6.4. Numerical Integration — The Basics and Newton - Cotes. Quadrature.

For closed Newton Cotes $\Delta x = \frac{b-a}{n}$ $\wedge$ abscissas $x_i = a + i\Delta x$

" open " $\Delta x = \frac{(b-a)}{(n+2)}$ $\wedge$ abcissas $x_i = a+(i+1)\Delta x$.

Closed Newton Cotes :-

(1) Trapezoidal rule :- It correspond when $n = 1$.

$x_0 = a \quad x_1 = b \qquad \Delta x = b-a$

$$I(f) \simeq I_{1,\text{closed}}(f) = \frac{\Delta x}{2}(f(a)+f(b)).$$

$$= \frac{b-a}{2}(f(a)+f(b)).$$

(2). Simpson rule :- It corresponds when $n=2$. (one-third rule).

$x_0 = a \quad x_1 = a+\Delta x = \frac{a+b}{2},$

$x_2 = a+2\Delta x = a+2\frac{(b-a)}{2} = b.$

$$I(f) \simeq I_{2,\text{closed}}(f) = \frac{(b-a)}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right].$$

(3) when $n=3$ we have three - eight rule.

$$I(f) \simeq I_{3,\text{closed}}(f) = \frac{(b-a)}{8}\left[f(a)+3f(a+\Delta x)+3f(a+2\Delta x)+f(b)\right].$$

(4) when $n=4$. we have Boole's rule.

$$I(f) \simeq I_{4,\text{closed}}(f) = \frac{b-a}{90}\left(7f(a)+32f(a+\Delta x)+12f(a+2\Delta x)+32f(a+3\Delta x)+7f(b)\right).$$

(5). Trapezoidal Error and degree of precission on Trapezoidal rule :—

$$I(f) - I_{1,\text{closed}}(f) = -\frac{(b-a)^3}{12}f''(\xi) \quad a \le \xi \le b$$

⑥ Error and degree of precission of Simpson Rule :-

$$I(f) \approx I_2 \text{ closed } (f) = \frac{-(b-a)^5}{2880} \cdot f^{(4)}(\hat{\xi}) . a < \hat{\xi} \leq b$$

⑦ Mid point Rule :- $n=0$

$$I(f) \approx I_{0,\text{ open}}(f) = (b-a) f\left(\frac{a+b}{2}\right).$$

⑧ $n=1,$

$$I(f) \approx I_{1,\text{ open}}(f) = \frac{b-a}{2}\left[f(a+\Delta x)+f(a+2\Delta x)\right]$$

$$\Delta x = \frac{b-a}{3}$$

⑨ Degree of precission of mid point rule and Error term

$$I(f) - I_{0,\text{ open}}(f) = (b-a) f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24} f''(\hat{\xi}).$$

$$a < \xi < b$$

⑩ Error term and degree of precission of simpson rule :-

$$I(f) - I_{1,\text{ open}}(f) = \frac{(b-a)^3}{36} f''(\xi).$$

Q1. Approx the value using Trapezoidal rule and verify the theorical error bound hold in each case.

a). $\int_1^2 \frac{1}{x} dx.$

Sol: By trapezoidal rule we have

$$I(f) \approx I_{1,\text{ closed}}(f) = \frac{b-a}{2}\left[f(a)+f(b)\right].$$

$f(x) = \frac{1}{x}.$

Here $a = 1,$ $b = 2.$

$f(a) = \frac{1}{1} = 1$ and $f(b) = \frac{1}{2} = 0.5$

$\therefore$ $I_{1,\text{closed}}(f) = \frac{1}{2}\left[1 + 0.5\right] = \frac{1.5}{2} = 0.75$

Exact Value, $I(f) = \int_1^2 \frac{1}{x}\,dx = \ln x \Big|_1^2 = \ln 2 - \ln(1)$
$= 0.6931471 8$

Then
Absolute Error $= |I(f) - I_{1,\text{closed}}(f)|$
$= |0.69314718 - 0.75|$

$= 0.056852819$

The error term associated with Trapezoidal rule is
$-\frac{(b-a)^3}{12} f''(\xi) = -\frac{1}{12} f''(\xi)$.

