6

Numerical Integration and Differentiation

CONTENTS

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to be obtained. Mover, if f is determined by given data, the integration and differentiation of function f is difficult to obtain. Thus, the numerical integration and differentiation will be discussed in this chapter.

6.1 Elements of Numerical Integration

If $F(x)$ is a differentiable function whose derivative is $f(x)$, then we can evaluate the definite integral as

$$\int_a^b f(x)\mathrm{d}x = F(b) - F(a).$$

The above formula is Newton-Leibniz formula. Most integrals can be evaluated by the formula and there exists many techniques for making such evaluations. However, in many applications in science and engineering,

(1) it may have no explicit antiderivative or whose antiderivative is not easy to obtain, such as $f(x)=\dfrac{\sin x}{x}$,e^{-x^2}, $\dfrac{1}{\ln x}$, $\sqrt{a+x^3}$;

(2) f may be specified as a tabulated list, for example,

x	x_0	x_1	$\cdots$	x_n
$f(x)$	$f(x_0)$	$f(x_1)$	$\cdots$	$f(x_n)$.

Numerical integration is required to solve the problem.

From the definition of the integration

$$\int_a^b f(x)\mathrm{d}x = \lim_{\substack{n\to\infty \\ \max\{\Delta x_k\}\to 0}} \sum_{k=1}^{n} f(x_k)\,\Delta x_k$$

where Δx_k is the length of the kth subinterval of [a,b] not related with $f(x)$. An approximation for the definite integral of a function is

$$\int_a^b f(x)\mathrm{d}x \approx \sum_{k=1}^{n} f(x_k)\,\Delta x_k. \tag{6.1}$$

In general, we want to construct

$$\int_a^b f(x)\mathrm{d}x \approx \sum_{k=0}^{n} A_k f(x_k), \tag{6.2}$$

where x_k and A_k are to be determined. The coefficient A_k is related with x_k and not related with the function $f(x)$.

6.1.1 Newton-Cotes Formula

Let

$$I(f)=\int_a^b f(x)\mathrm{d}x. \tag{6.3}$$

For given a set of nodes $a\leqslant x_0<x_1<\cdots<x_n\leqslant b$, and the functon f, the Lagrange interpolating polynomial is

$$L_n(x)=\sum_{k=0}^{n} f(x_k)\,l_k(x)$$

where $l_k(x)$ is

$$l_k(x)=\prod_{\substack{j=0\\ j\neq k}}^{n}\frac{x-x_j}{x_k-x_j}.$$

Then integrate the Lagrange interpolating polynomial and obtain

$$\begin{aligned} I_n(f) &= \int_a^b L_n(x)\mathrm{d}x = \int_a^b \sum_{k=0}^{n} f\left(x_k\right) l_k(x)\mathrm{d}x \\ &= \sum_{k=0}^{n} \left[\int_a^b l_k(x)\mathrm{d}x\right] f\left(x_k\right) = \sum_{k=0}^{n} A_k f\left(x_k\right), \end{aligned}$$

where $A_k = \int_a^b l_k(x)\mathrm{d}x$.

Definition 33. *The formula is called* **interpolating quadrature formula** *if*

$$I_n(f) = \sum_{k=0}^{n} A_k f\left(x_k\right), \tag{6.4}$$

where $A_k = \int_a^b l_k(x)\mathrm{d}x (k = 0, 1, \cdots, n)$.

The error is given by

$$\begin{aligned} R(f) = I(f) - I_n(f) &= \int_a^b f(x)\mathrm{d}x - \sum_{k=0}^{n} \left[\int_a^b l_k(x)\mathrm{d}x\right] f\left(x_k\right) \\ &= \int_a^b f(x)\mathrm{d}x - \int_a^b L_n(x)\mathrm{d}x \\ &= \int_a^b \left[f(x) - L_n(x)\right]\mathrm{d}x \\ &= \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{k=0}^{n} \left(x - x_k\right)\mathrm{d}x \end{aligned} \tag{6.5}$$

