Unit 6 Numerical Integrations

Numerical Analysis

EE/NTHU

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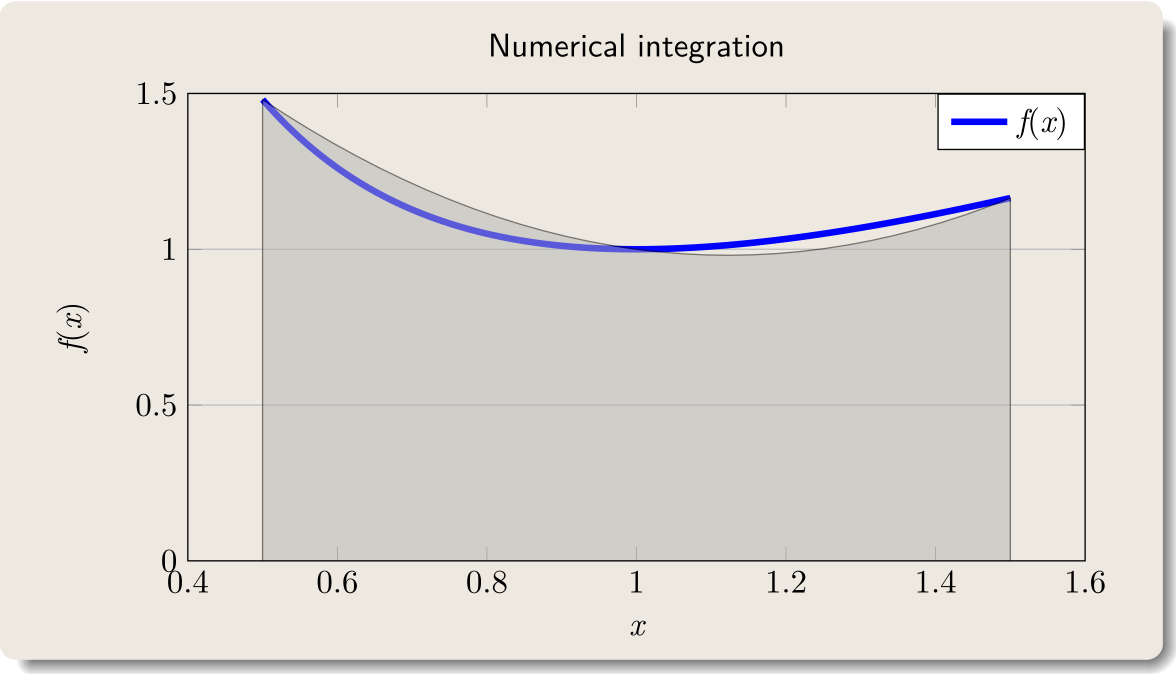
Numerical Integrations



- To find

$$\int_{0.5}^{1.5} (\log^2(x) + 1)\,dx$$

- Given function $f(x)$, $x \in [a, b]$, and $f(x)$ can be evaluate accurately, but costly.
- Closed form solution of the integral is not known.

Numerical Integrations, II

- Integration of a function $f(x)$ over an interval $[a, b]$ tends to have fewer explicit formulas than differentiation, thus there are more studies done on numerical integration.
- Function $f(x)$ needs to be integrable and the definite integral over the interval $[a, b]$ is sought for

$$I(f) = \int_a^b f(x)\, dx \tag{6.1.1}$$

- Finding the explicit formula to approximate of the integral $I(f)$ is called a quadrature formula or numerical integration formula.
- An example is to replace f by an approximation f_n, $n >= 0$, and compute $I(f_n)$ instead of $I(f)$. Denote $I_n(f) = I(f_n)$, then

$$I_n(f) = \int_a^b f_n(x)\, dx. \tag{6.1.2}$$

- If f is a continuous function over the range $[a, b]$, then the quadrature error $E_n(f) = I(f) - I_n(f)$ satisfies

$$|E_n(f)| \le \int_a^b |f(x) - f_n(x)|\, dx \le (b-a)\|f - f_n\|_\infty. \tag{6.1.3}$$

  If for some n, $\|f - f_n\|_\infty < \epsilon$, then $|E_n(f)| \le \epsilon(b-a)$.
- The quadrature error can be managed by choosing the right approximation of f_n.

