MA633L-Numerical Analysis

Lecture 34 : Numerical Integration - Newton-Cotes

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Open Newton-Cotes Formula

Open Newton-Cotes Formula

The general $(n+1)$-points closed Newton-Cotes formula using nodes $x_i = x_0 + ih$, for $i = 0, 1, 2, \cdots n$ where $x_0 = a, x_n = b, h = (b-a)/n$ is

$$\int_a^b f(x)dx \cong \sum_{i=0}^{n} \left[\int_{x_0}^{x_n} \ell_i(x)dx \right] f(x_i) \cong \sum_{i=0}^{n} A_i f(x_i) \tag{1}$$

- The open Newton-Cotes formula do not include the endpoints $[a, b]$ as nodes.
- They use only interior nodes.
- The numerical approximation for open Newton-Cotes formula is same as (1), but, $x_i \in (a, b)$.
- In order to use the same formula (1), we redefine the points by spacing as follows: $x_{-1} = a, x_0 = a + h, x_{n+1} = b, x_i = x_0 + ih$ for each $i = 0, 1, 2, \cdots, n$ where $h = (b-a)/(n+2)$.

Midpoint Rule

For the midpoint formula, we take $n = 0$, then $x_{-1} = a, x_0 = (a+b)/2, x_1 = b$. Therefore, the interior point is only $x_0 = (a+b)/2$. When we work on the interval $[0, 1]$, change of intervals and method of undetermined coefficients, we obtain that

$$\int_0^1 f(x)dx \cong A_0 f\left(\frac{1}{2}\right) \tag{2}$$

By the method of undetermined coefficients, we evaluate them on 1.

$$f(x) = 1 : \int_0^1 dx = A_0 \implies A_0 = 1$$

Midpoint Rule

The resulting formula is

$$\int_0^1 f(x)dx \approx f\left(\frac{1}{2}\right) \tag{3}$$

By (**??**), we obtain that

$$\begin{aligned}\int_a^b f(x)dx = (b-a)\int_0^1 f(\lambda(u))du &\cong (b-a)A_0 f\left(\lambda\left(\frac{1}{2}\right)\right)\\ &\approx (b-a)f\left(\frac{a+b}{2}\right)\end{aligned}$$

If $h = (b-a)/2$, then

$$\int_a^b f(x)dx \approx 2hf(a+h)$$

Midpoint Rule

Theorem 1 (Error in Midpoint Rule)
If $f \in C^2[a,b]$, then the error in Midpoint rule is given by

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

Proof: By Taylor polynomial about $(a+b)/2$ for each $x \in (a,b)$ is given by

$$f(x) = f\left(\frac{a+b}{2}\right) + f'\left(\frac{a+b}{2}\right)\left(x - \frac{a+b}{2}\right) + \frac{1}{2} f''(\xi)\left(x - \frac{a+b}{2}\right)^2$$

Midpoint Rule

Integrating on both sides we obtain that

$$\int_a^b f(x)dx = f\left(\frac{a+b}{2}\right)(b-a) + \frac{1}{2}f'\left(\frac{a+b}{2}\right)\underbrace{\left[\left(b-\frac{a+b}{2}\right)^2 - \left(a-\frac{a+b}{2}\right)^2\right]}_{0}$$

$$+\frac{1}{6}f''(\xi)\left[\left(b-\frac{a+b}{2}\right)^3 - \left(a-\frac{a+b}{2}\right)^3\right]$$

$$= f\left(\frac{a+b}{2}\right)(b-a) + \frac{1}{3}f''(\xi)\left(\frac{b-a}{2}\right)^3$$

Hence the proof.