Definition 34. *The formula* (6.4) *is called* **Newton-Cotes formula** *if*

$$x_k = a + kh \quad \left(k = 0, 1, \cdots, n; h = \frac{b-a}{n}\right).$$

Let

$$x = a + th,$$

then

$$\begin{aligned} A_k &= \int_a^b l_k(x)\mathrm{d}x = h \int_0^n \prod_{\substack{j=0 \\ j \neq k}}^{n} \frac{t-j}{k-j}\mathrm{d}c \\ &= \frac{(-1)^{n-k}(b-a)}{k!(n-k)!n} \int_0^n \prod_{\substack{j=0 \\ j \neq k}}^{n} (t-j)\mathrm{d}t \quad (k = 0, 1, 2, \cdots, n) \end{aligned} \tag{6.6}$$

Denote

$$C_{n,k} = \frac{(-1)^{n-k}}{k!(n-k)!n} \int_0^n \prod_{\substack{j=0 \\ j \neq k}}^{n} (t-j)\mathrm{d}t \quad (k = 0, 1, \cdots, n).$$

The Newton - Cotes formula is rewritten as

$$I_n(f) = (b-a) \sum_{k=0}^{n} C_{n,k} f(x_k). \tag{6.7}$$

Exercise 6.1. *Take* $n = 1, h = b - a, x_0 = a, x_1 = b$, *then*

$$C_{1,0} = \frac{(-1)^{1-0}}{0!(1-0)!} \int_0^1 (t-1)\mathrm{d}t = \frac{1}{2}$$
$$C_{1,1} = \frac{(-1)^{1-1}}{1!(1-1)!} \int_0^1 (t-0)\mathrm{d}t = \frac{1}{2}$$

Integrate the interpolating polynomial

$$I_1(f) = \frac{b-a}{2} f(x_0) + \frac{b-a}{2} f(x_1) = \frac{b-a}{2}[f(a) + f(b)],$$

then we obtain **Trapezoidal rule**

$$T(f) = \frac{b-a}{2}[f(a) + f(b)]. \tag{6.8}$$

Exercise 6.2. *Take* $n = 2, h = \frac{b-a}{2}, x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b$, *then*

$$C_{2,0} = \frac{(-1)^{2-0}}{0!(2-0)!2} \int_0^2 (t-1)(t-2)\mathrm{d}t = \frac{1}{6}$$
$$C_{2,1} = \frac{(-1)^{2-1}}{1!(2-1)!2} \int_0^2 (t-0)(t-2)\mathrm{d}t = \frac{4}{6}$$
$$C_{2,2} = \frac{(-1)^{2-2}}{2!(2-2)!2} \int_0^2 (t-0)(t-1)\mathrm{d}t = \frac{1}{6}$$

Thus

$$\begin{aligned} I_2(f) &= \frac{b-a}{6} f(x_0) + \frac{4(b-a)}{6} f(x_1) + \frac{b-a}{6} f(x_2) \\ &= \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \end{aligned}$$

It is called **Simpson's rule**

$$S(f) \equiv \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]. \tag{6.9}$$

Exercise 6.3. *Take* $n=4, h=\dfrac{b-a}{4}, x_0=a, x_1=\dfrac{3a+b}{4}, x_2=\dfrac{a+b}{2}, x_3=\dfrac{a+3b}{4}, x_4=b$, *then*

$$
\begin{aligned}
C_{4,0} &= \frac{(-1)^{4-0}}{0!(4-0)!4}\int_0^4 (t-1)(t-2)(t-3)(t-4)\mathrm{d}t = \frac{7}{90}\\
C_{4,1} &= \frac{(-1)^{4-1}}{1!(4-1)!4}\int_0^4 (t-0)(t-2)(t-3)(t-4)\mathrm{d}t = \frac{32}{90}\\
C_{4,2} &= \frac{(-1)^{4-2}}{2!(4-2)!4}\int_0^4 (t-0)(t-1)(t-3)(t-4)\mathrm{d}t = \frac{12}{90}\\
C_{4,3} &= \frac{(-1)^{4-3}}{3!(4-3)!4}\int_0^4 (t-0)(t-1)(t-2)(t-4)\mathrm{d}t = \frac{32}{90}\\
C_{4,4} &= \frac{(-1)^{4-4}}{4!(4-0)!4}\int_0^4 (t-0)(t-1)(t-2)(t-3)\mathrm{d}t = \frac{7}{90}
\end{aligned}
$$

