

Newton-Cotes Formulas

Introduction to Newton-Cotes Formulas

The *Newton-Cotes formulas* are a family of methods used for approximating the definite integral of a function. These formulas are derived by interpolating the function using polynomials based on equally spaced data points, and then integrating the polynomial exactly.

Numerical Integration and Interpolation

Given a function $f(x)$, the goal of numerical integration is to approximate the integral:

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

Newton-Cotes formulas work by dividing the interval $[a, b]$ into subintervals and approximating $f(x)$ using polynomials of various degrees over these subintervals.

General Form of Newton-Cotes Formulas

Let $f(x)$ be known at $n + 1$ equally spaced points x_0, x_1, \dots, x_n in the interval $[a, b]$, where:

$$h = \frac{b - a}{n}$$

Newton-Cotes formulas approximate the integral of $f(x)$ over $[a, b]$ by integrating the interpolating polynomial $P_n(x)$ passing through the points $(x_0, f(x_0))$, $(x_1, f(x_1))$, \dots , $(x_n, f(x_n))$.

The integral of the polynomial gives the approximate value of the integral:

$$I \approx \int_a^b P_n(x) dx = h \sum_{i=0}^n w_i f(x_i)$$

where w_i are the *weights* that depend on the interpolation formula used.

Types of Newton-Cotes Formulas

Newton-Cotes formulas can be categorized as **closed** or **open**:

- **Closed Newton-Cotes formulas** include the function values at both ends of the interval.
- **Open Newton-Cotes formulas** do not include the endpoints and instead use values inside the interval.

Common Newton-Cotes Formulas

Trapezoidal Rule (First-Order Polynomial)

The *Trapezoidal Rule* approximates $f(x)$ by a linear polynomial passing through two points $(x_0, f(x_0))$ and $(x_1, f(x_1))$. The formula is:

$$I \approx \frac{h}{2} (f(a) + f(b))$$

Simpson's Rule (Second-Order Polynomial)

The *Simpson's Rule* approximates $f(x)$ by a quadratic polynomial passing through three points $(x_0, f(x_0))$, $(x_1, f(x_1))$, and $(x_2, f(x_2))$. The formula is:

$$I \approx \frac{h}{3} \left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right)$$

Simpson's 3/8 Rule (Third-Order Polynomial)

The *Simpson's 3/8 Rule* uses a cubic polynomial and three subintervals. The formula is:

$$I \approx \frac{3h}{8} \left(f(a) + 3f\left(\frac{2a+b}{3}\right) + 3f\left(\frac{a+2b}{3}\right) + f(b) \right)$$

Example 1: $\int_0^1 e^x dx$

Exact solution:

$$\int_0^1 e^x dx = e - 1 \approx 1.7183$$

Numerical approximations:

- Trapezoidal Rule ($n = 1$): ≈ 1.8591
- Simpson's Rule ($n = 2$): ≈ 1.7189
- Simpson's 3/8 Rule ($n = 3$): ≈ 1.7186

Example 2: $\int_0^1 \sin(x^2) dx$

Numerical approximations:

- Trapezoidal Rule ($n = 1$): ≈ 0.4207
- Simpson's Rule ($n = 2$): ≈ 0.4553
- Simpson's 3/8 Rule ($n = 3$): ≈ 0.4597

Example 3: $\int_0^1 \frac{1}{1+x^2} dx$

Exact solution:

$$\int_0^1 \frac{1}{1+x^2} dx = \frac{\pi}{4} \approx 0.7854$$

Numerical approximations:

- Trapezoidal Rule ($n = 1$): ≈ 0.75
- Simpson's Rule ($n = 2$): ≈ 0.7849
- Simpson's 3/8 Rule ($n = 3$): ≈ 0.7852

Applications and Practical Considerations

Newton-Cotes formulas are widely used in numerical integration, particularly when function values are known at equally spaced points. Care must be taken when applying higher-order formulas, as they can suffer from numerical instability.

Formulation

Let $f(x)$ be a continuous function on $[a, b]$. We approximate the integral:

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

by dividing $[a, b]$ into n subintervals, where n is even. The width of each subinterval is $h = \frac{b-a}{n}$.

Let the points x_0, x_1, \dots, x_n be equally spaced, where $x_0 = a$, $x_n = b$, and $x_i = a + ih$ for $i = 0, 1, \dots, n$. The Newton-Cotes formula is applied to each subinterval, and the results are summed.