Numerical Integrations, III

- One approximation of Eq. (6.1.2) is as following

$$I_n(f) = \sum_{i=0}^n \alpha_i f(x_i). \tag{6.1.4}$$

- This is a weighted sum of f at each node x_i.
- $\alpha_i \in \mathbb{R}$ is the coefficient or weight.
- Note that Eq. (6.1.4) is a linear combination of f_i.
- The accuracy of the integration is heavily dependent on n.
- Interpolatory quadrature formulas are one example of the quadrature formulas, where f is replaced by interpolating polynomials.
- Define the degree of exactness of a quadrature formula as the maximum integer, $r \ge 0$ such that

$$I_n(f) = I(f), \quad \text{for all } f \in \mathbb{P}_r. \tag{6.1.5}$$

  $\mathbb{P}_r$ is the set of polynomial of degree less than or equal to r.
- Lagrange quadrature is

$$I_n(f) = \sum_{i=0}^n f(x_i) \int_a^b l_i(x)\, dx, \tag{6.1.6}$$

  where l_i is the characteristic Lagrange polynomial of degree n associated with node x_i, and Lagrange quadrature has the degree of exactness of n.

Rectangle Formula

- The rectangle integration formula is

$$I_0(f) = (b-a)f(\frac{a+b}{2}) \tag{6.1.7}$$

- Rectangle formula replaces f over $[a,b]$ with the constant function equals to the value of f at the midpoint of $[a,b]$.
- If $f \in C^2([a,b])$ then expand f around $x_0 = (a+b)/2$

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + f''(\xi)(x-x_0)^2/2,$$

And, let $H = (b-a)/2$, we have

$$\int_a^b f(x)\,dx = (b-a)f(x_0) + f'(x_0)\frac{y^2}{2}\Big|_{y=-H}^{H} + f''(\xi)\frac{y^3}{6}\Big|_{y=-H}^{H}$$
$$= (b-a)f(x_0) + f''(\xi)\frac{H^3}{3}.$$

Thus, the quadrature error is

$$E_0(f) = \frac{H^3}{3}f''(\xi), \quad H = \frac{b-a}{2} \tag{6.1.8}$$

where $\xi \in [a,b]$.
- The rectangle formula has the degree of exactness equal to 1.

Composite Rectangle Formula

- The quadrature error of rectangle formula is proportional to H^3.
- If $H = (b-a)/2$ is large then the quadrature error is large.
- In practice, we can reduce the quadrature error by adopting the composite quadrature formula: divide $[a,b]$ into m subintervals each with width of $h = (b-a)/m, m \geq 1$ and the quadrature nodes are $x_k = a + (2k+1)h/2$, $k = 0, \cdots, m-1$. Then the composite rectangle formula is

$$I_{0,m}(f) = h\sum_{k=0}^{m-1} f(x_k). \tag{6.1.9}$$

- The quadrature error is then

$$E_{0,m}(f) = I(f) - I_{0,m}(f) = \sum_{k=0}^{m-1}(I(f) - I_{0,m}(f))$$
$$= m \cdot \frac{1}{3} \cdot \left(\frac{h}{2}\right)^3 f''(\xi) = \frac{mh^3}{24}f''(\xi)$$
$$= \frac{(b-a)h^3}{24h}f''(\xi) = \frac{(b-a)h^2}{24}f''(\xi) \tag{6.1.10}$$

- By choosing appropriate m the quadrature error can be controlled.