Thus

$$
\begin{aligned}
I_4(f) =& \frac{7(b-a)}{90} f(x_0) + \frac{32(b-a)}{90} f(x_1) + \frac{12(b-a)}{90} f(x_2)\\
&+ \frac{32(b-a)}{90} f(x_3) + \frac{7(b-a)}{90} f(x_4)\\
=& \frac{b-a}{90}\left[7f(a) + 32f\left(\frac{3a+b}{4}\right) + 12f\left(\frac{a+b}{2}\right)\right.\\
&\left. +32f\left(\frac{a+3b}{4}\right) + 7f(b)\right]
\end{aligned}
$$

It is called **Boole's Rule**

$$
\begin{aligned}
C(f) \equiv \frac{b-a}{90}&\left[7f(a) + 32f\left(\frac{3a+b}{4}\right) + 12f\left(\frac{a+b}{2}\right)\right.\\
&\left. +32f\left(\frac{a+3b}{4}\right) + 7f(b)\right]. \qquad (6.10)
\end{aligned}
$$

6.1.2 Measuring Precision

From Eq. (6.5), the error is given by

$$R(f) = \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{k=0}^{n}(x-x_k)\,\mathrm{d}x.$$

The error is zero if

$$I_n(f) = I(f).$$

Definition 35. *The* **degree of accuracy**, *or* **precision**, *of a quadrature formula*

$$I_n(f)=\sum_{k=0}^{n} A_k f\left(x_k\right) \tag{6.11}$$

is the positive integer m such that the formula is exact for all the polynomial of degree at most m and is not exact for at least one polynomial of degree $m+1$.

Theorem 36. *The degree of precision of the quadrature formula*

$$I_n(f)=\sum_{k=0}^{n} A_k f\left(x_k\right)$$

is at least n if and only if

$$A_k=\int_a^b l_k(x) \mathrm{d} x \quad(k=0,1, \cdots, n).$$

Proof It is easy to know the degree of precision of the quadrature formula $I_n(f)$ with $A_k=\int_a^b l_k(x) \mathrm{d} x$ is at least n. On the other hand, if the degree of precision of the quadrature formula $I_n(f)$ is at least n, the formula is exact for the polynomial l_i of degree at most n

$$l_i(x)=\prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x-x_j}{x_i-x_j}.$$

Then

$$\int_a^b l_i(x) \mathrm{d} x=I\left(l_i\right)=I_n\left(l_i\right)=\sum_{k=0}^{n} A_k l_i\left(x_k\right)=A_i \quad(i=0,1,2, \cdots, n).$$

Thus

$$A_k=\int_a^b l_k(x) \mathrm{d} x \quad(k=0,1, \cdots, n).$$

□

Theorem 37. *The degree of precision of the quadrature formula* (6.11) *is m if and only if the formula is exact for $f(x)=1, x, \cdots, x^m$ and not exact for $f(x)=x^{m+1}$.*

Proof Let

$$g_k(x)=x^k \quad(k=0,1,2, \cdots, m+1).$$

1° **Necessity** Suppose the degree of precision of the quadrature (6.11) is

m, i.e. it is exact for any polynomial of degree at most m and not exact for a polynomial of degree $(m+1)$

$$p_{m+1}(x) = c_{n+1}x^{m+1} + p_m(x)$$

where $c_{m+1} \neq 0$. $p_m(x)$ is a polynomial of degree at most m. It is easy to know it is exact for $g_0, g_1, \cdots, g_m$. Since

$$\begin{aligned} I\left(p_{m+1}\right) &= I\left(c_{m+1}g_{m+1} + p_m\right) = c_{m+1}I\left(g_{m+1}\right) + I\left(p_m\right) \\ I_n\left(p_{m+1}\right) &= I_n\left(c_{m+1}g_{m+1} + p_m\right) = c_{m+1}I_n\left(g_{m+1}\right) + I_n\left(p_m\right) \end{aligned}$$

and

$$I\left(p_m\right) = I_n\left(p_m\right), \quad I\left(p_{m+1}\right) \neq I_n\left(p_{m+1}\right),$$

we have

$$I\left(g_{m+1}\right) \neq I_n\left(g_{m+1}\right).$$

2° **Sufficiency** Suppose $I\left(g_0\right) = I_n\left(g_0\right), I\left(g_1\right) = I_n\left(g_1\right), \cdots, I\left(g_m\right) = I_n\left(g_m\right), I\left(g_{m+1}\right) \neq I_n\left(g_{m+1}\right)$.