The theoretical error bound is given by,
$\max_{1 \le x \le 2} \left| -\frac{1}{12} f''(x) \right| = \frac{1}{12} \max_{1 \le x \le 2} |f''(x)| = \frac{1}{12} \max_{1 \le x \le 2}$

As, $f(x) = \frac{1}{x}$,
$f'(x) = -\frac{1}{x^2}$
$f''(x) = +\frac{2}{x^3}$

$\therefore$ $\max_{1 \le x \le 2} \left| -\frac{1}{12} f''(x) \right| = \frac{1}{12} \max_{1 \le x \le 2} \left| \frac{2}{x^3} \right| = \frac{1}{6}$
$= 0.16666666666$

~~$= \frac{2}{12} \left| \max_{1 \le x \le 2} \right| \frac{2}{x^3}$~~

let $g(x) = \frac{1}{x^3}$
$g'(x) = -\frac{3}{x^4}$
$g''(x) = 0$
$x = \infty$

$\frac{2}{8} \times \frac{1}{12} = \frac{1}{48}$

$= \frac{1}{6} = 0.6666666666$

$\therefore$ $0.056852819 < 0.66666666$

So, Theoritical error bound holds.

(b). $\int_0^1 e^{-x}\,dx$.

$a = 0, \quad b = 1.$

$f(a) = 1 \qquad f(b) = \cancel{0.3678794401}\ \frac{1}{e}.$

By Trapezoidal rule,

$I_{1,closed}(f) = \frac{b-a}{2}\left[f(a) + f(b)\right].$

$= \frac{1}{2}\left[1 + e^{-1}\right].$

$= 0.68393972.$

$I_{1,closed}(f) = \frac{b-a}{2}$

$I(f)$

Exact Value $I(f) = \int_0^1 e^{-x}\,dx = -e^{-x}\Big|_0^1$

$= -e^{-1} + e^{0}.$

$= -e^{-1} + 1.$

$= 1 - e^{-1} = 0.632120558$

Then Absolute Error.

$|I(f) - I_{1,closed}(f)| = |0.632120558 - 0.68393972|$

$= 0.05181916\,1.$

The error term associated with Trapezoidal is given as, $-\frac{(b-a)^3}{12} f''$

$\max_{0 \le x \le 1} \left| -\frac{(b-a)^3}{12} f''(\eta) \right| = \max_{0 \le x \le 1} \left| -\frac{1}{12} f''(\eta) \right|$

$= \max_{0 \le x \le 1} \frac{1}{12} \left| f''(\eta) \right|$

$f'(x) = -e^{-x}$

$f''(x) = e^{-x}$

$= \frac{1}{12} \max_{0 \le x \le 1} \left| e^{-x} \right| = \frac{1}{12} = 0.08333333333$

$\therefore$ $0.05181916\,1 < 0.08333333$ $\therefore$ Theoritical error holds.

Q. ii C $\int_0^1 \frac{1}{1+x^2}\,dx$.

Trapezoidal rule is given by,

$$I_{1,\text{closed}}(f) = \frac{(b-a)}{2}[f(a)+f(b)].$$

$a = 0,\ b = 1,$

$f(a) = 1,\ \text{n}\ f(b) = 0.5$

$$\therefore I_{1,\text{closed}}(f) = \frac{1}{2}[1+0.5] = \frac{1.5}{2} = 0.75$$

Exact value $I(f) = \int_0^1 \frac{1}{1+x^2} = \tan^{-1}(x)\Big|_0^1$

$$= \tan^{-1}(1) - \tan^{-1}(0)$$

$$= \pi/4 - 0$$

$$= 0.785390163$$

Absolute Error $= \left| I(f) - I_{1,\text{closed}}(f) \right|$.

$$= \left| \frac{\pi}{4} - 0.75 \right|$$

$$= 0.035398163.$$

The Error term is given by

$$\left| -\frac{(b-a)}{12} f''(\xi) \right| = \max_{0\le x\le 1} \left| -\frac{1}{12} f''(\xi) \right|.$$

$$= \frac{1}{12} \max_{0\le x\le 1} \left| f''(\xi) \right|.$$

$f(x) = \frac{1}{1+x^2}$.