Composite Trapezoidal Rule

The *Composite Trapezoidal Rule* is:

$$I \approx \frac{h}{2} \left(f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right) = T(n)$$

Composite Simpson's Rule

The *Composite Simpson's Rule* for an even number of subintervals is:

$$I \approx \frac{h}{3} \left(f(x_0) + 4 \sum_{i \text{ odd}} f(x_i) + 2 \sum_{i \text{ even}} f(x_i) + f(x_n) \right) = S(n)$$

General Composite Newton-Cotes Rule

In general, for any Newton-Cotes rule of degree n , the integral is approximated by:

$$I \approx \sum_{k=1}^n \int_{x_{k-1}}^{x_k} P(x) dx$$

where $P(x)$ is the interpolating polynomial

Example 1: $\int_0^1 e^x dx$

Exact solution:

$$\int_0^1 e^x dx = e - 1 \approx 1.7183$$

Numerical Approximations:

- **Composite Trapezoidal Rule** ($n = 1, m = 4$):

$$\int_0^1 e^x dx \approx \frac{1}{8} \left(e^0 + 2e^{\frac{1}{4}} + 2e^{\frac{1}{2}} + 2e^{\frac{3}{4}} + e^1 \right) \approx 1.7201$$

- **Composite Simpson's Rule** ($n = 2, m = 4$):

$$\int_0^1 e^x dx \approx \frac{1}{12} \left(e^0 + 4e^{\frac{1}{4}} + 2e^{\frac{1}{2}} + 4e^{\frac{3}{4}} + e^1 \right) \approx 1.7183$$

- **Composite Simpson's 3/8 Rule** ($n = 3, m = 3$):

$$\int_0^1 e^x dx \approx \frac{3}{32} \left(e^0 + 3e^{\frac{1}{3}} + 3e^{\frac{2}{3}} + e^1 \right) \approx 1.7184$$

Example 2: $\int_0^1 \sin(x^2) dx$

Exact solution: None (no closed form).

Numerical Approximations:

- **Composite Trapezoidal Rule** ($n = 1, m = 4$):

$$\int_0^1 \sin(x^2) dx \approx \frac{1}{8} \left(\sin(0) + 2 \sin\left(\frac{1}{4}\right) + 2 \sin\left(\frac{1}{2}\right) + 2 \sin\left(\frac{3}{4}\right) + \sin(1) \right) \approx 0.4550$$

- **Composite Simpson's Rule** ($n = 2, m = 4$):

$$\int_0^1 \sin(x^2) dx \approx \frac{1}{12} \left(\sin(0) + 4 \sin\left(\frac{1}{4}\right) + 2 \sin\left(\frac{1}{2}\right) + 4 \sin\left(\frac{3}{4}\right) + \sin(1) \right) \approx 0.4549$$

- **Composite Simpson's 3/8 Rule** ($n = 3, m = 3$):

$$\int_0^1 \sin(x^2) dx \approx \frac{3}{32} \left(\sin(0) + 3 \sin\left(\frac{1}{3}\right) + 3 \sin\left(\frac{2}{3}\right) + \sin(1) \right) \approx 0.4548$$

Properties of Newton-Cotes rule

1. Equally Spaced Nodes Newton-Cotes rules use equally spaced nodes x_i within the interval $[a, b]$, which simplifies the calculation of the interpolation polynomial. The nodes are given by:

$$x_i = a + i \cdot h, \quad i = 0, 1, \dots, n$$

where $h = \frac{b-a}{n}$ is the step size.

2. Degree of Accuracy The degree of accuracy (or precision) of a Newton-Cotes rule is the highest degree polynomial that the rule can integrate exactly.

For an n -point Newton-Cotes rule: - If n is odd, the degree of accuracy is n .
- If n is even, the degree of accuracy is $n + 1$.

For example: - The trapezoidal rule ($n = 1$) has a degree of accuracy of 1. - Simpson's rule ($n = 2$) has a degree of accuracy of 3.

3. Closed vs. Open Formulas Newton-Cotes rules can be classified as either ****closed**** or ****open****: - ****Closed Newton-Cotes rules**** use both endpoints of the interval $[a, b]$ as nodes (e.g., trapezoidal and Simpson's rules). - ****Open Newton-Cotes rules**** do not include the endpoints and use nodes only within the interval (a, b) .