For any polynomial $p_m(x)$ of degree m can be

$$p_m(x) = \sum_{k=0}^{m} a_k x^k = \sum_{k=0}^{m} a_k g_k(x),$$

we obtain

$$\begin{aligned} I_n\left(p_m\right) &= I_n\left(\sum_{k=0}^{m} a_k g_k\right) = \sum_{k=0}^{m} a_k I_n\left(g_k\right) \\ &= \sum_{k=0}^{m} a_k I\left(g_k\right) = I\left(\sum_{k=0}^{m} a_k g_k\right) = I\left(p_m\right). \end{aligned}$$

Moreover, the formula is not exact for $g_{m+1}(x) = x^{m+1}$. The proof is end. □

Remark: Integration and summation are linear operations; that is,

$$I(\alpha f + \beta g) = \alpha I(f) + \beta I(g), \quad I_n(\alpha f + \beta g) = aI_n(f) + \beta I_n(g)$$

for any $\alpha, \beta \in R$.

Exercise 6.4. *Show the degree of precision of Simpson's Rule*

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

is three.

n	1	2	3	4	5	6	$\cdots$
the degree of precision	1	3	3	5	5	7	$\cdots$

TABLE 6.1
The degree of precisionNewton-Cotes formula

Proof From Th. 37, the degree of the precision of the Simpson's Rule is at least 2. If $f(x) = x^3$, we have

$$I(f) = \int_a^b x^3 \mathrm{d}x = \frac{1}{4}\left(b^4 - a^4\right),$$

$$\begin{aligned} S(f) &= \frac{b-a}{6}\left[a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right] \\ &= \frac{b-a}{6}\left[(a+b)\left(a^2 - ab + b^2\right) + \frac{1}{2}(a+b)^3\right] \\ &= \frac{b^2-a^2}{12}\left[2\left(a^2 - ab + b^2\right) + (a+b)^2\right] \\ &= \frac{1}{4}\left(b^4 - a^4\right). \end{aligned}$$

If $f(x) = x^4$, then

$$I(f) = \int_a^b x^4 \mathrm{d}x = \frac{1}{5}\left(b^5 - a^5\right) \tag{6.12}$$

$$S(f) = \frac{b-a}{6}\left[a^4 + 4\left(\frac{a+b}{2}\right)^4 + b^4\right] \tag{6.13}$$

In Eq. (6.13), the coefficient of b^5 is $\frac{5}{24}$, while it is $\frac{1}{5}$ in Eq. (6.12).The formula is not exact for the function $f(x) = x^4$. Thus the degree of precision of Simpson's Rule is three.

□

Remark If n is odd, the degree of precision of Newton- Cotes formula is n; if n is even, the degree of precision of Newton-Cotes formula is $(n+1)$(see Table 6.1) .

6.1.3 Error of Trapezoidal Rule, Simpson's Rule and Boole's Rule

(1) The error of the Trapezoidal rule $T(f)$ is

$$R_T(f) = I(f) - T(f) = \int_a^b \frac{f''(\xi)}{2}(x-a)(x-b)\mathrm{d}x,$$

where $\xi \in (a,b)$ and is related with x. If $x \in (a,b)$, $(x-a)(x-b) < 0$. From the Weighted Mean Value Theorem for Integrals, we have

$$\begin{aligned} R_T(f) &= \frac{f''(\eta)}{2}\int_a^b (x-a)(x-b)\mathrm{d}x \\ &= -\frac{(b-a)^3}{12}f''(\eta), \quad \eta \in (a,b). \end{aligned} \tag{6.14}$$

(2) Construct an interpolating polynomial $H(x)$ satisfying

$$\begin{gathered} H(a) = f(a), H\left(\frac{a+b}{2}\right) = f\left(\frac{a+b}{2}\right), \quad H(b) = f(b) \\ H'\left(\frac{a+b}{2}\right) = f'\left(\frac{a+b}{2}\right). \end{gathered}$$

