

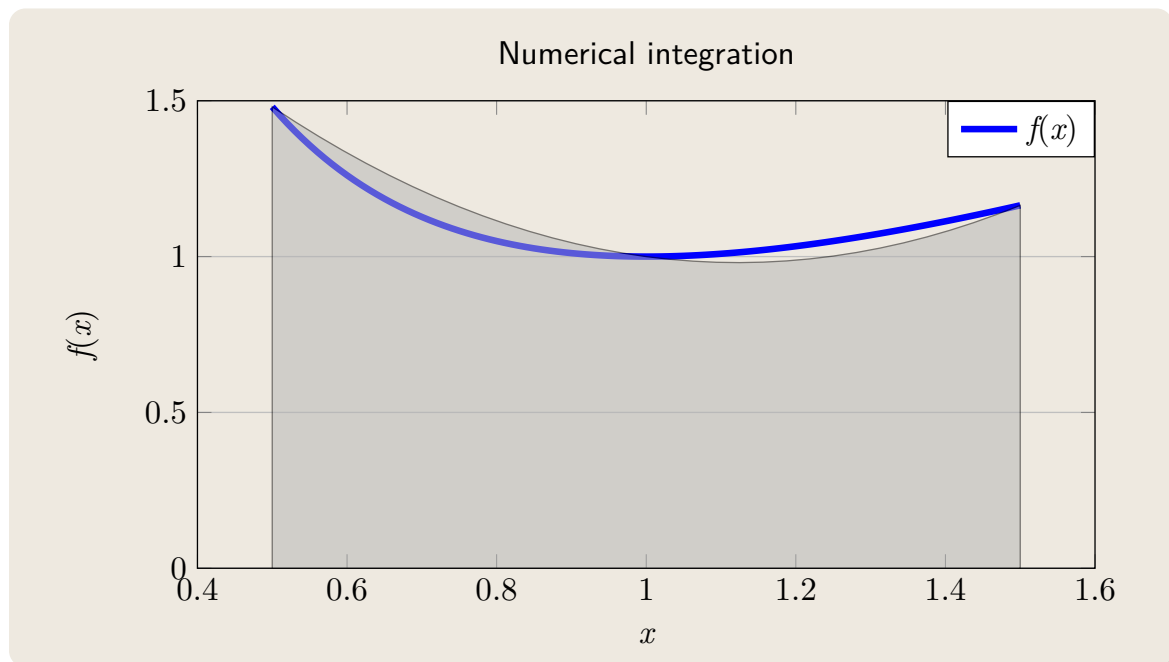
Unit 6 Numerical Integrations

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

$$I(f) = \int_a^b f(x) dx \quad (6.1.1)$$

- 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 , $n \geq 0$, and compute $I(f_n)$ instead of $I(f)$. Denote $I_n(f) = I(f_n)$, then

$$I_n(f) = \int_a^b f_n(x) dx. \quad (6.1.2)$$

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

$$|E_n(f)| \leq \int_a^b |f(x) - f_n(x)| dx \leq (b - a) \|f - f_n\|_\infty. \quad (6.1.3)$$

If for some n , $\|f - f_n\|_\infty < \epsilon$, then $|E_n(f)| \leq \epsilon(b - a)$.

- 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

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

- 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, $r \geq 0$ such that

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

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

- **Lagrange quadrature** is

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

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

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

- 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

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

Thus, the quadrature error is

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

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 $x_k = a + (2k + 1)h/2$, $k = 0, \dots, m - 1$. Then the composite rectangle formula is