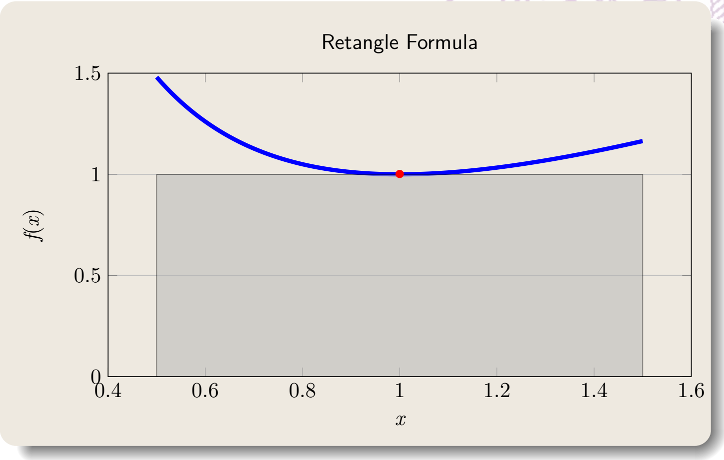
Composite Rectangle Formula, II

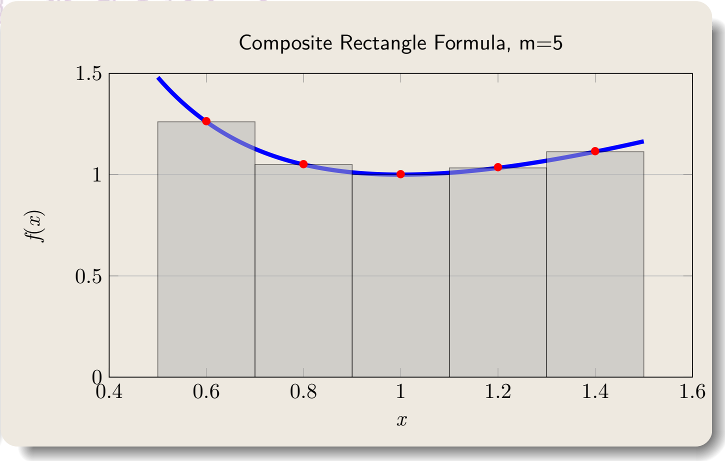
- In deriving the composite rectangle quadrature error, we have used the following theorem.

Theorem 6.1.1. Discrete mean-value theorem

Let $f \in C^0([a,b])$ and let x_j be $s+1$ points in $[a,b]$ and δ_j be $s+1$ constants, all having the same sign. Then there is an $\eta \in [a,b]$ such that

$$\sum_{j=0}^{s} \delta_j f(x_j) = f(\eta) \sum_{j=0}^{s} \delta_j. \tag{6.1.11}$$



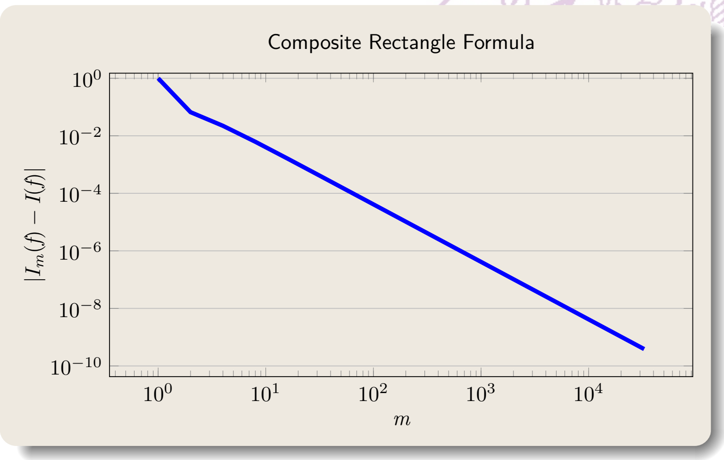


Composite Rectangle Formula, Algorithm

Algorithm 6.1.2. Composite Rectangle Formula

Given the function f in the interval $[a,b]$ and an integer m

let $h = \dfrac{b-a}{m}$; $x = a + \dfrac{h}{2}$; $I = 0$;
while $(x \leq b)\{$
  $I = I + f(x) * h;$
  $x = x + h;$
$\}$
I is the integral.



- As m increases, the rectangle quadrature produces more accurate result.
- It converges to $I(f)$ as $m \to \infty$.
- The convergence rate is constant, $O(m^{-2})$.

The Trapezoidal Formula

- The trapezoidal quadrature approximates function f by a first order polynomial of $f_1(x) = a_0 + a_1 x$.
  With $f_1(a) = f(a)$ and $f_1(b) = f(b)$. Thus,

$$f_1(x) = \frac{x-a}{b-a} f(b) + \frac{x-b}{a-b} f(a) = \frac{f(b)-f(a)}{b-a} x + \frac{bf(a)-af(b)}{b-a} \tag{6.1.12}$$

$$I_1(f) = \int_a^b f_1(x)\,dx = (b-a)\frac{f(a)+f(b)}{2}. \tag{6.1.13}$$

- By Theorem (5.1.16), the quadrature error is then

$$E_1(f) = \int_a^b \frac{1}{2}(x-a)(x-b) f''(\xi)\,dx = -\frac{H^3}{12} f''(\xi), \quad H = b-a, \tag{6.1.14}$$

  where $\xi \in [a, b]$.
- The trapezoidal quadrature method has degree of exactness equal to 1.
  - The same as the rectangle quadrature method.

