Chapter 4. Numerical Integration

Section 1. Newton-Cotes Formulas

In most cases, the antiderivative of a given function $f(x)$ is not known, and then the explicit expression of the integral

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

can not be obtained. Thus, approximation to this integral is necessary, which is called numerical quadrature,

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

1. Trapezoidal rule. (Burden & Faires, 4.3)

If $f(x)$ is approximated by the linear interpolation polynomial

$$P(x) = \frac{(x-x_1)}{(x_0-x_1)}f(x_0) + \frac{(x-x_0)}{(x_1-x_0)}f(x_1)$$

where $x_0 = a$ and $x_1 = b$, then we have

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_1}\left[\frac{(x-x_1)}{(x_0-x_1)}f(x_0) + \frac{(x-x_0)}{(x_1-x_0)}f(x_1)\right]dx \\ &\quad +\frac{1}{2}\int_{x_0}^{x_1} f''(\xi)(x-x_0)(x-x_1)dx \\ &= \frac{h}{2}[f(a)+f(b)] - \frac{h^3}{12}f''(\xi)\end{aligned}$$

where $h = b - a$. This is called the Trapezoidal rule.

2. Simpson's rule. (Burden & Faires, 4.3)

Let $x_0 = a$, $x_2 = b$, and $x_1 = a+h$, where $h = (b-a)/2$. Let $x \in [a,b]$, using Taylor's theorem we have

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(4)}(\xi)}{24}(x-x_1)^4$$

Then we have

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_2}\left[f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3\right]dx + \\ &\quad \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi)(x-x_1)^4 dx \\ &= 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4 dx \\ &= 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{60}h^5 dx\end{aligned}$$

Using Taylor's theorem we have

$$f''(x_1) = \frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2)$$

Thus, we have the Simpson's rule,

$$\int_a^b f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi)$$

Definition 4.1. The **degree of accuracy**, or **precision**, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, $k = 0, 1, 2, \cdots, n$. ■

By this definition, the Trapezoidal rule has the degree of precision one, and the Simpson's rule has the degree of precision three.

3. Newton-Cotes Formulas (Burden & Faires, 4.3) In general, if we use the Lagrange interpolation polynomial $P_n(x)$ to approximate $f(x)$, we obtain the Newton-Cotes Formula,

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

where $x_0 = a$, $x_n = b$, $x_i = x_0 + ih$ with $h = (b - a)/n$, and

$$a_i = \int_{x_0}^{x_n} L_i(x)dx = \int_{x_0}^{x_n} \prod_{j=0, j\neq i}^{n} \frac{(x - x_j)}{(x_i - x_j)}dx$$

Theorem 4.2. **(Closed Newton-Cotes Formulas)** Let $x_0 = a, x_n = b$, and $x_i = x_0 + ih$ with $h = (b - a)/n$. If n is even and $f \in C^{n+2}[a, b]$, then

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n + 2)!} \int_0^n t^2(t - 1)\cdots(t - n)dt$$

If n is odd and $f \in C^{n+1}[a, b]$, then

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n + 1)!} \int_0^n t(t - 1)\cdots(t - n)dt \quad ■$$

This quadrature formula is called closed Newton-Cotes Formula since the endpoints of $[a, b]$ are included as nodes. The Trapezoidal Rule and Simpson's Rule are the special cases of the Newton-Cotes Formula when $n = 1$ and $n = 2$.

- $n = 1$: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12}f''(\xi)$$

- $n = 2$: Simpsom's rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi)$$

- $n = 3$: Simpsom's Three-Eights rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80}f^{(4)}(\xi)$$

- $n = 4$:

$$\int_{x_0}^{x_4} f(x)dx = \frac{2h}{45}[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] - \frac{8h^7}{945}f^{(6)}(\xi)$$

Similarly, open Newton-Cotes Formula can also be obtained, which does not include the endpoints of $[a, b]$ as nodes.

Theorem 4.3. (Open Newton-Cotes Formulas) Let $x_{-1} = a, x_{n+1} = b$, and $x_i = x_0 + ih$ with $h = (b - a)/(n + 2)$. If n is even and $f \in C^{n+2}[a, b]$, then

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3}f^{(n+2)}(\xi)}{(n+2)!}\int_{-1}^{n+1} t^2(t-1)\cdots(t-n)dt$$

If n is odd and $f \in C^{n+1}[a, b]$, then

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2}f^{(n+1)}(\xi)}{(n+1)!}\int_{-1}^{n+1} t(t-1)\cdots(t-n)dt \quad \blacksquare$$

- $n = 0$: Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi)$$

- $n = 1$:

$$\int_{x_{-1}}^{x_2} f(x)dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4}f''(\xi)$$

- $n = 2$:

$$\int_{x_{-1}}^{x_3} f(x)dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45}f^{(4)}(\xi)$$

- $n = 3$:

$$\int_{x_{-1}}^{x_4} f(x)dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95h^5}{144}f^{(4)}(\xi)$$

Section 2. Composite Numerical Integration

As we have seen in the last chapter, high order interpolations may led to large errors in the resulting approximations. For numerical integrations, we face the same problem. High order quadrature rules may give inaccurate results due to the stability problem. Similar to piecewise polynomial interpolations, we can also introduce piecewise lower order quadrature formulas, which are called composite quadrature rules.