Two-Point Newton-Cotes Open Rule

For the Two-point formula, we take $n = 1$, then $x_{-1} = a, x_0 = (a+b)/3, x_0 = 2(a+b)/3, x_2 = b$. Therefore, the interior points are only $x_0 = (a+b)/3$ and $x_1 = 2(a+b)/3$. When we work on the interval $[0, 1]$, change of intervals and method of undetermined coefficients, we obtain that

$$\int_0^1 f(x)dx \cong A_0 f\left(\frac{1}{3}\right) + A_1 f\left(\frac{2}{3}\right) \tag{4}$$

Two-Point Newton-Cotes Open Rule

By the method of undetermined coefficients, we evaluate them on $\{1, x\}$.

$$
\begin{aligned}
f(x) = 1 : \int_0^1 dx = A_0 + A_1 &\implies A_0 + A_1 = 1 \\
f(x) = x : \int_0^1 x dx = A_0 \frac{1}{3} + A_1 \frac{2}{3} &\implies \frac{1}{3} A_0 + \frac{2}{3} A_1 = \frac{1}{2}
\end{aligned}
$$

Solving for A_0, A_1, we obtain that $A_0 = 1/2, A_1 = 1/2$.

Two-Point Newton-Cotes Open Rule

The resulting formula is

$$\int_0^1 f(x)dx \approx \frac{1}{2}f\left(\frac{1}{3}\right) + \frac{1}{2}f\left(\frac{2}{3}\right) \tag{5}$$

By (**??**), we obtain that

$$\begin{aligned}
\int_a^b f(x)dx &= (b-a)\int_0^1 f(\lambda(u))du \\
&\cong (b-a)A_0 f\left(\lambda\left(\frac{1}{3}\right)\right) + (b-a)A_1 f\left(\lambda\left(\frac{2}{3}\right)\right) \\
&\approx \frac{(b-a)}{2}\left[f\left(a+\frac{b-a}{3}\right) + f\left(a+2\frac{b-a}{3}\right)\right]
\end{aligned}$$

Two-Point Newton-Cotes Open Rule

If $h = (b-a)/3$, then

$$\int_a^b f(x)dx \approx \frac{3h}{2}[f(a+h) + f(a+2h)]$$

Two-Point Newton-Cotes Open Rule

Theorem 2 (Error in Two-point Newton-Cotes Open Rule)
If $f \in C^2[a, b]$, then the error in Two-point rule is given by

$$\frac{(b-a)^3}{36} f''(\xi)$$

for some $\xi \in (a, b)$

Midpoint Rule

Example 3

Evaluate

$$\int_0^1 e^{-x^2}\,dx$$

using Midpoint rule.

$$a = 0, b = 1, \frac{a+b}{2} = 0.5, f\left(\frac{a+b}{2}\right) = 0.7788$$

$$\int_0^1 e^{-x^2}\,dx = (1-0)f(0.5) = 0.7788$$

Two-Point Newton-Cotes Open Rule

Example 4

Using Two-Point Newton-Cotes open rule, the following numerical integration can be obtained.

$$
\begin{aligned}
\int_0^2 x^2 dx &= \tfrac{3-0}{2}\left[\tfrac{4}{9} + \tfrac{16}{9}\right] = \tfrac{10}{3}, & E_t &= \frac{2}{3} \\
\int_0^3 \frac{1}{1+x} dx &= \tfrac{3-0}{2}\left[0.5 + \tfrac{1}{3}\right] = 1.25, & E_t &= 0.1363 \\
\int_0^3 \sqrt{1+x^2} dx &= \tfrac{3-0}{2}\left[\sqrt{2} + \sqrt{5}\right] = 5.0673, & E_t &= -0.5853 \\
\int_0^3 e^x dx &= \tfrac{3-0}{2}\left[e + e^2\right] = 15.16, & E_t &= 3.9246
\end{aligned}
$$

