation 11 is the second-order approximation of the first derivative.
  - However, the second-order approximation of the first derivative requires knowledge of the second derivative.
  - So, we need an expression for the second-order approximation in terms of the data points.

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- Second-Order Approximation for the First Derivative

  If we let $f'(x)$ be the first derivative of $f(x)$ with respect to x, then the forward difference approximation of the second derivative is given by

$$\frac{d^2 f(x)}{dx^2} = \frac{f'(x+\Delta x) - f'(x)}{\Delta x} \qquad (12)$$

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- Second-Order Approximation for the First Derivative

But

$$f'(x+\Delta x)=\frac{f(x+2\Delta x)-f(x+\Delta x)}{\Delta x} \qquad (13)$$

and

$$f'(x)=\frac{f(x+\Delta x)-f(x)}{\Delta x} \qquad (14)$$

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- Second-Order Approximation for the First Derivative

Substituting Eqs. 13 and 14 into Eq. 12 will provide the following results

$$\frac{d^2 f(x)}{dx^2}=\frac{\dfrac{f(x+\Delta 2x)-f(x+\Delta x)}{\Delta x}-\dfrac{f(x+\Delta x)-f(x)}{\Delta x}}{\Delta x}$$

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- Second-Order Approximation for the First Derivative

$$\frac{d^2 f(x)}{dx^2} = \frac{f(x+\Delta 2x) - f(x+\Delta x) - f(x+\Delta x) + f(x)}{(\Delta x)^2}$$

or

$$\frac{d^2 f(x)}{dx^2} = \frac{f(x+\Delta 2x) - 2f(x+\Delta x) + f(x)}{(\Delta x)^2} \qquad (15)$$

Equation 15 is the first-order approximation of the second derivative.

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- Second-Order Approximation for the First Derivative

Bt substituting Eq. 15 into Eq. 11

$$\begin{aligned}
\frac{df(x)}{dx} &= \frac{f(x+\Delta x) - f(x)}{\Delta x} - \frac{d^2 f(x)}{dx^2}\frac{\Delta x}{2} \\
&= \frac{f(x+\Delta x) - f(x)}{\Delta x} - \frac{f(x+2x) - 2f(x+\Delta x) + f(x)}{(\Delta x)^2}\frac{\Delta x}{2} \\
&= \frac{2f(x+\Delta x) - 2f(x) - f(x+2x) + 2f(x+\Delta x) - f(x)}{2\Delta x} \\
&= \frac{-f(x+2x) + 4f(x+\Delta x) - 3f(x)}{2\Delta x}
\end{aligned} \qquad (16)$$

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- Second-Order Approximation for the First Derivative

$$\frac{df(x)}{dx} \approx \frac{-f(x+2x)+4f(x+\Delta x)-3f(x)}{2\Delta x} \qquad (17)$$

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- In a similar manner, a forward difference, second-order approximation of the second derivative can be derived from Taylor series.
- Also, other formulas as provided in the following viewgraphs, for the first and second derivatives can be derived from Taylor series expansion.

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- First Derivative
  - Forward Difference
    - First-order Approximation

$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x} \qquad (18)$$

    - Second-order Approximation

$$\frac{df(x)}{dx} \approx \frac{-f(x+2x) + 4f(x+\Delta x) - 3f(x)}{2\Delta x} \qquad (19)$$

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- First Derivative
  - Backward Difference
    - First-order Approximation

$$\frac{df(x)}{dx} \approx \frac{f(x) - f(x-\Delta x)}{\Delta x} \qquad (20)$$

    - Second-order Approximation

$$\frac{df(x)}{dx} \approx \frac{3f(x) - 4f(x-\Delta x) + f(x-2x)}{2\Delta x} \qquad (21)$$

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- First Derivative
  - Two-Step Method
    - First-order Approximation

$$\frac{df(x)}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} \quad (22)$$

