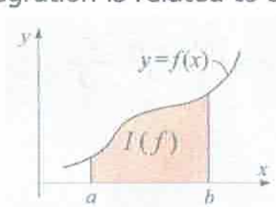
MCEN3030 COMPUTATIONAL METHODS

CHAPTER 9

NUMERICAL INTEGRATION

Background

- Engineering measurements require the calculation of both derivatives and integrals:
  -
- Analytical integration can be difficult
  -
- Same code can be used for many functions
  -
- Numerical integration is related to solving ODE's



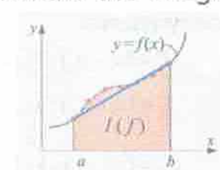
Example

Measuring the volumetric flow across a pipe using a Pitot tube:

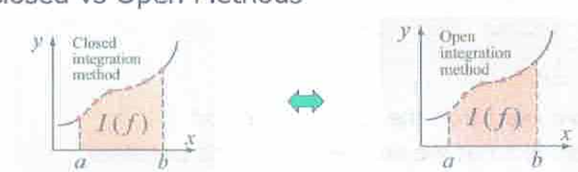
- Formula: $Q = \int_A v\,dA = \int v(r)\cdot dA$
- Approximation:

Numerical Integration Approaches

- First approach consist on using the end points to approximate the integral to a trapezoid

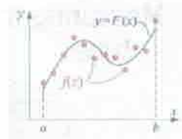


- Closed vs Open Methods

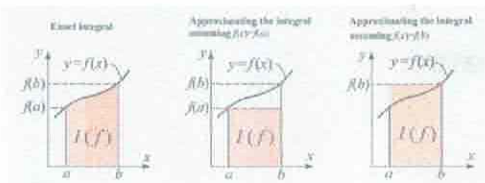


Initial Approaches

- Newton-Cotes Integration: Closed Method
  - Data is fitted into a curve (function), which is easy to integrate: polynomial

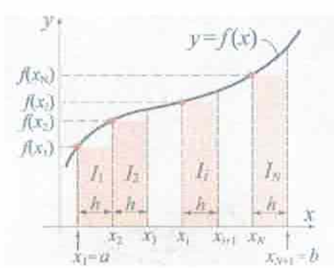


- Rectangle Method: Closed Method
  - Assume a constant value for the function:



Rectangle Method

- Composite Rectangle Method:
  - The domain [a,b] is divided into N intervals: (N+1) points
  - Each integral is calculated on every interval



$$I_1 \approx (x_2 - x_1) f(x_1) = h \cdot f(x_1)$$

$$I_2 \approx (x_3 - x_2) f(x_2) = h \cdot f(x_2)$$

$$\vdots$$

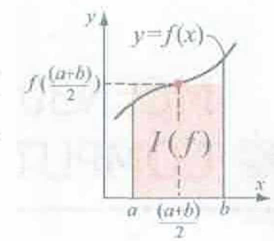
$$I_N \approx (x_{N+1} - x_N) f(x_N) = h \cdot f(x_N)$$

- More exact than the rectangle method
- More exact as the number of intervals increases

Mid Point Methods

- Midpoint Method: Open Method
  - Instead of the extreme points, the midpoint is used to calculated the integral

$$I = \int_a^b f(x)dx \approx \int_a^b f\left(\frac{a+b}{2}\right)dx = f\left(\frac{a+b}{2}\right)\int_a^b dx$$



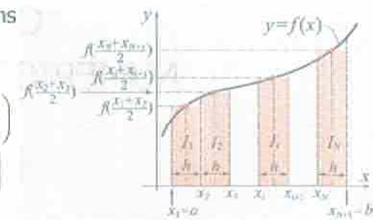
  - Composite Midpoint Method
    - Domain is again divided in N sections

$$I_1 \approx (x_2 - x_1) f\left(\frac{x_1 + x_2}{2}\right) = h \cdot f\left(\frac{x_1 + x_2}{2}\right)$$

$$\vdots$$

$$I_N \approx (x_{N+1} - x_N) f\left(\frac{x_N + x_{N+1}}{2}\right) = h \cdot f\left(\frac{x_N + x_{N+1}}{2}\right)$$

$$I = \int_a^b f(x)dx \approx \sum_{i=1}^{N} I_i = \sum_{i=1}^{N} h \cdot f\left(\frac{x_i + x_{i+1}}{2}\right)$$