Gaussian Quadrature

Using the change of interval $\lambda : [-1, 1] \to [a, b]$ as

$$\lambda(x) = \frac{1}{2}(b-a)x + \frac{1}{2}(a+b)$$

we obtain that

$$\begin{aligned}
\int_a^b f(x)dx &= \frac{b-a}{2} \int_{-1}^{1} f(\lambda(u))du \\
\int_a^b f(x)dx &\approx \frac{b-a}{2} \left[f\left(\lambda\left(\frac{-1}{\sqrt{3}} \right) \right) + f\left(\lambda\left(\frac{1}{\sqrt{3}} \right) \right) \right] \\
\implies \int_a^b f(x)dx &\approx \frac{b-a}{2} \left[f\left(\frac{a-b}{2\sqrt{3}} + \frac{1}{2}(a+b) \right) + f\left(\frac{b-a}{2\sqrt{3}} + \frac{1}{2}(a+b) \right) \right]
\end{aligned}$$

Example

Example 5

Determine the coefficients A_0, A_1, A_2 when the interval is $[-2, 2]$ and the points are $-1, 0$ and 1.

$$\int_{-2}^{2} f(x)dx \cong A_0 f(-1) + A_1 f(0) + A_2 f(1) \tag{6}$$

Example

We use the polynomials $\{1, x, x^2\}$ to determine the coefficients

$$f(x) = 1 : \int_{-2}^{2} dx = A_0 + A_1 + A_2 \implies A_0 + A_1 + A_2 = 4$$

$$f(x) = x : \int_{-2}^{2} x dx = -A_0 + A_2 = 0 \implies A_0 = A_2$$

$$f(x) = x^2 : \int_{-2}^{2} x^2 dx = A_0 + A_2 = \frac{16}{3}$$

$$\implies A_0 = A_2 = \frac{8}{3} \implies A_1 = -\frac{4}{3}$$

Example

Therefore,

$$\int_{-2}^{2} f(x)dx \cong \frac{8}{3}f(-1) - \frac{4}{3}f(0) + \frac{8}{3}f(1) \tag{7}$$

Verify! that the above formula produces exact values for all quadratic polynomials.

Some Open Newton-Cotes Formula

Some Open Newton-Cotes Formula

When $n = 0$, open Newton-Cotes formula provides Midpoint rule. Similarly, when $n = 1$, it yields the two-point Newton-Cotes open rule. When $n = 3$, the following three point Newton-Cotes open rule is obtained

$$\int_a^b f(x)dx \approx \frac{4h}{3}[2f(a+h) - f(a+2h) + 2f(a+3h)]$$

with error as

$$E_3(t) = \frac{14}{45}h^5 f^{(4)}(\xi), \xi \in (a,b)$$

Some Open Newton-Cotes Formula

When $n = 4$, we obtain the following four-point Newton-Cotes open rule

$$\int_a^b f(x)dx \approx \frac{5h}{24}[11f(a+h) + f(a+2h) + f(a+3h) + 11f(a+4h)]$$

where the error is

$$E_4(t) = \frac{95}{144}h^5 f^{(4)}(\xi), \xi \in (a,b)$$

Some Open Newton-Cotes Formula

When $n = 5$, we obtain the following five-point Newton-Cotes open rule

$$\int_a^b f(x)dx \approx \frac{6h}{20}[11f(a+h) - 14f(a+2h) + 26f(a+3h) - 14f(a+4h) + 11f(a+5h)]$$

where the error is

$$E_5(t) = -\frac{41}{140}h^7 f^{(6)}(\xi), \xi \in (a, b)$$

The following theorem gives the general error term for an $(n+1)$-points closed Newton-Cotes formula.

Some Open Newton-Cotes Formula

Theorem 6

Suppose that $\sum_{i=0}^{n} A_i f(x_i)$ denotes the open Newton-Cotes formula with $x_{-1} = a, x_{n+1} = b, x_0 = a+h, x_i = x_0 + ih, i = 0, 1, 2, \cdots, n$ where $h = (b-a)/(n+2)$. There exists $\xi \in (a, b)$ for which

$$\int_a^b f(x)dx = \sum_{i=0}^{n} A_i f(x_i) + E_n(t)$$

where the error is given by

$$E_n(t) = \begin{cases} \dfrac{h^{n+3}}{(n+2)!} f^{(n+2)}(\xi) \displaystyle\int_{-1}^{n+1} t^2(t-1)\cdots(t-n)dt & n \text{ is even, } f \in C^{n+2} \\ \dfrac{h^{n+2}}{(n+1)!} f^{(n+1)}(\xi) \displaystyle\int_{-1}^{n+1} t(t-1)\cdots(t-n)dt & n \text{ is odd, } f \in C^{n+1} \end{cases}$$