Then the polynomial of degree three is unique and the error is

$$f(x) - H(x) = \frac{f^{(4)}(\xi)}{4!}(x-a)\left(x - \frac{a+b}{2}\right)^2 (x-b),$$

where $\xi \in (\min(x,a,b), \max(x,a,b))$ and is related with x. Thus

$$\begin{aligned} \int_a^b H(x)\mathrm{d}x = S(H) &= \frac{b-a}{6}\left[H(a) + 4H\left(\frac{a+b}{2}\right) + H(b)\right] \\ &= \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] = S(f). \end{aligned}$$

Hence

$$\begin{aligned} R_S(f) = I(f) - S(f) &= \int_a^b f(x)\mathrm{d}x - \int_a^b H(x)\mathrm{d}x \\ &= \int_a^b [f(x) - H(x)]\mathrm{d}x \\ &= \int_a^b \frac{f^{(4)}(\xi)}{4!}(x-a)\left(x - \frac{a+b}{2}\right)^2 (x-b)\mathrm{d}x. \end{aligned}$$

By Weighted Mean Value Theorem for Integrals and the $x = \dfrac{a+b}{2} + \dfrac{b-a}{2}t$, there is

$$\begin{aligned} R_S(f) &= \frac{f^{(4)}(\eta)}{4!}\int_a^b (x-a)\left(x - \frac{a+b}{2}\right)^2 (x-b)\mathrm{d}x \\ &= \frac{f^{(4)}(\eta)}{4!}\left(\frac{b-a}{2}\right)^5 \int_{-1}^1 (t+1)t^2(t-1)\mathrm{d}t \\ &= \frac{f^{(4)}(\eta)}{4!}\left(\frac{b-a}{2}\right)^5 2\int_0^1 t^2\left(t^2-1\right)\mathrm{d}t \\ &= -\frac{b-a}{180}\left(\frac{b-a}{2}\right)^4 f^{(4)}(\eta), \quad \eta \in (a,b) \end{aligned} \tag{6.15}$$

(3) The error of Boole's rule can be obtained

$$R_C(f) = I(f) - C(f) = -\frac{2(b-a)}{945}\left(\frac{b-a}{4}\right)^6 f^{(6)}(\eta), \quad \eta \in (a,b) \tag{6.16}$$

6.1.4 Stability

In science and engineering, the values of $f(x_k)\,(k = 0, 1, \cdots, n)$ are often approximated by $\widetilde{f}_k$. Thus $I_n(f)$ is calculated by

$$I_n(\tilde{f}) = \sum_{k=0}^{n} A_k \widetilde{f}_k.$$

Definition 36. *$I_n(f) = \sum\limits_{k=0}^{n} A_k f(x_k)$ is approximated by $I_n(\widetilde{f}) = \sum\limits_{k=0}^{n} A_k \widetilde{f}_k$. $I_n(f)$ is said* **stable** *with for any $\varepsilon > 0$, there exists $\delta > 0$, such that $\left|I_n(f) - I_n(\tilde{f})\right| < \varepsilon$, when $\max\limits_{0 \leqslant k \leqslant n}\left|f(x_k) - \widetilde{f}_k\right| < \delta$.*

6.2 Composite Numerical Integration

The Newton-Cotes formulas are generally unsuitable for use over large integration intervals. High-degree formulas would be required, and the values of the coefficients in these formulas are difficult to obtain. Also, the Newton-Cotes formulas are based on interpolatory polynomials that use equally-spaced nodes, a procedure that is inaccurate over large intervals because of the oscillatory nature of high-degree polynomials.

In this section, we discuss a piecewise approach to numerical integration that uses the low-order Newton-Cotes formulas. Since definite integrals are additive over subintervals, we can evaluate an integral by dividing the interval up into several subintervals, applying the rule separately on each one, and then totaling up. This strategy is called **composite numerical integration**.