For example: - Trapezoidal rule (closed) uses nodes $x_0 = a$ and $x_1 = b$. - Midpoint rule (open) uses a single node at $x = \frac{a+b}{2}$ without including endpoints.

4. Weights The weights w_i in the Newton-Cotes formulas depend on the number of points n and are chosen to minimize the error of the rule. The weights are derived by integrating Lagrange basis polynomials over $[a, b]$.

For example, in Simpson's rule (for $n = 2$), the weights are:

$$w_0 = \frac{1}{3}, \quad w_1 = \frac{4}{3}, \quad w_2 = \frac{1}{3}$$

5. Error Term The error E in a Newton-Cotes formula of degree n for a sufficiently smooth function $f(x)$ can be expressed as:

$$E = -\frac{(b-a)^{n+3}}{(n+3)!} f^{(n+2)}(\xi)$$

for some $\xi \in [a, b]$. This error term indicates that the accuracy of the rule depends on both the step size h and the smoothness of $f(x)$.

6. Stability and Oscillatory Behavior Newton-Cotes rules are generally stable for small n , but as n increases, these rules can become unstable, particularly for open formulas with high n . This instability is due to **Runge's phenomenon**, where oscillations occur near the endpoints of the interval as the degree of the interpolating polynomial increases.

Gauss-Legendre Quadrature

The Gauss-Legendre quadrature rule is used to approximate the integral of a function $f(x)$ over the interval $[-1, 1]$:

$$\int_{-1}^1 f(x) dx \approx \sum_{i=1}^n w_i f(x_i),$$

where x_i and w_i are nodes and weights that depend on n , the number of points.

Case $n = 1$

For $n = 1$, we have:

$$x_1 = 0, \quad w_1 = 2.$$

Thus,

$$\int_{-1}^1 f(x) dx \approx 2 \cdot f(0).$$

Case $n = 2$

For $n = 2$:

$$x_1 = -\frac{1}{\sqrt{3}}, \quad x_2 = \frac{1}{\sqrt{3}},$$

with weights:

$$w_1 = 1, \quad w_2 = 1.$$

So,

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

Case $n = 3$

For $n = 3$:

$$x_1 = -\sqrt{\frac{3}{5}}, \quad x_2 = 0, \quad x_3 = \sqrt{\frac{3}{5}},$$

with weights:

$$w_1 = \frac{5}{9}, \quad w_2 = \frac{8}{9}, \quad w_3 = \frac{5}{9}.$$

Therefore,

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

Example 1: $\int_{-1}^1 e^x dx$

Exact solution:

$$\int_{-1}^1 e^x dx = e - \frac{1}{e} \approx 2.3504$$

Numerical approximations:

- For $n = 1$: $2 \cdot e^0 = 2$
- For $n = 2$: $e^{-\frac{1}{\sqrt{3}}} + e^{\frac{1}{\sqrt{3}}} \approx 2.3366$
- For $n = 3$: $\frac{5}{9} e^{-\sqrt{\frac{3}{5}}} + \frac{8}{9} e^0 + \frac{5}{9} e^{\sqrt{\frac{3}{5}}} \approx 2.3497$

Example 2: $\int_{-1}^1 \sin(x^2) dx$

Numerical approximations:

- For $n = 1$: $2 \cdot \sin(0) = 0$
- For $n = 2$: $\sin\left(\frac{1}{\sqrt{3}}\right) + \sin\left(-\frac{1}{\sqrt{3}}\right) \approx 0.6325$
- For $n = 3$: $\frac{5}{9} \sin\left(\sqrt{\frac{3}{5}}\right) + \frac{8}{9} \sin(0) + \frac{5}{9} \sin\left(-\sqrt{\frac{3}{5}}\right) \approx 0.6340$

Example 3: $\int_{-1}^1 \frac{1}{1+x^2} dx$

Exact solution:

$$\int_{-1}^1 \frac{1}{1+x^2} dx = \pi \approx 3.1416$$

Numerical approximations:

- For $n = 1$: $2 \cdot \frac{1}{1+0^2} = 2$
- For $n = 2$: $\frac{1}{1+\frac{1}{3}} + \frac{1}{1+\frac{1}{3}} \approx 3.079$
- For $n = 3$: $\frac{5}{9} \cdot \frac{1}{1+\frac{3}{5}} + \frac{8}{9} \cdot \frac{1}{1+0} + \frac{5}{9} \cdot \frac{1}{1+\frac{3}{5}} \approx 3.136$

The Gauss-Legendre integration rule approximates an integral of the form:

$$\int_a^b f(x) dx$$

by transforming the interval to $[-1, 1]$ and using predefined points (nodes) and weights.