Composite Rules

Composite Rules

- The Newton-Cotes formulas are generally unsuitable for use over large integration intervals.
- High-degree formulas would be required and the values of these formulas are difficult to obtain.
- Also, the Newton-Cotes formulas are based on interpolation polynomials that use equally spaced nodes, a procedure that is inaccurate over large intervals because of the oscillatory nature of high-degree polynomials,
- On the other hand, piecewise approach to numerical integration uses the low-order Newton-Cotes formulas.
- These are the techniques most often applied.

Composite Rules

Theorem 7

Suppose that $c \in [a, b]$, then

$$\int_a^b f(x)dx = \int_a^c f(x)dx + \int_c^b f(x)dx$$

If we subdivide the interval into n equal subintervals by points $x_0 = a, x_1 = a + h, x_2 = a + 2h, \cdots, x_i = a + ih, \cdots, x_n = b$ with spacing $h = (b - a)/n$. Then by integration property, we have

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx$$

Composite Rules

Then we can apply the basic rules in each subinterval $[x_i, x_{i+1}]$, that is,

$$\int_{x_i}^{x_{i+1}} f(x)dx = \sum_{j=0}^{m} A_j f(x_j)$$

where m is the number of points considered in the Newton-Cotes rule in the interval $[x_i, x_{i+1}]$. The general composite Newton-Cotes formula is given by

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} \sum_{j=0}^{m} A_{ij} f(x_{ij}) \tag{8}$$

Composite trapezoidal Rule

The composite trapezoidal rule is obtained by keeping the $m = 2$ in (8). That is,

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{h}{2}[f(x_i) + f(x_{i+1})]$$

and

$$\int_{a}^{b} f(x)dx \approx \frac{h}{2}\sum_{i=0}^{n-1}[f(x_i) + f(x_{i+1})] \tag{9}$$

Composite trapezoidal Rule

For each interval $[x_i, x_{i+1}]$, the error is given by

$$E_t^i = -\frac{h^3}{12} f''(\xi_i)$$

Therefore, the error of the composite trapezoidal rule is obtained as

$$E_t = -\frac{h^3}{12} \sum_{i=0}^{n-1} f''(\xi_i) = O(h^2)$$

The last equation is obtained by using the reason that

$$-\frac{h^3}{12} \sum_{i=0}^{n-1} f''(\xi_i) = -\frac{h^2}{12}(b-a) \sum_{i=0}^{n-1} \frac{1}{n} f''(\xi_i) = -\frac{b-a}{12} h^2 f''(\zeta)$$

for some $\zeta \in (a, b)$.

Composite trapezoidal Rule

The composite trapezoidal rule can also be written as

$$\int_a^b f(x)dx \approx h\sum_{i=1}^{n-1} f(x_i) + \frac{h}{2}[f(a) + f(b)] \tag{10}$$

Composite trapezoidal Rule

Example 8

If the composite trapezoidal rule is to be used to compute

$$\int_0^1 e^{-x^2}\,dx$$

with an error of at most $\frac{1}{2} \times 10^{-4}$, how many points should be used?

Solution The error formula is

$$-\frac{b-a}{12}h^2 f''(\zeta)$$

Now,

$$f''(x) = (4x^2 - 2)e^{-x^2}$$

Therefore,

$$|f''(\zeta)| \leq 2$$

Composite trapezoidal Rule

To have an error of at most $\frac{1}{2} \times 10^{-4}$, we must choose h such that

$$-\frac{1-0}{12}h^2 2 \leq \frac{1}{2} \times 10^{-4} \implies h \leq 0.01733$$

As $h = 1/n$, we need at least 59 or more points to obtain the desired accuracy.