The Composite Trapezoidal Formula

- The composite trapezoidal formula divides the interval $[a, b]$ into m equal subintervals and apply the trapezoidal formula in each region. Let the points be $a = x_0, x_1, x_2, \cdots, x_{m-1}, x_m = b$,

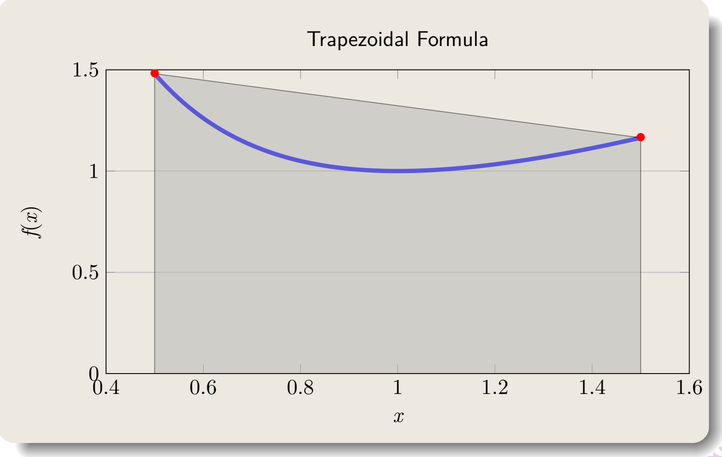
$$\begin{aligned} I_{1,m}(f) &= \sum_{k=0}^{m-1} (x_{k+1} - x_k) \frac{f(x_k) + f(x_{k+1})}{2} = \frac{h}{2} \sum_{k=0}^{m-1} (f(x_k) + f(x_{k+1})) \\ &= h \left(\frac{f(x_0)}{2} + f(x_1) + f(x_2) + \cdots + f(x_{m-2}) + \frac{f(x_m)}{2} \right), \end{aligned} \tag{6.1.15}$$

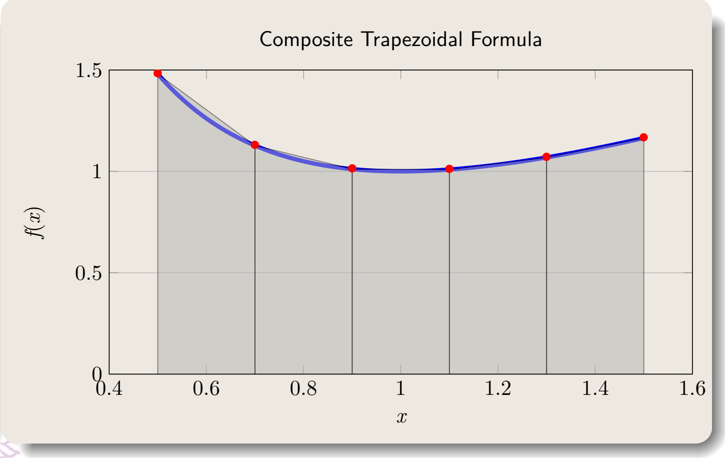
  where $h = \dfrac{b-a}{m}$.
- Note that the series summation has the values at both end points ($f(a)$ and $f(b)$) with the weight of $1/2$, while all other points have the weight of 1.
- And the quadrature error is

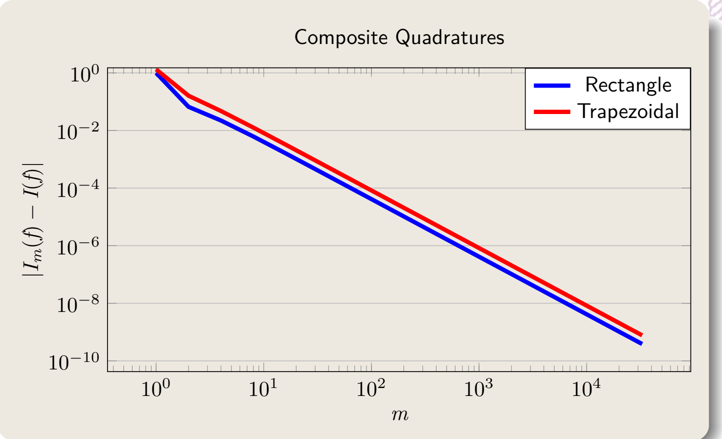
$$\begin{aligned} E_{1,m}(f) &= I(f) - I_{1,m}(f) = \sum_{k=0}^{m-1} (I(f) - I_{1,k}(f)) \\ &= -\frac{b-a}{12} h^2 f''(\xi), \end{aligned} \tag{6.1.16}$$

  assuming $f \in C^2([a, b])$ and $\xi \in (a, b)$.