Suppose the interval $[a, b]$ is divided into n subintervals, apply the Trapezoidal rule in each of the subinterval we obtain

Theorem 4.5. (Composite Trapezoidal rule) Let $f \in C^2[a, b]$, $h = (b - a)/n$, and $x_j = a + jh$, $j = 0, 1, \cdots, n$. There exists a $\mu \in (a, b)$ such that

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu)$$

Similarly, if n is even, apply Simpson's rule on each consecutive pair of subinterval we obtain

Theorem 4.4. (Composite Simpson's rule) Let $f \in C^4[a, b]$, n be even, $h = (b - a)/n$, and $x_j = a + jh$, $j = 0, 1, \cdots, n$. There exists a $\mu \in (a, b)$ such that

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180}h^4 f^{(4)}(\mu)$$

Section 3. Romberg Method

Romberg integration is a acceleration technique to increase the convergence speed. Romberg integration uses the Composite Trapezoidal rule to give preliminary approximations and then applies the Richardson extrapolation process to improve the approximation. Let $m_n = 2^{n-1}, n = 1, 2, 3, \cdots$, and let $h_k = (b-a)/m_k$. Use the Composite Trapezoidal rule we have

$$\int_a^b f(x)dx = \frac{h_k}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{2^{k-1}-1} f(a + ih_k)\right] - \frac{(b-a)}{12}h_k^2 f''(\mu_k)$$

Introduce the notations

$$\begin{aligned}
R_{1,1} &= \frac{h_1}{2}[f(a) + f(b)] = \frac{(b-a)}{2}[f(a) + f(b)] \\
R_{2,1} &= \frac{h_2}{2}[f(a) + f(b) + 2f(a + h_2)] \\
&= \frac{(b-a)}{4}\left[f(a) + f(b) + 2f\left(a + \frac{b-a}{2}\right)\right] \\
&= \frac{1}{2}[R_{1,1} + h_1 f(a + h_2)] \\
R_{3,1} &= \frac{1}{2}[R_{2,1} + h_2(f(a + h_3) + f(a + 3h_3))]
\end{aligned}$$

and in general

$$R_{k,1} = \frac{1}{2}\left[R_{k-1,1} + h_{k-1}\sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k)\right]$$

Suppose $f \in C^\infty[a, b]$, then the Composite Trapezoidal rule has the form

$$\int_a^b f(x)dx - R_{k,1} = \sum_{i=1}^{\infty} K_i h_k^{2i} = K_1 h_k^2 + \sum_{i=2}^{\infty} K_i h_k^{2i}$$

Then we have

$$\int_a^b f(x)dx - R_{k+1,1} = \sum_{i=1}^{\infty} K_i h_{k+1}^{2i} = \sum_{i=2}^{\infty} \frac{K_i h_k^{2i}}{2^{2i}} = \frac{K_1 h_k^2}{4} + \sum_{i=2}^{\infty} \frac{K_i h_k^{2i}}{4^i}$$

From these two equations we obtain

$$\begin{aligned}
\int_a^b f(x)dx - \left[R_{k+1,1} + \frac{R_{k+1,1} - R_{k,1}}{3}\right] &= \sum_{i=2}^{\infty} \frac{K_i}{3}\left(\frac{h_k^{2i}}{4^{i-1}} - h_k^{2i}\right) \\
&= \sum_{i=2}^{\infty} \frac{K_i}{3}\left(\frac{1 - 4^{i-1}}{4^{i-1}}\right) h_k^{2i}
\end{aligned}$$

or

$$\int_a^b f(x)dx - R_{k+1,2} = -\frac{K_2}{4}h_k^4 + \sum_{i=3}^{\infty} \frac{K_i}{3}\left(\frac{1-4^{i-1}}{4^{i-1}}\right) h_k^{2i}$$

where

$$R_{k+1,2} = R_{k+1,1} + \frac{R_{k+1,1} - R_{k,1}}{3}$$

which gives the $O(h_k^4)$ approximation. Similarly, using $R_{k,2}$ and $R_{k+1,2}$ we can obtain an $O(h_k^6)$ approximation, and so on. In general,

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$
$$j = 2, 3, \cdots, n, \quad k = j, j+1, \cdots, n.$$

will give an $O(h_{k-1}^{2j})$ approximation. The process is given in the following table

Table 4.9

$R_{1,1}$					
$R_{2,1}$	$R_{2,2}$				
$R_{3,1}$	$R_{3,2}$	$R_{3,3}$			
$R_{4,1}$	$R_{4,2}$	$R_{4,3}$	$R_{4,4}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
$R_{n,1}$	$R_{n,2}$	$R_{n,3}$	$R_{n,4}$	$\cdots$	$R_{n,n}$