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

- The quadrature error is then

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

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

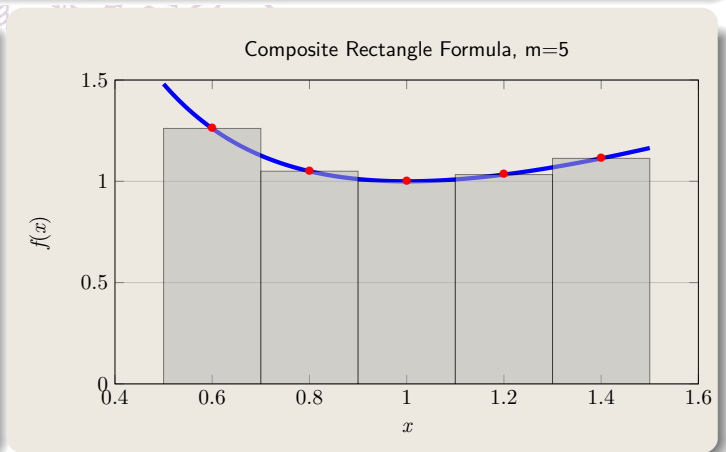
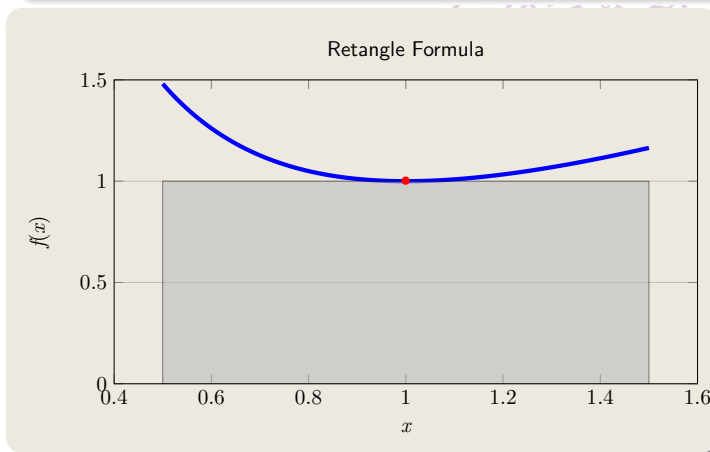
Composite Rectangle Formula, II

- 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

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



Composite Rectangle Formula, Algorithm

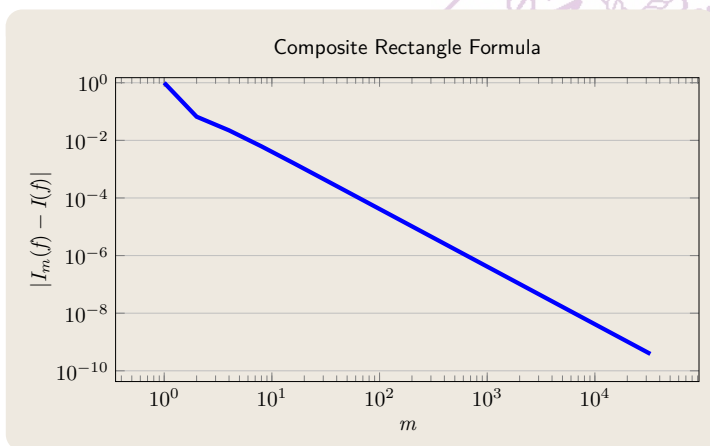
Algorithm 6.1.2. Composite Rectangle Formula

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

let $h = \frac{b-a}{m}$; $x = a + \frac{h}{2}$; $I = 0$;

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 $m \rightarrow \infty$.
- The convergence rate is constant, $O(m^{-2})$.

The Trapezoidal Formula

- The trapezoidal quadrature approximates function f by a first order polynomial of $f_1(x) = a_0 + a_1x$.

With $f_1(a) = f(a)$ and $f_1(b) = f(b)$. Thus,

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

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

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

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

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 $a = x_0, x_1, x_2, \dots, x_{m-1}, x_m = b$,

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

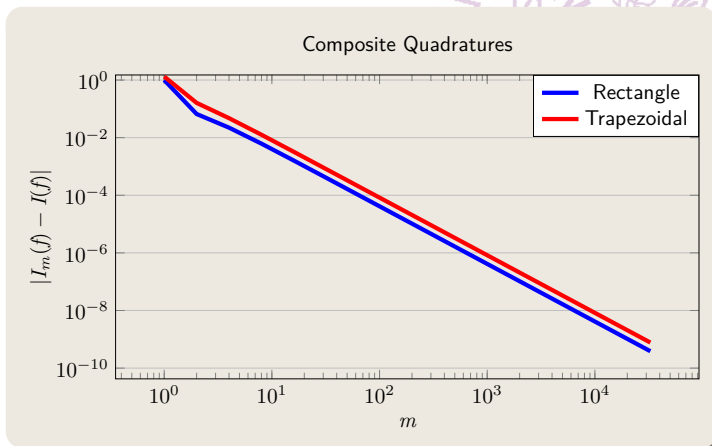
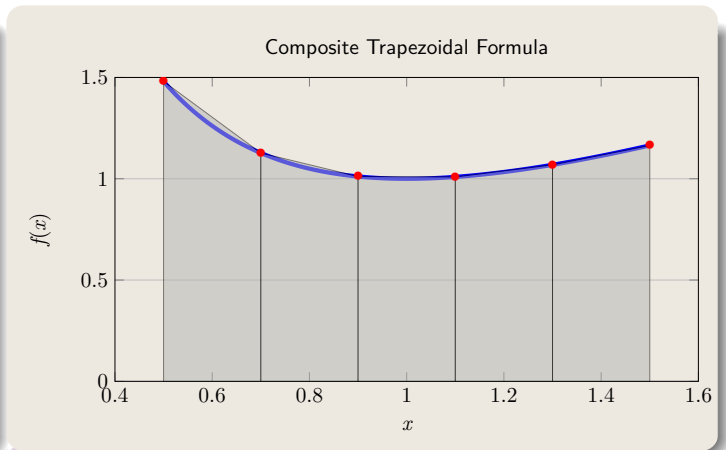
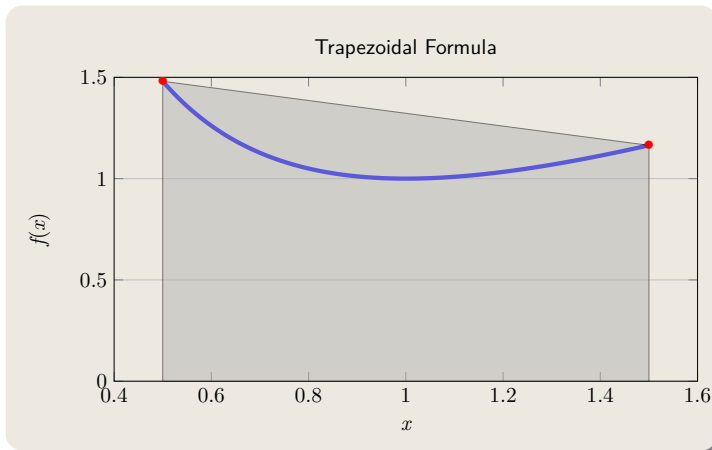
where $h = \frac{b-a}{m}$.