For an arbitrary interval $[a, b]$, we use the transformation:

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

Example 1: Integral of $f(x) = x^2$ over $[0, 1]$ Transform the interval $[0, 1]$ to $[-1, 1]$:

$$\int_0^1 x^2 dx = \frac{1}{2} \int_{-1}^1 \left(\frac{x}{2} + \frac{1}{2}\right)^2 dx$$

Applying the Gauss-Legendre rule with $n = 1, 2, 3$:

1. For $n = 1$:

$$\int_0^1 x^2 dx \approx \frac{1}{2} \times w_1 \times f\left(\frac{x_1}{2} + \frac{1}{2}\right) = \frac{1}{2} \times 2 \times \left(\frac{0}{2} + \frac{1}{2}\right)^2 = 0.25$$

2. For $n = 2$:

$$\begin{aligned} \int_0^1 x^2 dx &\approx \frac{1}{2} \left(w_1 f\left(\frac{x_1}{2} + \frac{1}{2}\right) + w_2 f\left(\frac{x_2}{2} + \frac{1}{2}\right) \right) \\ &= \frac{1}{2} \left(1 \times \left(\frac{-0.5774}{2} + \frac{1}{2}\right)^2 + 1 \times \left(\frac{0.5774}{2} + \frac{1}{2}\right)^2 \right) \approx 0.3333 \end{aligned}$$

3. For $n = 3$:

$$\begin{aligned} \int_0^1 x^2 dx &\approx \frac{1}{2} \left(w_1 f\left(\frac{x_1}{2} + \frac{1}{2}\right) + w_2 f\left(\frac{x_2}{2} + \frac{1}{2}\right) + w_3 f\left(\frac{x_3}{2} + \frac{1}{2}\right) \right) \\ &= \frac{1}{2} \left(\frac{5}{9} \times \left(\frac{-0.7746}{2} + \frac{1}{2}\right)^2 + \frac{8}{9} \times \left(\frac{0}{2} + \frac{1}{2}\right)^2 + \frac{5}{9} \times \left(\frac{0.7746}{2} + \frac{1}{2}\right)^2 \right) \approx 0.3333 \end{aligned}$$

Properties of the Gauss-Legendre Rule

1. Orthogonality of Legendre Polynomials: The nodes x_i are the roots of the n -th Legendre polynomial $P_n(x)$, which are orthogonal on the interval $[-1, 1]$. The orthogonality condition for Legendre polynomials $P_m(x)$ and $P_n(x)$ is:

$$\int_{-1}^1 P_m(x) P_n(x) dx = 0 \quad \text{for } m \neq n.$$

2. Exactness for Polynomials of Degree $2n - 1$: The Gauss-Legendre rule with n nodes is exact for all polynomials $f(x)$ of degree up to $2n - 1$. This means that if $f(x)$ is a polynomial of degree $\leq 2n - 1$, then:

$$\int_{-1}^1 f(x) dx = \sum_{i=1}^n w_i f(x_i).$$

3. Symmetry of Nodes and Weights: The nodes x_i and weights w_i are symmetric about the origin. Specifically, for each x_i in the interval $(0, 1]$, there exists a corresponding node $-x_i$ with the same weight:

$$x_i = -x_{n+1-i} \quad \text{and} \quad w_i = w_{n+1-i}.$$

4. Range of Nodes: The nodes x_i are strictly within the interval $(-1, 1)$. For a given n , the nodes are distinct and lie in the open interval $(-1, 1)$:

$$-1 < x_1 < x_2 < \cdots < x_n < 1.$$

5. Transformation for General Intervals: For an interval $[a, b]$ other than $[-1, 1]$, the Gauss-Legendre rule can be transformed using the change of variables:

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

After transforming, the rule becomes:

$$\int_a^b f(x) dx \approx \frac{b-a}{2} \sum_{i=1}^n w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right).$$

6. Computational Efficiency: Since the Gauss-Legendre rule requires fewer nodes than other quadrature methods for a given degree of accuracy (due to its exactness for polynomials of degree $2n-1$), it is computationally efficient, especially for high-precision applications.