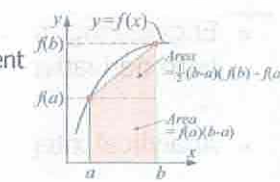


Trapezoidal Method

$$f(x) = \frac{f(b) - f(a)}{b-a}(x-a) + f(a)$$

- Closed Method
- A linear approximation is used to represent the function:

$$I = \int_a^b f(x)dx \approx \int_a^b \left[\frac{f(b) - f(a)}{b-a}(x-a) + f(a)\right]dx$$

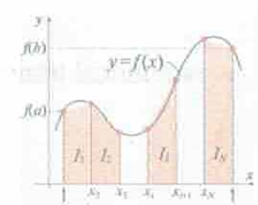


- Composite Trapezoidal Method

$$I_1 \approx \left[\frac{f(x_1) + f(x_2)}{2}\right](x_2 - x_1) = \left[\frac{f(x_1) + f(x_2)}{2}\right]h$$

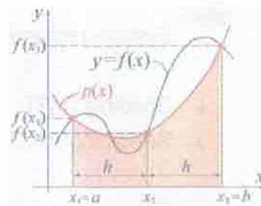
$$\vdots$$

$$I_N \approx \left[\frac{f(x_N) + f(x_{N+1})}{2}\right](x_{N+1} - x_N) = \left[\frac{f(x_N) + f(x_{N+1})}{2}\right]h$$



Simpson's Methods

- This technique approximates the function to higher order polynomial instead of a line
- Quadratic function: 1/3 method
  - 3 points needed: $x_1, x_2, x_3 \quad f(x_1), f(x_2), f(x_3)$
  - Newton's Polynomial:



$$p(x) = \alpha + \beta(x - x_1) + \gamma(x - x_1)(x - x_2)$$

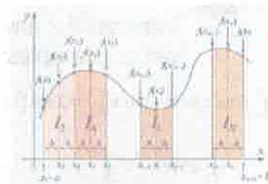
$$p(x) = f(x_1) + \left[\frac{f(x_2) - f(x_1)}{h}\right](x - x_1) + \left[\frac{f(x_3) - 2f(x_2) + f(x_1)}{2h^2}\right](x - x_1)(x - x_2) \quad h = \frac{b-a}{2}$$

$$I = \int_a^b f(x)dx \approx \int_a^b p(x)dx = \int_a^b \left[\alpha + \beta(x - x_1) + \gamma(x - x_1)(x - x_2)\right]dx$$

$$I \approx \alpha\int_a^b dx + \beta\int_a^b (x - x_1)dx + \gamma\int_a^b (x - x_1)(x - x_2)dx$$

Simpson's Methods

- Composite Simpson's 1/3 method
  - Use N several subintervals: different N equations
  - Each quadratic equation will involve two intervals
  - Number of intervals must be an even number
- The case for same width is shown: $h = \frac{b-a}{N}$



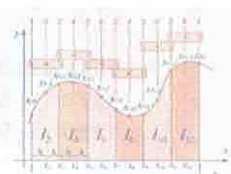
$$I = \int_a^b f(x)dx = \int_{x_1=a}^{x_3} f(x)dx + \int_{x_3}^{x_5} f(x)dx + \ldots + \int_{x_{i-1}}^{x_{i+1}} f(x)dx + \ldots + \int_{x_{N-1}}^{x_{N+1}} f(x)dx$$

$$I = \sum_{i=2,4,6,\ldots}^{N} \int_{x_{i-1}}^{x_{i+1}} f(x)dx \approx \sum_{i=2,4,6,\ldots}^{N} \int_{x_{i-1}}^{x_{i+1}} p(x)dx \Rightarrow I \approx \sum_{i=2,4,6,\ldots}^{N} \frac{h}{3}\left[f(x_{i-1}) + 4f(x_i) + f(x_{i+1})\right]$$