The Composite Trapezoidal Formula, II







- Composite trapezoidal method seems to track the function curve well.
- But the quadrature errors are compatible to rectangle method.
- Both have the degree of exactness equal to 1.

The Cavalieri-Simpson Formula

- The Cavalieri-Simpson formula is obtained when f is replaced by the interpolating polynomial of degree 2 at the nodes, $x_0 = a$, $x_1 = (a+b)/2$, and $x_2 = b$. It can be derived that the resulting formula is

$$I_2(f) = \frac{b-a}{6}\left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right]. \tag{6.1.17}$$

and the quadrature error is

$$E_2(f) = -\frac{H^5}{90} f^{(4)}(\xi), \quad H = \frac{b-a}{2}. \tag{6.1.18}$$

- Thus, the Cavalieri-Simpson formula has the degree of exactness equal to 3.
- The composite Cavalieri-Simpson formula has the following form, assuming the quadrature nodes are $x_k = a + kh/2$, $k = 0, \cdots, 2m$ and $h = (b-a)/m$.

$$I_{2,m}(f) = \frac{h}{6}\left[f(x_0) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{k=0}^{m-1} f(x_{2k+1}) + f(x_{2m})\right]. \tag{6.1.19}$$

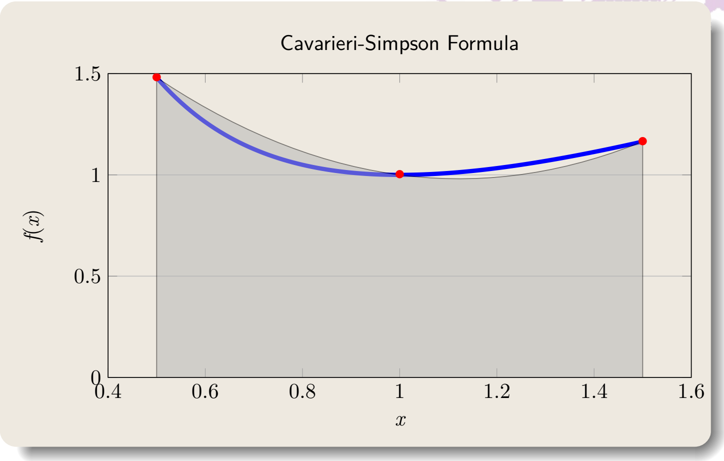
with the quadrature error

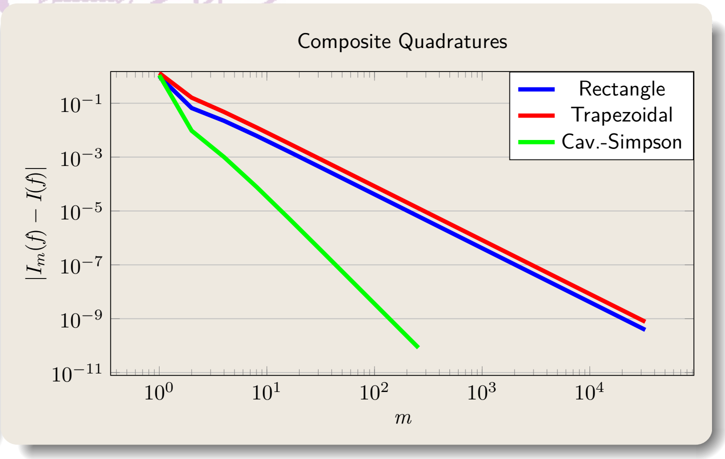
$$E_{2,m}(f) = -\frac{b-a}{180}(h/2)^4 f^{(4)}(\xi), \tag{6.1.20}$$

if $f \in C^4([a,b])$, and $\xi \in (a,b)$. The degree of exactness is 3.

The Cavalieri-Simpson Formula, II

- Composite quadrature formulas are effective in performing numerical integrations.
- Formulas with higher degree of exactness can produce more accurate integration with fewer nodes.
- Integrations by composite quadrature are easy to implement and very efficient in CPU time and memory space.