7. Positive Weights: The weights w_i of the Gauss-Legendre quadrature rule are always positive, which helps ensure numerical stability:

$$w_i > 0, \quad \text{for all } i = 1, 2, \dots, n.$$

Problem : Determine constants c_j , $j = -1, 0, 1, 2$, such that the quadrature

$$Q(f) = c_{-1}f(-1) + c_0f(0) + c_1f(1) + c_2f(2)$$

satisfies

$$Q(p) = \int_0^1 p(x) dx$$

for every polynomial p of degree ≤ 3 . Show that, with these weights and under appropriate smoothness assumptions on f ,

$$\left| \int_0^1 f(x) dx - Q(f) \right| \leq \frac{11}{720} M_4,$$

where M_4 is a suitable bound on the fourth derivative of f . State the hypotheses needed.

Determine the weights

Exactness for all polynomials of degree ≤ 3 is equivalent to the moment conditions: for $k = 0, 1, 2, 3$,

$$\sum_{j=-1}^2 c_j x_j^k = \int_0^1 x^k dx,$$

where $x_{-1} = -1$, $x_0 = 0$, $x_1 = 1$, $x_2 = 2$. Writing $c_{-1} = a$, $c_0 = b$, $c_1 = c$, $c_2 = d$ we obtain the linear system

$$\begin{aligned} (k=0) \quad & a + b + c + d = \int_0^1 1 dx = 1, \\ (k=1) \quad & -a + 0 \cdot b + c + 2d = \int_0^1 x dx = \frac{1}{2}, \\ (k=2) \quad & a + 0 \cdot b + c + 4d = \int_0^1 x^2 dx = \frac{1}{3}, \\ (k=3) \quad & -a + 0 \cdot b + c + 8d = \int_0^1 x^3 dx = \frac{1}{4}. \end{aligned}$$

Subtract the $k = 1$ equation from the $k = 3$ equation to eliminate a and c :

$$(-a + c + 8d) - (-a + c + 2d) = \frac{1}{4} - \frac{1}{2} \implies 6d = -\frac{1}{4},$$

hence

$$d = c_2 = -\frac{1}{24}.$$

Substitute d into the $k = 1$ and $k = 2$ equations:

$$\begin{aligned} -a + c + 2\left(-\frac{1}{24}\right) &= \frac{1}{2} \implies c - a = \frac{1}{2} + \frac{1}{12} = \frac{7}{12}, \\ a + c + 4\left(-\frac{1}{24}\right) &= \frac{1}{3} \implies a + c = \frac{1}{3} + \frac{1}{6} = \frac{1}{2}. \end{aligned}$$

Solve these two equations for a, c :

$$\begin{cases} c - a = \frac{7}{12}, \\ a + c = \frac{1}{2}, \end{cases} \implies c = \frac{13}{24}, \quad a = -\frac{1}{24}.$$

Finally use the $k = 0$ equation to get b :

$$b = 1 - (a + c + d) = 1 - \left(-\frac{1}{24} + \frac{13}{24} - \frac{1}{24}\right) = 1 - \frac{11}{24} = \frac{13}{24}.$$

Thus the unique weights making the rule exact on \mathbb{P}_3 are

$$\boxed{c_{-1} = -\frac{1}{24}, \quad c_0 = \frac{13}{24}, \quad c_1 = \frac{13}{24}, \quad c_2 = -\frac{1}{24}}.$$

One may check directly that these satisfy the four moment equations.

Error representation (Peano / generalized Taylor form)

Because Q is exact on polynomials up to degree 3, the quadrature error functional

$$\mathcal{E}[f] := \int_0^1 f(x) dx - Q(f)$$

annihilates \mathbb{P}_3 . By the Peano kernel representation (or by repeated integration of the Taylor remainder) there exists $\xi \in (0, 1)$ such that

$$\mathcal{E}[f] = \frac{f^{(4)}(\xi)}{4!} \int_0^1 \omega(x) dx,$$

where the *node polynomial* ω is

$$\omega(x) = \prod_{j=-1}^2 (x - x_j) = (x + 1)x(x - 1)(x - 2).$$

(Heuristically this follows from writing f as its degree-3 Taylor polynomial plus remainder and using exactness of Q on degree ≤ 3 .)

