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NUMERICAL METHODS & OPTIMISATION

Part I: 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

Overview

Numerical Differentiation and Integration

- **Newton-Cotes Integration Formulas**
  - Trapezoidal rule
  - Simpson’s rules
- **Integration of Equations**
  - Gauss Quadrature
- **Numerical Differentiation**
  - High-accuracy formulas
  - Richardson extrapolation
  - Unequal-spaced data

Numerical methods for differentiation and integration

- The function to be differentiated or integrated will typically be in one of the following three forms:
  - A simple continuous function such as polynomial, an exponential, or a trigonometric function.
  - A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
  - A tabulated function where values of x and f(x) are given at a number of discrete points, as is often the case with experimental or field data.

New Cotes Integration Formulas

- Most common numerical integration schemes
- Based on strategy of replacing a complicated function or tabulated data with an approximating function

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

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$$

- n is the order of polynomial

a) First order polynomial is used as approximation
b) Parabola for the same purpose

The Trapezoidal Rule

- The *Trapezoidal rule* is the first of Newton-Cotes integration formulas, for cases in which the polynomial is **first order**:

$$I = \int_a^b f(x)dx \cong \int_a^b f_1(x)dx$$

- The area under curve is an estimate of *f(x)* between the limits of *a* and *b*:

  I ≅ width x average height

$$I = (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

The Multiple Application of Trapezoidal Rule

- One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from *a* to *b* into *n* number of segments and apply the method to each segment.
- The areas of individual segments can then be added to yield the integral for the entire interval.

$$h = \frac{b-a}{n} \qquad a = x_0 \quad b = x_n$$

$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

The Simpson's Rule

- A more accurate estimation of an integral can be obtained if a higher-order polynomial is used to connect the points.
- The formulas that result from taking the integrals under such polynomials are called *Simpson's rules*.

Simpson's 1/3 Rule

- Results when a **second-order Lagrange** interpolating polynomial is used.

$$I \cong (b-a)\left[\frac{f(x_0)+4f(x_1)+f(x_2)}{6}\right]$$

$$E_a = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Multiple Application of Simpson's 1/3 Rule

- Just as the trapezoidal rule, Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width.
- Yields accurate results and considered superior to trapezoidal rule for most applications.
- Can be employed only if the number of segments is even

$$I \cong (b-a)\left[\frac{f(x_0)+4\sum_{i=1,3,5}^{n-1} f(x_i)+2\sum_{j=2,4,6}^{n-2} f(x_j)+f(x_n)}{3n}\right]$$

$$E_a = -\frac{(b-a)^5}{180n^4}\bar{f}^{(4)}$$

Simpson's 3/8 Rule: Cubic

- Results when a **third-order Lagrange** interpolating polynomial is used.
- This polynomial can be fit to four points and integrated to yield:

$$I \cong (b-a)\left[\frac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}\right]$$

$$E_a = -\frac{(b-a)^5}{6480} f^{(4)}(\xi)$$

Illustration of how Simpson's rule 1/3 and 3/8 can be applied in tandem to handle multiple application with odd numbers of intervals

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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