Newton-Cotes Formulas

- Newton-Cotes formulas are based on Lagrange interpolation with equally spaced nodes in $[a, b]$.
- For an $n > 0$, the nodes are placed at $x_k = x_0 + kh$, $k = 0, \cdots, n$ with $h = (b-a)/n$. Note that $x_0 = a$ and $x_n = b$.
- Rectangle, trapezoidal and Simpson formulas are special instances of the Newton-Cotes formulas, with $n = 0$, $n = 1$ and $n = 2$.
    - In the case $n = 0$, $h = b - a$ and $x_0 = a$, $x_1 = b$, we have retangle formula.
- With Lagrange interpolation,

$$f = \sum_{i=0}^{n} \prod_{k=0,k\neq i}^{n} \frac{x - x_k}{x_i - x_k} f(x_i) = \sum_{i=0}^{n} \prod_{k=0,k\neq i}^{n} \frac{t-k}{i-k} f(x_i). \tag{6.1.21}$$

The second part of the above equation is obtained by a change of variable $x = x_0 + th$. Thus,

$$I_n(f) = \int_{x=a}^{b} \sum_{i=0}^{n} \prod_{k=0,k\neq i}^{n} \frac{x - x_k}{x_i - x_k} f(x_i)\, dx = \sum_{i=0}^{n} f(x_i) \int_{t=0}^{n} \prod_{k=0,k\neq i}^{n} \frac{t-k}{i-k} h dt = h \sum_{i=0}^{n} w_i f(x_i). \tag{6.1.22}$$

with

$$w_i = \int_{t=0}^{n} \prod_{k=0,k\neq i}^{n} \frac{t-k}{i-k} dt. \tag{6.1.23}$$

Newton-Cotes Formulas, II

- In the case $n = 0$, $f(x) = f(\frac{a+b}{2})$ is a constant, and

$$w_0 = \int_{t=0}^{1} 1\,dt = 1.$$

Thus,

$$I_0(f) = hf(\frac{a+b}{2}). \tag{6.1.24}$$

- When $n = 1$,

$$\begin{aligned} w_0 &= \int_{t=0}^{1} \frac{t-1}{0-1}\,dt = -\left[\frac{t^2}{2} - t\right]_{t=0}^{1} = \frac{1}{2} \\ w_1 &= \int_{t=0}^{1} \frac{t-0}{1-0}\,dt = \left[\frac{t^2}{2}\right]_{t=0}^{1} = \frac{1}{2} \end{aligned}$$

Thus,

$$I_1(f) = \frac{h}{2}(f(x_0) + f(x_1)) = h\frac{f(a) + f(b)}{2}. \tag{6.1.25}$$

Newton-Cotes Formulas, III

- When $n = 2$,

$$\begin{aligned} w_0 &= \int_{t=0}^{2} \frac{(t-1)(t-2)}{(0-1)(0-2)}\,dt = \frac{1}{2}\left[\frac{t^3}{3} - \frac{3t^2}{2} + 2t\right]_{t=0}^{2} = \frac{1}{3} \\ w_1 &= \int_{t=0}^{2} \frac{(t-2)(t-0)}{(1-2)(1-0)}\,dt = -\left[\frac{t^3}{3} - \frac{2t^2}{2}\right]_{t=0}^{2} = \frac{4}{3} \\ w_2 &= \int_{t=0}^{2} \frac{(t-0)(t-1)}{(2-0)(2-1)}\,dt = \frac{1}{2}\left[\frac{t^3}{3} - \frac{t^2}{2}\right]_{t=0}^{2} = \frac{1}{3} \end{aligned}$$

Thus,

$$\begin{aligned} I_2(f) &= h\left(\frac{1}{3}f(x_0) + \frac{4}{3}f(x_1) + \frac{1}{3}f(x_2)\right) \\ &= \frac{b-a}{6}\Big(f(x_0) + 4f(x_1) + f(x_2)\Big). \end{aligned} \tag{6.1.26}$$

Newton-Cotes Formulas, IV

- When $n = 3$,

$$w_0 = \int_{t=0}^{3} \frac{(t-1)(t-2)(t-3)}{(0-1)(0-2)(0-3)}\,dt = \frac{-1}{6}\left[\frac{t^4}{4} - \frac{6t^3}{3} + \frac{11t^2}{2} - 6t\right]_{t=0}^{3} = \frac{3}{8}$$

$$w_1 = \int_{t=0}^{3} \frac{(t-2)(t-3)(t-0)}{(1-2)(1-3)(1-0)}\,dt = \frac{1}{2}\left[\frac{t^4}{4} - \frac{5t^3}{3} + \frac{6t^2}{2}\right]_{t=0}^{3} = \frac{9}{8}$$