Evaluation of the kernel integral

Expand $\omega(x)$:

$$\omega(x) = (x + 1)x(x - 1)(x - 2) = x^4 - 2x^3 - x^2 + 2x.$$

Integrate termwise on $[0, 1]$:

$$\int_0^1 \omega(x) dx = \int_0^1 (x^4 - 2x^3 - x^2 + 2x) dx = \left[\frac{1}{5} - \frac{2}{4} - \frac{1}{3} + 1 \right] = \frac{1}{5} - \frac{1}{2} - \frac{1}{3} + 1.$$

Compute the rational sum:

$$\frac{1}{5} - \frac{1}{2} - \frac{1}{3} + 1 = \frac{6 - 15 - 10 + 30}{30} = \frac{11}{30}.$$

Hence from the Peano representation,

$$\mathcal{E}[f] = \frac{f^{(4)}(\xi)}{4!} \cdot \frac{11}{30} = \frac{11}{720} f^{(4)}(\xi).$$

Therefore the exact error has the pointwise form

$$\int_0^1 f(x) dx - Q(f) = \frac{11}{720} f^{(4)}(\xi) \quad \text{for some } \xi \in (0, 1).$$

Uniform bound and definition of M_4

If $f \in C^4[0, 1]$ and we define

$$M_4 := \max_{x \in [0, 1]} |f^{(4)}(x)|,$$

then taking absolute values in the pointwise remainder yields the uniform bound

$$\left| \int_0^1 f(x) dx - Q(f) \right| = \left| \frac{11}{720} f^{(4)}(\xi) \right| \leq \frac{11}{720} M_4.$$

Thus the claimed bound holds with M_4 defined as above.

Notation and definitions

Let $a = b_0 < b = b_{2m}$ and consider a uniform partition of $[a, b]$ into $2m$ subintervals of equal length

$$h = \frac{b - a}{2m}.$$

Then the coarser partition with m subintervals has step size $H = 2h$. Denote the nodes by

$$x_i = a + ih, \quad i = 0, 1, \dots, 2m.$$

The composite trapezoidal rule with $2m$ subintervals is

$$T(2m) = \frac{h}{2} \left(f(x_0) + 2 \sum_{i=1}^{2m-1} f(x_i) + f(x_{2m}) \right).$$

The composite trapezoidal rule with m subintervals (step $H = 2h$)—sampling only even nodes—can be written as

$$T(m) = \frac{H}{2} \left(f(x_0) + 2 \sum_{j=1}^{m-1} f(x_{2j}) + f(x_{2m}) \right) = h \left(f(x_0) + 2 \sum_{j=1}^{m-1} f(x_{2j}) + f(x_{2m}) \right).$$

The composite Simpson rule over $2m$ subintervals (i.e. m Simpson panels, each using 3 points) is

$$S(2m) = \frac{h}{3} \left(f(x_0) + 4 \sum_{\substack{i=1 \\ i \text{ odd}}}^{2m-1} f(x_i) + 2 \sum_{\substack{i=2 \\ i \text{ even}}}^{2m-2} f(x_i) + f(x_{2m}) \right).$$

Prove that $S(2m) = \frac{4}{3}T(2m) - \frac{1}{3}T(m)$

We expand the right-hand side in terms of the nodal values $f(x_i)$.

First compute $\frac{4}{3}T(2m)$:

$$\frac{4}{3}T(2m) = \frac{4}{3} \cdot \frac{h}{2} \left(f_0 + 2 \sum_{i=1}^{2m-1} f_i + f_{2m} \right) = \frac{2h}{3} f_0 + \frac{4h}{3} \sum_{i=1}^{2m-1} f_i + \frac{2h}{3} f_{2m},$$

where for brevity $f_i := f(x_i)$.