- 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

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

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

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

and the quadrature error is

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

- 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 $x_k = a + kh/2$, $k = 0, \dots, 2m$ and $h = (b-a)/m$.

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

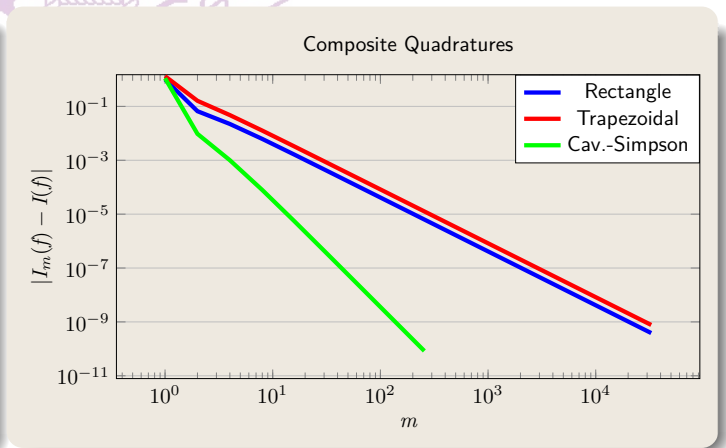
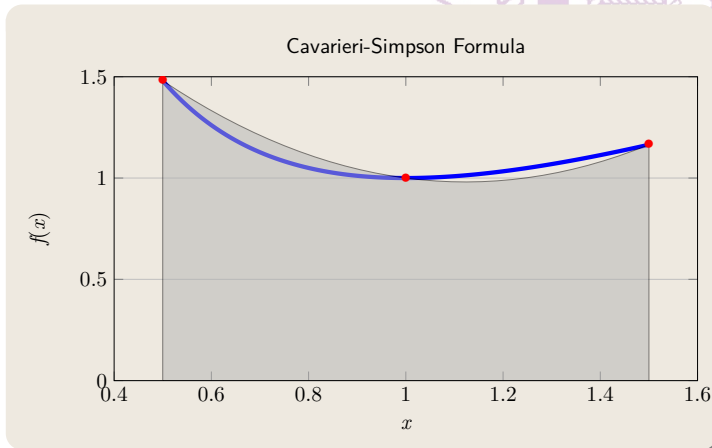
with the quadrature error

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

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 $x_k = x_0 + kh$, $k = 0, \dots, n$ 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 rectangle formula.
- With Lagrange interpolation,

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

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

$$I_n(f) = \int_{x=a}^b \sum_{i=0}^n \prod_{k=0, k \neq i}^n \frac{x - x_k}{x_i - x_k} f(x_i) dx = \sum_{i=0}^n f(x_i) \int_{t=0}^1 \prod_{k=0, k \neq i}^n \frac{t - k}{i - k} h dt = h \sum_{i=0}^n w_i f(x_i). \quad (6.1.22)$$

with

$$w_i = \int_{t=0}^1 \prod_{k=0, k \neq i}^n \frac{t - k}{i - k} dt. \quad (6.1.23)$$