$$w_2 = \int_{t=0}^{3} \frac{(t-3)(t-0)(t-1)}{(2-3)(2-0)(2-1)}\,dt = \frac{-1}{2}\left[\frac{t^4}{4} - \frac{4t^3}{3} + \frac{3t^2}{2}\right]_{t=0}^{3} = \frac{9}{8}$$

$$w_3 = \int_{t=0}^{3} \frac{(t-0)(t-1)(t-2)}{(3-0)(3-1)(3-2)}\,dt = \frac{1}{6}\left[\frac{t^4}{4} - \frac{3t^3}{3} + \frac{2t^2}{2}\right]_{t=0}^{3} = \frac{3}{8}$$

Thus,

$$I_3(f) = h\left(\frac{3}{8}f(x_0) + \frac{9}{8}f(x_1) + \frac{9}{8}f(x_2) + \frac{3}{8}f(x_3)\right)$$
$$= \frac{b-a}{24}\Big(3f(x_0) + 9f(x_1) + 9f(x_2) + 3f(x_3)\Big). \qquad (6.1.27)$$

Newton-Cotes Formulas, V

- The n-th order Newton-Cotes integration formula is

$$I_n(f) = h\sum_{i=0}^{n} w_i f(x_i), \qquad (6.1.28)$$

where $h = \dfrac{b-a}{n}$, $x_i = a + ih$, and the coefficients, w_i are shown below.

n	w_0	w_1	w_2	w_3	w_4	w_5	w_6
1	1/2	1/2					
2	1/3	4/3	1/3				
3	3/8	9/8	9/8	3/8			
4	14/45	64/45	24/45	64/45	14/45		
5	95/288	375/288	250/288	250/288	375/288	95/288	
6	41/140	216/140	27/140	272/140	27/140	216/140	41/140

Newton-Cotes Formulas, VI

Theorem 6.1.3.

Given the Newton-Cotes integration formula as shown in Eq. (6.1.28), then

$$w_i = w_{n-i}, \tag{6.1.29}$$

$$\sum_{i=0}^{n} w_i = n. \tag{6.1.30}$$

Eq. (6.1.29) is due to the symmetry of the quadrature, and Eq. (6.1.30) can be proved by applying to a constant $f = 1$. In this case

$$I_n(f) = b - a = \frac{b-a}{n} \sum_{i=0}^{n} w_i.$$

Newton-Cotes Formulas, VII

Theorem 6.1.4.

Given the Newton-Cotes integration formula as shown in Eq. (6.1.28), then the quadrature error is

$$E_n(f) = \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t \prod_{i=0}^{n} (t-i)\, dt, \quad \text{if } n \text{ is even}, \tag{6.1.31}$$

$$= \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n \prod_{i=0}^{n} (t-i)\, dt, \quad \text{if } n \text{ is odd}. \tag{6.1.32}$$

- Thus, the degree of exactness of Newton-Cotes integration formula is $n+1$ when n is even; and it is n when n is odd.
- And

$$E_n(f) \approx O(h^{n+3}) \quad \text{when } n \text{ is even}, \tag{6.1.33}$$

$$\approx O(h^{n+2}) \quad \text{when } n \text{ is odd}. \tag{6.1.34}$$

- Also note that

$$\int_0^n t \prod_{i=0}^{n} (t-i)\, dt < 0, \quad \text{if } n \text{ is even}, \tag{6.1.35}$$

$$\int_0^n \prod_{i=0}^{n} (t-i)\, dt < 0, \quad \text{if } n \text{ is odd}. \tag{6.1.36}$$

Composite Newton-Cotes Formulas

- The composite Newton-Cotes Formulas divide the integration interval $[a, b]$ into m subintervals, $[a_i, b_i]$, $i = 0, \cdots, m-1$, with $a_0 = a$; $a_{i+1} = b_i = a + (b-a)/m$, $i = 0, \cdots, m-2$; $b_{m-1} = b$.
- Then carry out Newton-Cotes integration on each subinterval $[a_i, b_i]$.
- The overall integration is the sum of the integrations of the subintervals.

$$\begin{aligned} I(f) &= \int_a^b f(x)\,dx = \sum_{i=0}^{m-1} \int_{a_i}^{b_i} f(x)\,dx \\ &= h \sum_{i=0}^{m-1} \sum_{k=0}^{n} w_k f(a_i + kh) \end{aligned} \tag{6.1.37}$$

where an n-th order quadrature is assumed and $h = (b-a)/mn$.