$$I \approx \frac{h}{3}\left[\sum_{i=2,4,6,\ldots}^{N} f(x_{i-1}) + 4\sum_{i=2,4,6,\ldots}^{N} f(x_i) + \sum_{i=2,4,6,\ldots}^{N} f(x_{i+1})\right]$$

$$I \approx \frac{h}{3}\left[\sum_{i=1,3,5,\ldots}^{N-1} f(x_i) + 4\sum_{i=2,4,6,\ldots}^{N} f(x_i) + \sum_{i=3,5,7,\ldots}^{N+1} f(x_i)\right]$$

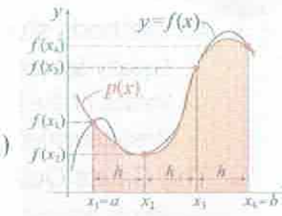
$$I \approx \frac{h}{3}\left[f(x_1) + \sum_{i=3,5,\ldots}^{N-1} f(x_i) + 4\sum_{i=2,4,6,\ldots}^{N} f(x_i) + \sum_{i=3,5,7,\ldots}^{N-1} f(x_i) + f(x_{N+1})\right]$$



3/8 Simpson's Methods

- Cubic function: 3/8 method
- Four points are needed: equally spaced

$x_1, x_2, x_3, x_4 \quad f(x_1), f(x_2), f(x_3), f(x_4)$

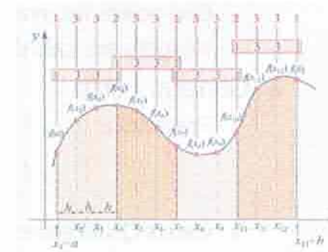


$$p(x) = \alpha + \beta(x - x_1) + \gamma(x - x_1)(x - x_2) + \delta(x - x_1)(x - x_2)(x - x_3)$$

$$I = \int_a^b f(x)dx \approx \frac{3}{8}h\left[f(a) + 3f(x_2) + 3f(x_3) + f(b)\right]$$

- Composite 3/8 methods:
  - N has to be a multiple of 3

$$I \approx \sum_{i=1,4,7,\ldots} \frac{3}{8}h\left[f(x_i) + 3f(x_{i+1}) + 3f(x_{i+2}) + f(x_{i+3})\right]$$



Summary Table

- Single Methods

Integration Method	Values of the function used in evaluating the integral.
Rectangle Equation (7.2)	$f(a)$ or $f(b)$ (Either one of the endpoints.)
Midpoint Equation (7.5)	$f((a+b)/2)$ (The middle point.)
Trapezoidal Equation (7.9)	$f(a)$ and $f(b)$ (Both endpoints.)
Simpson's 1/3 Equation (7.16)	$f(a)$, $f(b)$, and $f((a+b)/2)$ (Both endpoints and the middle point.)
Simpson's 3/8 Equation (7.20)	$f(a)$, $f(b)$, $f\left(a+\frac{1}{3}(a+b)\right)$, and $f\left(a+\frac{2}{3}(a+b)\right)$ (Both endpoints and two points that divide the interval into three equal-width subintervals.)

- Composite Methods include several intervals

Gauss Quadrature

- All methods studied previously use:
  - Equally spaced points
  - Values of the function at those points.
  - Predetermined constant weights
- The Gauss Quadrature Method:
  - Points are not equally spaced
  - End points are not included
  - Weights are calculated to minimize the error
- General Form
  - Previously: $I=\int_a^b f(x)dx \approx f(a)\cdot(b-a)$

    $I=\int_a^b f(x)dx \approx \frac{h}{3}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$
  - Gauss Quadrature:

Gauss Quadrature

- Basic Integral on domain [-1,1]: $\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} C_i f(x_i)$
- Coefficients and Weights are calculated by enforcing the results for: $f(x)=1,x,x^2,x^3,...$
- Example: n=2
  - 4 unknowns: $x_1,x_2,C_1,C_2 \rightarrow$ 4 equations
  - Procedure: Take first four functions:
    - First: $\int_{-1}^{1}(1)dx = C_1\cdot 1 + C_2\cdot 1 \Rightarrow x\Big|_{-1}^{1} = 2 = C_1 + C_2$
    - Second: $\int_{-1}^{1} x dx = C_1x_1 + C_2x_2 \Rightarrow \left[\frac{x^2}{2}\right]_{-1}^{1} = 0 = C_1x_1 + C_2x_2$
    - Third: $\int_{-1}^{1} x^2 dx = C_1x_1^2 + C_2x_2^2 \Rightarrow \left[\frac{x^3}{3}\right]_{-1}^{1} = \frac{2}{3} = C_1x_1^2 + C_2x_2^2$
    - Fourth: $\int_{-1}^{1} x^3 dx = C_1x_1^3 + C_2x_2^3 \Rightarrow \left[\frac{x^4}{4}\right]_{-1}^{1} = 0 = C_1x_1^3 + C_2x_2^3$

Gauss Quadrature

- System reduces to:
- Dividing IV/II:
- Replacing in (III): , from (I):
- Taking the positive root:
- Choosing x_1 to be symmetrically opposite to x_2:
- Replacing in (II): $C_1(-1/\sqrt{3}) = -C_2(1/\sqrt{3}) \Rightarrow C_1 = C_2 \Rightarrow C_1 = C_2 = 1$
- Finally:
- Previous 2-term expression will calculate the exact integral for the 4 functions presented: $f(x)=1,x,x^2,x^3$

Gauss Quadrature

- Integrals for any other function will have an approximated value. Examples:

$$\int_{-1}^{1}\cos(x)dx = [\sin x]_{-1}^{1} = 2\sin(1) = 1.683 \Rightarrow$$

$$\int_{-1}^{1} e^x dx = \left[e^x\right]_{-1}^{1} = e^1 - e^{-1} = 2.350 \Rightarrow$$

$$\int_{-1}^{1} x^4 dx = \left[\frac{x^5}{5}\right]_{-1}^{1} = \frac{1^5}{5} - \frac{-1^5}{5} = 0.4 \Rightarrow$$

$$\int_{-1}^{1} x^8 dx = \left[\frac{x^9}{9}\right]_{-1}^{1} = \frac{1^9}{9} - \frac{-1^9}{9} = 0.222 \Rightarrow$$

- Accuracy can be improved by increasing the number of terms:
  - 3 terms $\rightarrow$ 6 unknowns: Use 6 functions: $f(x)=1,x,x^2,x^3,x^4,x^5$
  - 4 terms $\rightarrow$ 8 unknowns: Use 8 functions: ...

Gauss Quadrature: General Case

- Simple Integral: $\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{2} C_i f(x_i)$
- General Integral: $I = \int_a^b f(x)dx$
- Changing variable: $x \to t$ $\quad \Big\} \; x = mt + p$
- Then:

$$I = \int_a^b f(x)dx = \int_{-1}^{1} f\left(\frac{1}{2}[t(b-a)+b+a]\right)\frac{1}{2}(b-a)\,dt$$

$$\int_a^b f(x)dx = \frac{1}{2}(b-a)\int_{-1}^{1} f\left(\frac{1}{2}[t(b-a)+b+a]\right)dt$$

Matlab Commands

- quad(function,a,b)
  - Function and limits are needed within a tolerance of 10^{-6}
  - Tolerance is specified for the case: quad(function,a,b,tol)
  - Modified Simpson's Method is used
- trapz(x,y)
  - Data is entered as two column vectors
  - Trapezoid method is used
- dblquad
  - Used for double integrals

Improper Integrals

- Not all integrals are continuous:
  - Check for discontinuity points in the function domain
- Integral may have singularities
  - Numerical Integration must be performed by dividing the whole domain into several domains
  - Limit of integrations may need to be approximated
  - Consider changing variables to avoid singularities
- Unbounded Limits
  - Numerical integrations is possible if the integral converges
  - Number of intervals is increased until variation becomes small