Subdivide the interval $[a, b]$ into n subintervals, and let

$$h = \frac{b-a}{n}, \quad x_k = a + kh \quad (k = 0, 1, \cdots, n),$$

for simplicity. Then

$$I(f) = \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} f(x)\mathrm{d}x.$$

6.2.1 Composite Trapezoidal Rule

The **composite Trapezoidal Rule** is simply the sum of Trapezoidal Rule approximations on adjacent subinterval $[x_k, x_{k+1}]$, i.e.

$$T_n(f) = \sum_{k=0}^{n-1} \frac{h}{2} \left[f(x_k) + f(x_{k+1}) \right], \tag{6.17}$$

or

$$T_n(f) = \frac{h}{2} \left[f(x_0) + 2 \sum_{k=1}^{n-1} f(x_k) + f(x_n) \right].$$

Suppose $f(x) \in C^2[a,b]$. From Eq. (6.14), we have

$$\int_{x_k}^{x_{k+1}} f(x) \mathrm{d}x - \frac{h}{2} \left[f(x_k) + f(x_{k+1}) \right] = -\frac{h^3}{12} f''(\eta_k), \quad \eta_k \in (x_k, x_{k+1}).$$

The error of composite Trapezoidal Rule $T_n(f)$ is

$$\begin{aligned} I(f) - T_n(f) &= \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} f(x) \mathrm{d}x - \sum_{k=0}^{n-1} \frac{h}{2} \left[f(x_k) + f(x_{k+1}) \right] \\ &= \sum_{k=0}^{n-1} \left\{ \int_{x_k}^{x_{k+1}} f(x) \mathrm{d}x - \frac{h}{2} \left[f(x_k) + f(x_{k+1}) \right] \right\} \\ &= \sum_{k=0}^{n-1} \left[-\frac{h^3}{12} f''(\eta_k) \right] \\ &= -\frac{h^3}{12} \sum_{k=0}^{n-1} f''(\eta_k). \end{aligned} \tag{6.18}$$

From Extreme Value Theorem, there exists $\eta \in (a,b)$ such that

$$\frac{1}{n} \sum_{k=0}^{n-1} f''(\eta_k) = f''(\eta).$$

Taking the above equation to Eq. (6.18), there is

$$I(f) - T_n(f) = -\frac{h^3}{12} n f''(\eta) = -\frac{b-a}{12} h^2 f''(\eta). \tag{6.19}$$

Let $M_2 = \max\limits_{a \leq x \leq b} | f''(x)|$. For given precision ε, we can choose h, such that

$$\frac{b-a}{12} M_2 h^2 \leqslant \varepsilon.$$

Then

$$|I(f) - T_n(f)| = \frac{b-a}{12} h^2 \left| f''(\eta) \right| \leqslant \frac{b-a}{12} M_2 h^2 \leqslant \varepsilon.$$

On the other hand, from Eq. (6.18), we have

$$\frac{I(f)-T_n(f)}{h^2}=-\frac{1}{12}h\sum_{k=0}^{n-1}f''(\eta_k). \tag{6.20}$$

Then

$$\lim_{h\to 0}h\sum_{k=0}^{n-1}f''(\eta_k)=\int_a^b f''(x)\mathrm{d}x=f'(b)-f'(a)$$

Let $h\to 0$ on both side of the Eq. (6.20), and we obtain

$$\begin{aligned}\lim_{h\to 0}\frac{I(f)-T_n(f)}{h^2}&=-\frac{1}{12}\lim_{h\to 0}h\sum_{k=0}^{n}f''(\eta_k)\\&=\frac{1}{12}\left[f'(a)-f'(b)\right].\end{aligned}$$

For smaller h, there is

$$\frac{I(f)-T_n(f)}{h^2}\approx\frac{1}{12}\left[f'(a)-f'(b)\right],$$

or

$$I(f)-T_n(f)\approx\frac{1}{12}\left[f'(a)-f'(b)\right]h^2. \tag{6.21}$$

Similarly,

$$I(f)-T_{2n}(f)\approx\frac{1}{12}\left[f'(a)-f'(b)\right]\left(\frac{h}{2}\right)^2. \tag{6.22}$$

From Eqs. (6.21) and (6.22), we have

$$I(f)-T_{2n}(f)\approx\frac{1}{4}\left[I(f)-T_n(f)\right].$$

That is

$$I(f)-T_{2n}(f)\approx\frac{1}{3}\left[T_{2n}(f)-T_n(f)\right]. \tag{6.23}$$

For the given precision ε, if

$$\frac{1}{3}\left|T_{2n}(f)-T_n(f)\right|<\varepsilon$$

we have

$$\left|I(f)-T_{2n}(f)\right|\approx\frac{1}{3}\left|T_{2n}(f)-T_n(f)\right|<\varepsilon.$$