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,

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

- When $n = 1$,

$$w_0 = \int_{t=0}^1 \frac{t-1}{0-1} dt = -\left[\frac{t^2}{2} - t\right]_{t=0}^1 = \frac{1}{2}$$

$$w_1 = \int_{t=0}^1 \frac{t-0}{1-0} dt = \left[\frac{t^2}{2}\right]_{t=0}^1 = \frac{1}{2}$$

Thus,

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

Newton-Cotes Formulas, III

- When $n = 2$,

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

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

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

Thus,

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

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,

$$\begin{aligned} I_3(f) &= h \left(\frac{3}{8}f(x_0) + \frac{9}{8}f(x_1) + \frac{9}{8}f(x_2) + \frac{3}{8}f(x_3) \right) \\ &= \frac{b-a}{24} (3f(x_0) + 9f(x_1) + 9f(x_2) + 3f(x_3)). \end{aligned} \quad (6.1.27)$$

Newton-Cotes Formulas, V

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

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

where $h = \frac{b-a}{n}$, $x_i = a + ih$, 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

Theorem 6.1.3.

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

$$w_i = w_{n-i}, \quad (6.1.29)$$

$$\sum_{i=0}^n w_i = n. \quad (6.1.30)$$

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

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

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

- 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

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

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

- Also note that

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

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

Composite Newton-Cotes Formulas

- The composite Newton-Cotes Formulas divide the integration interval $[a, b]$ into m subintervals, $[a_i, b_i]$, $i = 0, \dots, m-1$, with $a_0 = a$; $a_{i+1} = b_i = a + (b-a)/m$, $i = 0, \dots, m-2$; $b_{m-1} = b$.
- 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.

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

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

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

$$= \frac{b-a}{(n+1)!} \frac{H^{n+1}}{n^{n+2}} f^{(n+1)}(\xi) \int_0^n \prod_{i=0}^n (t-i) dt, \quad \text{if } n \text{ is odd} \quad (6.1.39)$$

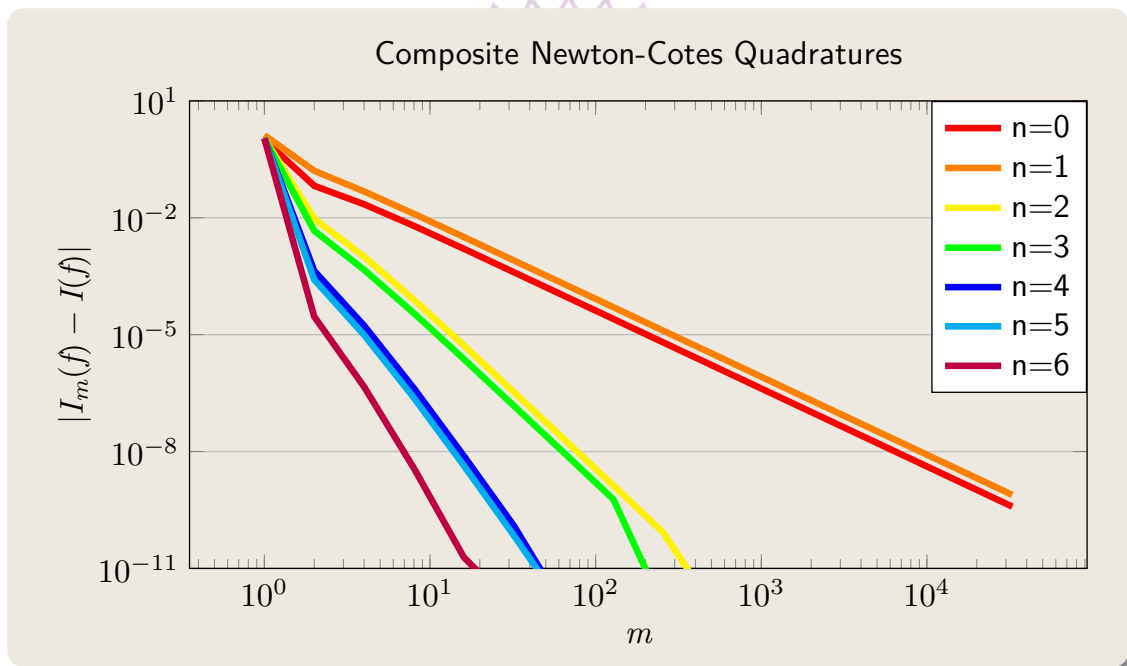
where $H = (b-a)/m$ and $\xi \in (a, b)$.

- 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