Composite Newton-Cotes Formulas, II

- The quadrature error of the composite Newton-Cotes Formula can be derived as

Theorem 6.1.5.

Given an $f \in C^{n+2}([a, b])$ the n-th order and m subintervals composite Newton-Cotes formula, then

$$\begin{aligned} E_{n,m}(f) &= \frac{b-a}{(n+2)!} \frac{H^{n+2}}{n^{n+3}} f^{(n+2)}(\xi) \int_0^n t \prod_{i=0}^{n} (t-i)\,dt, \quad \text{if } n \text{ is even}, && (6.1.38) \\ &= \frac{b-a}{(n+1)!} \frac{H^{n+1}}{n^{n+2}} f^{(n+1)}(\xi) \int_0^n \prod_{i=0}^{n} (t-i)\,dt, \quad \text{if } n \text{ is odd} && (6.1.39) \end{aligned}$$

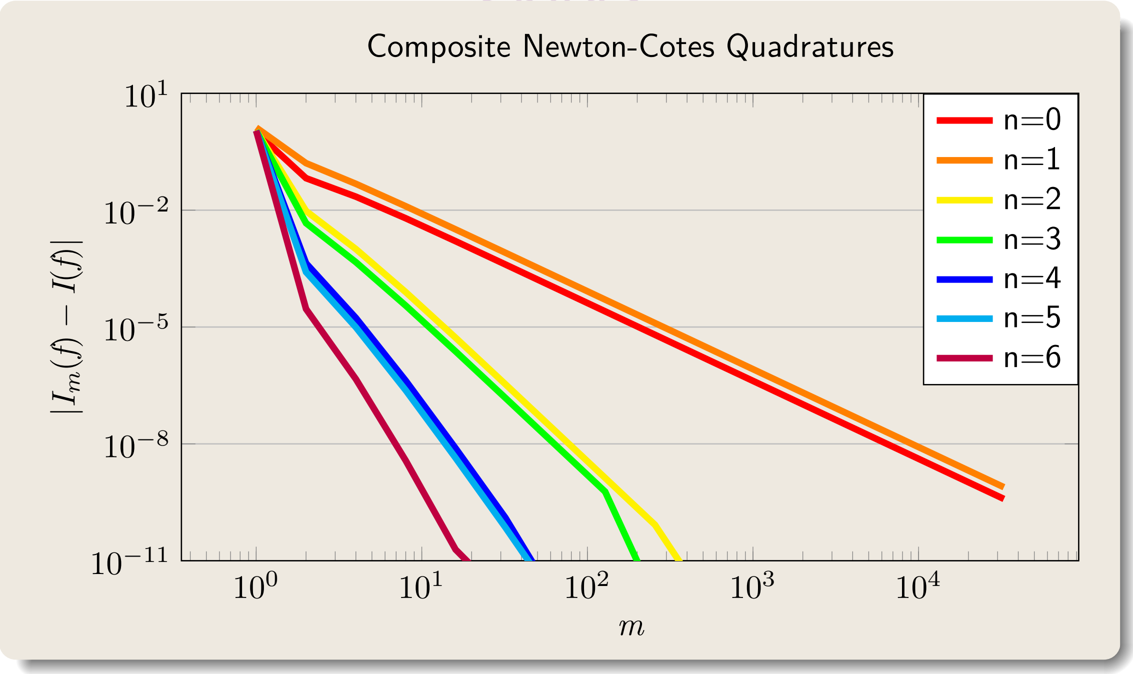
where $H = (b-a)/m$ and $\xi \in (a, b)$.

- Thus the composite Newton-Cotes formulas have very significant improvement on quadrature errors.

Composite Newton-Cotes Formulas, III

- The quadrature errors of composite Newton-Cotes quadratures are shown below

$$I = \int_{0.5}^{1.5} (\log^2(x) + 1)\, dx$$



- Note that $n = 0$ and $n = 1$ quadratures have similar errors
  - So do $n = 2$ and n=3; and $n = 4$ and $n = 5$.
- Higher order quadratures need smaller number of m to get accurate integration

Summary

- Numerical integration and quadrature formula
- Rectangle formula
  - Composite formula
- Trapezoidal formula
  - Composite formula
- Cavalieri-Simpson formula
- Newton-Cotes formulas
  - Composite formulas