Next compute $-\frac{1}{3}T(m)$ (recall $T(m) = h(f_0 + 2 \sum_{j=1}^{m-1} f_{2j} + f_{2m})$):

$$-\frac{1}{3}T(m) = -\frac{h}{3} f_0 - \frac{2h}{3} \sum_{j=1}^{m-1} f_{2j} - \frac{h}{3} f_{2m}.$$

Add these two contributions:

$$\frac{4}{3}T(2m) - \frac{1}{3}T(m) = \left(\frac{2h}{3} - \frac{h}{3} \right) f_0 + \left(\frac{4h}{3} \sum_{i=1}^{2m-1} f_i - \frac{2h}{3} \sum_{j=1}^{m-1} f_{2j} \right) + \left(\frac{2h}{3} - \frac{h}{3} \right) f_{2m}.$$

Simplify endpoint coefficients:

$$\frac{2h}{3} - \frac{h}{3} = \frac{h}{3},$$

so the coefficient of f_0 and f_{2m} is $h/3$, matching Simpson's rule.

Now split the interior sum over $i = 1, \dots, 2m-1$ into odd and even indices:

$$\sum_{i=1}^{2m-1} f_i = \sum_{\substack{i=1 \\ i \text{ odd}}}^{2m-1} f_i + \sum_{\substack{i=2 \\ i \text{ even}}}^{2m-2} f_i.$$

Thus the interior contribution becomes

$$\frac{4h}{3} \left(\sum_{i \text{ odd}} f_i + \sum_{i \text{ even}} f_i \right) - \frac{2h}{3} \sum_{i \text{ even}} f_i = \frac{4h}{3} \sum_{i \text{ odd}} f_i + \left(\frac{4h}{3} - \frac{2h}{3} \right) \sum_{i \text{ even}} f_i.$$

But $\frac{4h}{3} - \frac{2h}{3} = \frac{2h}{3}$. Hence the total expression is

$$\frac{h}{3} f_0 + \frac{4h}{3} \sum_{i \text{ odd}} f_i + \frac{2h}{3} \sum_{i \text{ even}} f_i + \frac{h}{3} f_{2m},$$

which is exactly the composite Simpson rule $S(2m)$. Therefore

$$\boxed{S(2m) = \frac{4}{3}T(2m) - \frac{1}{3}T(m)}$$

as required. □

Remarks

- The identity $S(2m) = \frac{4}{3}T(2m) - \frac{1}{3}T(m)$ is precisely the Richardson extrapolation that raises the order of accuracy of the trapezoidal rule from $O(h^2)$ to $O(h^4)$; in fact the combination equals the composite Simpson rule.

Statement of Simpson's rule (single panel)

Let f be sufficiently smooth on $[a, b]$. Put

$$x_0 = a, \quad x_1 = \frac{a+b}{2}, \quad x_2 = b, \quad h = \frac{b-a}{2}.$$

The Simpson (1/3) approximation to the integral $\int_a^b f(x) dx$ is

$$S[f] := \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)).$$

We will prove that this rule is exact for all polynomials of degree ≤ 3 and that, for $f \in C^4[a, b]$, there exists $\xi \in (a, b)$ such that

$$\int_a^b f(x) dx - S[f] = -\frac{(b-a)^5}{2880} f^{(4)}(\xi).$$

Proof

Making the change of variable

$$x = \frac{b+a}{2} + t \frac{b-a}{2}, \quad t \in [-1, 1],$$

and defining the function $t \rightarrow F(t)$ by $F(t) = f(x)$, we see that

$$\begin{aligned} \int_a^b f(x) dx - \frac{h}{3}(f(a) + 4f((a+b)/2) + f(b)) \\ = \frac{b-a}{2} \left(\int_{-1}^1 F(\tau) d\tau - \frac{1}{3}(F(-1) + 4F(0) + F(1)) \right) \end{aligned}$$

We now introduce the function $t \rightarrow G(t)$ by

$$G(t) = \frac{b-a}{2} \left(\int_{-t}^t F(\tau) d\tau - \frac{t}{3}(F(-t) + 4F(0) + F(t)) \right)$$

Moreover, we obtain

$$\begin{aligned}
\int_a^b f(x)dx - \frac{h}{3}(f(a) + 4f((a+b)/2) + f(b)) \\
= \frac{b-a}{2} \left(\int_{-1}^1 F(\tau)d\tau - \frac{1}{3}(F(-1) + 4F(0) + F(1)) \right) \\
= \frac{b-a}{2} G(1).
\end{aligned}$$