$f'(x) = \frac{-2x}{(1+x^2)^2}$.

$$= -2\left[\frac{(1+x^2)^2(1) - x\,2(1+x^2)(2x)}{(1+x^2)^4} \right]$$

$$= -2\left[\frac{(1+x^2)^2 - 4x^2(1+x^2)}{(1+x^2)^4} \right]$$

$$= -2\,\frac{(1-3x)}{(1+x^2)^3}$$

$$f''(x) = -2\left[\frac{1-3x^2}{(1+x^2)^3}\right].$$

$$\therefore \frac{1}{12}\max_{0\le x\le 1}\left|-2\,\frac{(1-3x^2)}{(1+x^2)^3}\right| = \frac{2\times 1}{12}\max_{0\le x\le 1}\left|-\frac{2}{8}\right|.$$

$$= \frac{2}{12}\times\frac{2}{8} = \frac{1}{4}\times\frac{1}{4}.$$

$$= \frac{1}{6}\times\frac{1}{4} = \frac{1}{24}.$$

$$= 0.041\,66666666$$

$\because$ absolute error < Theoritical error.

$\therefore$ Theoritical error bounds holds

Q2 Apply Simpson's Rule and verify the Theoritical error bound in this case.

(1) $\int_1^2 \frac{1}{x}\,dx$

By Simpson's Rule (or one-third rule), we get

$$I_{2,\text{closed}}(f) = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

$a = 1, \quad b = 2.$

$f(a) = 1, \quad f(b) = 0.5$

$$\therefore I_{2,\text{closed}}(f) = \frac{1}{6}\left[1 + 4f(1.5) + 0.5\right].$$

$$= \frac{1}{6}\left[1 + 4\times\frac{1}{1.5} + 0.5\right].$$

$$= \frac{1}{6}\left[1 + \frac{4}{1.5} + 0.5\right].$$

$= 0.6944444449.$

Exact value $I(f) = \int_1^2 \frac{1}{x}\,dx = \ln(x)\Big|_1^2 = \ln(2) - \ln(1)$

$= \ln(2)$

$\therefore$ Absolute error $= \left| I(f) - I_{2,\text{closed}}(f) \right|.$

$= \left| \ln(2) - 0.694444444 \right|.$

$= 0.0012972 6344.$

The error term associated with Simpson's rule is

$$-\frac{(b-a)^5}{2880} \cdot f^{(4)}(\xi) \qquad 1 < \xi < 2$$

$$= \frac{-1}{2880} \cdot f^{(4)}(\xi).$$

Theoretical error bound is

$$\max_{1 \le x \le 2} \left| -\frac{1}{2880} \cdot f^{(iv)}(\xi) \right| = \frac{1}{2880} \max_{1 \le x \le 2} \left| f^{(4)}(x) \right|.$$

$f(x) = \frac{1}{x} \quad f'(x) = -\frac{1}{x^2} \quad f''(x) = \frac{2}{x^3} \quad f'''(x) = -\frac{6}{x^4} \quad f^{iv}(x) = \frac{24}{x^5}$

$$\therefore \; = \frac{1}{2880} \max_{1 \le x \le 2} \left| \frac{24}{x^5} \right|$$

$= \frac{24}{2880} \times \frac{1}{32}$

$= \frac{192}{2880} \times \frac{1}{16}$

$= \frac{7}{2880} \times \frac{1}{8}$

$= 0.0002$

$= \frac{6}{2880} \times \frac{1}{8}.$

$= \frac{3}{2880} \times \frac{1}{4}.$

$= 0.000260416667.$

$= 0.00333333334.$

$\frac{24}{32}$

$\frac{12}{16}$

$\frac{6}{8}$

(2) The constants c and c' depend on both n and the type of formula (open vs. closed). For given n, the constant for the closed formula is typically smaller than the constant for the open formula, so closed formulas are used most often in practice. Because open formulas do not evaluate the integrand at the endpoints of the integration interval, open formulas can be useful for certain problems with endpoint singularities. Open formulas also find use in the construction of numerical methods for the solution of initial value problems.