    - Second-order Approximation

$$\frac{df(x)}{dx} \approx \frac{-f(x+2\Delta x) + 8f(x+\Delta x) - 8f(x-\Delta x) + f(x-2\Delta x)}{12\Delta x} \quad (23)$$

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- Second Derivative
  - Forward Difference
    - First-order Approximation

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x+\Delta 2x) - 2f(x+\Delta x) + f(x)}{(\Delta x)^2} \quad (24)$$

    - Second-order Approximation

$$\frac{d^2 f(x)}{dx^2} \approx \frac{-f(x+3\Delta x) + 4f(x+2\Delta x) - 5f(x+\Delta x) + 2f(x)}{(\Delta x)^2} \quad (25)$$

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- Second Derivative
  - Backward Difference
    - First-order Approximation

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x) - 2f(x-\Delta x) + f(x-2\Delta x)}{(\Delta x)^2} \qquad (26)$$

    - Second-order Approximation

$$\frac{d^2 f(x)}{dx^2} \approx \frac{2f(x) - 5f(x-\Delta x) + 4f(x-2\Delta x) - f(x-3\Delta x)}{(\Delta x)^2} \qquad (27)$$

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- Second Derivative
  - Two-Step Method
    - First-order Approximation

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2} \qquad (28)$$

    - Second-order Approximation

$$\frac{d^2 f(x)}{dx^2} \approx \frac{-f(x+2\Delta x) + 16f(x+\Delta x) - 30f(x) - 16f(x-\Delta x) - f(x-2\Delta x)}{12(\Delta x)^2} \qquad (29)$$

Numerical Differentiation

■ Example 6 – Evaporation Rates

A design engineer must make estimate of evaporation rates when the amount of needed water to meet irrigation demands is required. One input to frequently used formula for estimating evaporation rates is the slope of the saturation vapor pressure curve at air temperature *T*. The following data are collected to make such design estimates.

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■ Example 6 (cont'd):

Using the second-order approximation for the first derivative for forward, backward, and two-step methods estimate the slope of the saturation vapor at $T = 22^0$C.

T (^{0}C)	e_s (mm Hg)
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

Numerical Differentiation

■ Example 6 – Evaporation Rates

Using forward difference of Eq. 19, the slope is as follows:

$$\frac{df(x)}{dx} \approx \frac{-f(x+2x)+4f(x+\Delta x)-3f(x)}{2\Delta x}$$

$$= \frac{-e_s(24)+4e_s(23)-3e_s(22)}{2(1)}$$

$$= \frac{-22.37+4(21.05)-3(19.82)}{2(1)} = 1.185 \text{ mm Hg}/{}^0\text{C}$$

T (⁰C)	e_s (mm Hg)
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

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■ Example 6 – Evaporation Rates

Using backward difference of Eq. 21, the slope is as follows:

$$\frac{df(x)}{dx} \approx \frac{3f(x)-4f(x-\Delta x)+f(x-2\Delta x)}{2\Delta x}$$

$$= \frac{3e_s(22)-4e_s(21)+e_s(20)}{2(1)}$$

$$= \frac{3(19.82)-4(18.65)+(17.53)}{2(1)} = 1.195 \text{ mm Hg}/{}^0\text{C}$$

T (⁰C)	e_s (mm Hg)
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

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■ Example 6 – Evaporation Rates

Using backward difference of Eq. 23, the slope is as follows:

$$\frac{df(x)}{dx} \approx \frac{-f(x+2\Delta x)+8f(x+\Delta x)-8f(x-\Delta x)+f(x-2\Delta x)}{12\Delta x}$$

T (^{0}C)	e_s (mm Hg)
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

$$= \frac{-e_s(24)+8e_s(23)-8e_s(21)+e_s(20)}{12(1)}$$

$$= \frac{-(22.37)+8(21.05)-8(18.65)+(17.53)}{12(1)} = 1.1966 \text{ mm Hg}/^0\text{C}$$