The remainder of the proof is devoted to showing that $\frac{b-a}{2}G(1)$ is, in turn, equal to the right-hand side of the desired result for some ξ in (a, b) . To do so, we define

$$H(t) = G(t) - t^5 G(1) \quad t \in [-1, 1],$$

and apply Rolle's Theorem repeatedly to the function H . Noting that $H(0) = 0$ and $H(1) = 0$, we deduce that there exists $\xi_1 \in (0, 1)$ such that $H'(\xi_1) = 0$. But it is easy to show that $H'(0) = 0$, so there exists $\xi_2 \in (0, \xi_1)$, such that $H''(\xi_2) = 0$. Again we see that $H''(0) = 0$, so there exists $\xi_3 \in (0, \xi_2)$ such that $H'''(\xi_3) = 0$. Now,

$$G'''(t) = -\frac{t}{3}[F'''(t) - F'''(-t)],$$

and therefore

$$H'''(\xi_3) = -\frac{\xi_3}{3}[F''''(\xi_3) - F''''(-\xi_3)] - 60\xi_3^2 G(1).$$

Applying the Mean Value Theorem to the function F''' this shows that there exists $\xi_4 \in (-\xi_3, \xi_3)$ such that

$$\begin{aligned}
H'''(\xi_3) &= -\frac{\xi_3}{3}[2\xi_3 F^{IV}(\xi_4)] - 60\xi_3^2 G(1), \\
&= -\frac{2\xi_3^2}{3}[F^{IV}(\xi_4) + 90\xi_3^2 G(1)].
\end{aligned}$$

Since $H'''(\xi_3) = 0$ and $\xi_3 \neq 0$, this means that

$$G(1) = -\frac{1}{90}F^{IV}(\xi_4) = -\frac{(b-a)^4}{1440}f^{iv}(\xi),$$

and the required result follows.

Example : Two-Point Gauss-Legendre Rule on a General Interval

Evaluate

$$I = \int_0^2 e^{-x^2} dx.$$

Step 1. Transform interval: Let

$$x = \frac{b+a}{2} + t \frac{b-a}{2} = 1+t, \quad dx = dt,$$

so that $t \in [-1, 1]$. Then

$$I = \int_{-1}^1 e^{-(1+t)^2} dt.$$

Step 2. Apply 2-point formula:

$$I \approx f(-1/\sqrt{3}) + f(1/\sqrt{3}), \quad f(t) = e^{-(1+t)^2}.$$

Compute

$$f(-1/\sqrt{3}) = e^{-(1-1/\sqrt{3})^2}, \quad f(1/\sqrt{3}) = e^{-(1+1/\sqrt{3})^2}.$$

Hence,

$$I \approx e^{-(1-1/\sqrt{3})^2} + e^{-(1+1/\sqrt{3})^2}.$$

Numerically,

$$I \approx 0.6386 + 0.1041 = 0.7427.$$

Exact (by table):

$$\int_0^2 e^{-x^2} dx \approx 0.8821.$$

Error ≈ 0.14 .

Example : Three-Point Gauss–Legendre Quadrature

Approximate

$$I = \int_{-1}^1 e^x dx$$

using the 3-point Gauss–Legendre rule.

Step 1. Nodes and weights:

$$x_1 = -\sqrt{\frac{3}{5}}, \quad w_1 = \frac{5}{9},$$

$$x_2 = 0, \quad w_2 = \frac{8}{9},$$

$$x_3 = \sqrt{\frac{3}{5}}, \quad w_3 = \frac{5}{9}.$$

Step 2. Function values:

$$f(x) = e^x, \quad f(x_1) = e^{-\sqrt{3/5}}, \quad f(x_2) = 1, \quad f(x_3) = e^{\sqrt{3/5}}.$$

Step 3. Apply the rule:

$$I \approx \frac{5}{9}e^{-\sqrt{3/5}} + \frac{8}{9}(1) + \frac{5}{9}e^{\sqrt{3/5}}.$$

Numerically,

$$\sqrt{3/5} = 0.7746, \quad e^{0.7746} = 2.169, \quad e^{-0.7746} = 0.461.$$

Hence,

$$I \approx \frac{5}{9}(0.461 + 2.169) + \frac{8}{9} = \frac{5}{9}(2.63) + \frac{8}{9} = 2.347.$$

Step 4. Exact value:

$$\int_{-1}^1 e^x dx = e - e^{-1} = 2.3504.$$

So,

$I \approx 2.347 \quad (\text{error} \approx 0.0034).$
--