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NUMERICAL METHODS & OPTIMISATION

Part II: Numerical Differentiation

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Chapter Description

- Aims
  - Apply numerical methods in solving engineering problem and optimisation
- Expected Outcomes
  - Calculate the area under the curve by using different differentiation and integration methods
  - Apply the different differentiation and integration methods to solve engineering problems
- References
  - Steven C. Chapra and Raymond P. Canale (2009), Numerical Methods for Engineers, McGraw-Hill, 6th Edition

Integration of Equation

- The types of functions that can be integrated numerically exist in two forms:
  - A table of values: This form of data is limited by the number of points that are given.
  - A function: The values of f(x) can be generated as needed to attain the acceptable accuracy.

Derivation of the Two-Point Gauss-Legendre Formula

- The general form of this formula is given by:

$$I \cong c_0 f(x_0) + c_1 f(x_1)$$

- Rearrangement and substitution of the above equation yield:

$$I \cong f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

- In the presence of limit of integration, one should modify/ transform the given function using the following equations:

$$x = \frac{(b+a)+(b-a)x_d}{2} \qquad dx = \frac{b-a}{2}dx_d$$

Higher Points Gauss-Legendre Formula

- The general form of this formula is given by:

$$I \cong c_0 f(x_0) + c_1 f(x_1) + \ldots + c_{n-1} f(x_{n-1})$$

where n is the number of points.

- The values of c's and x's for up to the two points formula are summarized in the following table

Points	Weighting Factors (c)	Function Arguments (x)
1	$c_0 = 1.000000$ $c_1 = 1.000000$	$x_0 = -0.577350$ $x_1 = 0.577350$
2	$c_0 = 0.555556$ $c_1 = 0.888889$ $c_2 = 0.555556$	$x_0 = -0.774597$ $x_1 = 0.0$ $x_2 = 0.774597$

Numerical Differentiation

- This topic has been previously covered in Chapter 1 – Taylor Series Expansion was used to derive finite-divided-difference approximations of derivatives
- The finite-divided-difference approximations can be divided to:
  - Forward
  - Backward
  - Centered
- The errors are developed based on the step size used during the estimation
- In this chapter, a more accurate estimation will be developed – reduced error

Higher accuracy differentiation formulas

- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.
  - First derivative

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} \quad \text{; Error = O(h)}$$

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

  - Second derivative

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

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

Richardson Extrapolation

- There are two ways to improve derivative estimates when employing finite divided differences:
  - By decreasing the step size, or
  - By using a higher-order formula that employs more points.

- A third approach, based on Richardson extrapolation, uses two derivative estimates to compute a third, more accurate approximation.

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

Derivatives of unequally spaced data

- Data from experiments or field studies are often collected at unequal intervals.
- One way to handle such data is to fit a second-order Lagrange interpolating polynomial.

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

Discussion

- A jet fighter's position on an aircraft carrier's runway was timed during landing:

t, s	0	0.52	1.04	1.75	2.37	3.25	3.83
x, m	153	185	210	249	261	271	273

- Where x is the distance from the end of the carrier. Using numerical differentiation, estimate:
  - Velocity (dx/dt)
  - Acceleration (dv/dt)

Conclusion

- The area under the curve can be estimated by using different differentiation and integration methods
- Different differentiation and integration methods can be applied to solve engineering problems

Main Reference

Steven C. Chapra and Raymond P. Canale (2009), Numerical Methods for Engineers, McGraw-Hill, 6th Edition

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