EXERCISES

Q1 **1.** Approximate the value of each of the following integrals using the trapezoidal rule. Verify that the theoretical error bound holds in each case.

(a) $\int_1^2 \frac{1}{x}\,dx$

(b) $\int_0^1 e^{-x}\,dx$

(c) $\int_0^1 \frac{1}{1+x^2}\,dx$

(d) $\int_0^1 \tan^{-1} x\,dx$.

Q2 **2.** Repeat Exercise 1 using Simpson's rule rather than the trapezoidal rule.

3. Repeat Exercise 1 using the midpoint rule rather than the trapezoidal rule.

4. Verify directly that the midpoint rule has degree of precision equal to 1.

5. Verify directly that the open Newton-Cotes formula with $n = 1$ has degree of precision equal to 1.

6. (a) Determine values for the coefficients A_0, A_1, and A_2 so that the quadrature formula

$$I(f) = \int_{-1}^{1} f(x)\,dx = A_0 f\left(-\frac{1}{2}\right) + A_1 f(0) + A_2 f\left(\frac{1}{2}\right)$$

has degree of precision at least 2.

(b) Once the values of A_0, A_1, and A_2 have been computed, determine the overall degree of precision for the quadrature rule.

7. (a) Determine values for the coefficients A_0, A_1, and A_2 so that the quadrature formula

$$I(f) = \int_{-1}^{1} f(x)\,dx = A_0 f\left(-\frac{1}{3}\right) + A_1 f\left(\frac{1}{3}\right) + A_2 f(1)$$

has degree of precision at least 2.

(b) Once the values of A_0, A_1, and A_2 have been computed, determine the overall degree of precision for the quadrature rule.

8. (a) Determine values for the coefficients A_0, A_1, and x_1 so that the quadrature formula

$$I(f) = \int_{-1}^{1} f(x)\,dx = A_0 f(-1) + A_1 f(x_1)$$

has degree of precision at least 2.

(b) Once the values of A_0, A_1, and x_1 have been computed, determine the overall degree of precision for the quadrature rule.

9. Consider the quadrature rule

$$\int_{-1}^{1} f(x)\,dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right).$$

Determine the degree of precision of this formula.

10. Consider the quadrature rule

$$\int_{-1}^{1} f(x)\,dx \approx \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right).$$

Determine the degree of precision of this formula.

11. Derive the error term for the midpoint rule:

$$\frac{(b-a)^3}{24} f''(\xi),$$

where $a < \xi < b$.

12. (a) Derive the closed Newton-Cotes formula with $n = 3$:

$$I(f) \approx I_{3,\text{closed}}(f) = \frac{b-a}{8}[f(a) + 3f(a+\Delta x) + 3f(a+2\Delta x) + f(b)].$$

(b) Verify that this formula has degree of precision equal to 3.

(c) Derive the error term associated with this quadrature rule.

13. (a) Derive the closed Newton-Cotes formula with $n = 4$:

$$I(f) \approx I_{4,\text{closed}}(f) = \frac{b-a}{90}[7f(a) + 32f(a+\Delta x) + 12f(a+2\Delta x) + 32f(a+3\Delta x) + 7f(b)]$$

(b) Verify that this formula has degree of precision equal to 5.

(c) Derive the error term associated with this quadrature rule.

14. (a) Derive the open Newton-Cotes formula with $n = 2$:

$$I(f) \approx I_{2,\text{open}}(f) = \frac{b-a}{3}[2f(a+\Delta x) - f(a+2\Delta x) + 2f(a+3\Delta x)].$$

(b) Verify that this formula has degree of precision equal to 3.

(c) Derive the error term associated with this quadrature rule.

15. (a) Derive the open Newton-Cotes formula with $n = 3$:

$$I(f) \approx I_{3,\text{open}}(f) = \frac{b-a}{24}[11f(a+\Delta x) + f(a+2\Delta x) + f(a+3\Delta x) + 11f(a+4\Delta x)].$$

(b) Verify that this formula has degree of precision equal to 3.