Composite Simpson's 1/3 Rule

The composite Simpson's 1/3 rule is obtained by keeping the $m = 3$ in (8).

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{h}{3}[f(x_i) + 4f\left(\frac{x_i + x_{i+1}}{2}\right) + f(x_{i+1})]$$

Composite Simpson's 1/3 Rule

*Now choose n such that n is divisible by 2, then

$$\int_a^b f(x)dx \approx \frac{h}{3}\sum_{i=0}^{n-1}\left[f(x_i) + 4f\left(\frac{x_i + x_{i+1}}{2}\right) + f(x_{i+1})\right] \tag{11}$$

For each interval $[x_i, x_{i+1}]$, the error is given by

$$E_t^i = -\frac{h^5}{90} f^{(4)}(\xi_i)$$

Composite Simpson's 1/3 Rule

Therefore, the error of the composite Simpson's rule is obtained as

$$E_t = -\frac{h^5}{90}\sum_{i=0}^{n-1} f^{(4)}(\xi_i) = O(h^4)$$

When n is divisible by 2, the composite Simpson's 1/3 rule can also be written as

$$\int_a^b f(x)dx \approx 4\sum_{i=1}^{n/2}[f(a+(2i-1)h)] + 4\sum_{i=1}^{(n-2)/2}[f(a+2ih)] + \frac{h}{3}[f(a)+f(b)] \quad (12)$$

Composite Simpson's 1/3 Rule

Example 9

The calculation of work is an important equation in science and engineering. The general formula is given by

$$\text{Work} = \text{Force} \times \text{Distance}$$

Although, this formula seems to be simple, when apply this to realistic problem, we obtain a complicated function. For example, when the force varies during the course of calculation which results in

$$W = \int_{x_0}^{x_n} F(x)dx$$

Composite Simpson's 1/3 Rule

When the angle between the force and direction of the movement also varies as a function of position, we obtain that

$$W = \int_{x_0}^{x_n} F(x)\cos(\theta(x))dx$$

The following table shows the force and angle as a function of position x.

x	0	5	10	15	20	25	30
$F(x), N$	0.0	9.0	13.0	14.0	10.5	12.0	5.0
$\theta(x), rad$	0.50	1.40	0.75	0.90	1.30	1.48	1.50

Evaluate W using the Simpson's 1/3 rule and composite Simpson's 1/3 rules

Composite Simpson's 1/3 Rule

Solution:

By Simpson's rule, we have $h = (30 - 0)/2$

$$\begin{aligned} W &= \frac{15}{3}[F(0)\cos(\theta(0)) + 4F(15)\cos(\theta(0.9)) + F(30)\cos(\theta(1.50))] \\ &= 5[0 + 34.81 + 0.3537] = 175.82 \end{aligned}$$

By composite Simpson's 1/3 rule, we have $h = (30 - 0)/6$

$$\begin{aligned} W = &\frac{5}{3}[F(0)\cos(\theta(0)) + 4F(5)\cos(\theta(1.4)) + F(10)\cos(\theta(0.75))] \\ &+ \frac{5}{3}[F(10)\cos(\theta(0.75)) + 4F(15)\cos(\theta(0.90)) + F(20)\cos(\theta(1.30))] \\ &+ \frac{5}{3}[F(20)\cos(\theta(1.30)) + 4F(25)\cos(\theta(1.48)) + F(30)\cos(\theta(1.50))] \\ &= 117.13 \end{aligned}$$

Composite Midpoint Rule

Let $f \in c^2[a,b]$, n be even, $h = (b-a)/(n+2)$ and $x_i = a + (i+1)h$ for each $i = -1, 0, \cdots, n+1$. Then the composite midpoint rule is given by

$$\int_a^b f(x)dx \approx 2h \sum_{i=0}^{n/2} f(x_{2i}) \tag{13}$$

The error of the composite midpoint rule is given by

$$\frac{b-a}{6} h^2 f''(\zeta), \zeta \in (a,b)$$

Romberg Integration

Romberg Integration

- The idea behind Romberg integration is to successfully use the trapezoidal rule with increasing intervals and stop as soon as the two successive approximations agree to each other by a desired accuracy.
- The Romberg algorithm produces a triangular array of numbers, all of which are numerical estimates of the definite integral

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

Romberg Integration

The array is denoted by the following notation

$$
\begin{array}{llllll}
R(0,0) & & & & & \\
R(1,0) & R(1,1) & & & & \\
R(2,0) & R(2,1) & R(2,2) & & & \\
R(3,0) & R(3,1) & R(3,2) & R(3,3) & & \\
\vdots & \vdots & \vdots & \vdots & \ddots & \\
R(n,0) & R(n,1) & R(n,2) & R(n,3) & \cdots & R(n,n)
\end{array}
$$

The first column of this table is obtained by employing trapezoidal rule recursively by decreasing values of the step size.

Romberg Integration

The value $R(n, 0)$ is obtained by applying the trapezoidal rule with 2^n equal subintervals. The value of $R(0, 0)$ is obtained with one trapezoid

$$R(0,0) = \frac{1}{2}(b-a)[f(a) + f(b)] \tag{14}$$

Similarly, $R(1, 0)$ is obtained with two trapezoids

$$\begin{aligned}
R(1,0) &= \frac{1}{4}(b-a)[f(a) + f\left(\frac{a+b}{2}\right)] + \frac{1}{4}(b-a)[f\left(\frac{a+b}{2}\right) + f(b)] \\
&= \frac{1}{4}(b-a)[f(a) + f(b)] + \frac{1}{2}(b-a)f\left(\frac{a+b}{2}\right) \\
&= \frac{1}{2}R(0,0) + \frac{1}{2}(b-a)f\left(\frac{a+b}{2}\right)
\end{aligned}$$

Romberg Integration

In particular, the value of $R(n,0)$ is obtained by

$$R(n,0) = \frac{1}{2}R(n-1,0) + h\sum_{k=1}^{2^{n-1}} f(a+(2k-1)h)$$

The general $R(m,n)$ is generated by the following extrapolation formula

$$R(n,m) = R(n,m-1) + \frac{1}{4^m-1}[R(n,m-1) - R(n-1,m-1)] \qquad (15)$$

This formula is obtained from Richardson extrapolation.

Romberg Integration

We can stop this recursive computation with an accuracy of ϵ, when

$$|R(n,n) - R(n-1,n-1)| < \epsilon$$

The error of the Romberg integration is given $O(h^{2m+2})$.

Romberg Integration

Example 10

Using the Romberg integration, obtain the result of

$$\int_0^1 \frac{4}{1+x^2}dx$$

with $n = 5$

3.000000				
3.099999	3.133333			
3.131176	3.141568	3.142117		
3.138988	3.141592	3.141594	3.141585	
3.140941	3.141592	3.141592	3.141592	3.141592

Romberg Integration

Example 11

Using the Romberg integration, obtain the result of

$$\int_{1}^{1.5} x^2 \ln x dx$$

with $n = 2$

$$\begin{array}{lll} 0.228071 & & \\ 0.201225 & 0.1922453 & \\ 0.1944945 & 0.1922585 & 0.1922593 \end{array}$$

Romberg Integration

- Romberg integration applied to a function f on the interval $[a, b]$ relies on the assumption that the Composite Trapezoidal rule has an error term that can be expressed $O(h^2)$, that is, we must have $f \in C^{2m+2}[a, b]$ for the m^{th} row to be generated.
- General-purpose algorithms using Romberg integration include a check at each stage to ensure that this assumption is fulfilled.
- These methods are known as cautious Romberg algorithms.
- This algorithm takes less time to compute and it is not difficult to write the algorithm, however, it can not deal with unequally spaced intervals.

Thanks

Doubts and Suggestions

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