Denote

$$x_{k+\frac{1}{2}}=\frac{1}{2}\left(x_k+x_{k+1}\right)\quad(k=0,1,\cdots,n-1).$$

The T_{2n} can be calculted by

$$\begin{aligned}
T_{2n}(f) &= \sum_{k=0}^{n-1}\left\{\frac{1}{2}\cdot\frac{h}{2}\left[f\left(x_k\right)+f\left(x_{x+\frac{1}{2}}\right)\right]+\frac{1}{2}\cdot\frac{h}{2}\left[f\left(x_{k+\frac{1}{2}}\right)+f\left(x_{k+1}\right)\right]\right\}\\
&= \frac{1}{2}\sum_{k=0}^{n-1}\frac{h}{2}\left[f\left(x_k\right)+f\left(x_{k+1}\right)\right]+\frac{1}{2}h\sum_{k=0}^{n-1}f\left(x_{k+\frac{1}{2}}\right)\\
&= \frac{1}{2}\left[T_n(f)+h\sum_{k=0}^{n-1}f\left(x_{k+\frac{1}{2}}\right)\right]. \qquad (6.24)
\end{aligned}$$

Exercise 6.5. *Use composite Trapezoidal rule to approximate*

$$I(f)=\int_1^5\frac{\sin x}{x}\,\mathrm{d}x$$

with seven significant figures.

Solution Let $a=1, b=5, f(x)=\dfrac{\sin x}{x}$. Then

$$T_1(f)=\frac{5-1}{2}[f(1)+f(5)]=1.29937226,$$

$$T_2(f)=\frac{1}{2}\left[T_1(f)+4f(3)\right]=0.74376614,$$

$$T_4(f)=\frac{1}{2}\left[T_2(f)+2(f(2)+f(4))\right]=0.63733116,$$

$$\begin{aligned}
T_8(f) &= \frac{1}{2}\left[T_4(f)+(f(1.5)+f(2.5)+f(3.5)+f(4.5))\right]\\
&= 0.61213199.
\end{aligned}$$

Applying the Eq. (6.24) over and over again, the computed results are listed in Table 6.2. Hence

$$\int_1^5\frac{\sin x}{x}\,\mathrm{d}x\approx 0.6038482.$$

The number of nodes used in the composite Trapezoidal rule is 4097.

6.2.2 Composite Simpson's Rule

Let $x_{k+\frac{1}{2}}=\frac{1}{2}\left(x_k+x_{k+1}\right)$. The **composite Simpson's rule** is obtained by applying Simpson's rule on each consecutive pair of subintervals

$$S_n(f)=\sum_{k=0}^{n-1}\frac{h}{6}\left[f\left(x_k\right)+4f\left(x_{k+\frac{1}{2}}\right)+f\left(x_{k+1}\right)\right] \qquad (6.25)$$

TABLE 6.2
Example of composite Trapezoidal rule

k	2^k	T_{2^k}	$\frac{1}{3}\left(T_{2^k}-T_{2^{-1}}\right)$
0	1	1.29937226	
1	2	0.74376614	-0.18520204
2	4	0.63733116	-0.03547833
3	8	0.61213199	-0.00839972
4	16	0.60591379	-0.00207273
5	32	0.60436425	-0.00051651
6	64	0.60397717	-0.00012902
7	128	0.60388042	-0.00003225
8	256	0.60385624	-0.00000806
9	512	0.60385019	-0.00000202
10	1024	0.60384868	-0.00000050
11	2048	0.60384830	-0.00000013
12	4096	0.60384821	-0.00000003

or

$$S_n(f)=\frac{h}{6}\left[f\left(x_0\right)+2\sum_{k=1}^{n-1} f\left(x_k\right)+f\left(x_n\right)+4\sum_{k=0}^{n-1} f\left(x_{k+\frac{1}{2}}\right)\right].$$

Suppose $f(x)\in C^4[a,b]$. From Eq. (6.15), we have

$$\int_{x_k}^{x_{k+1}} f(x)\mathrm{d}x-\frac{h}{6}\left[f\left(x_k\right)+4f\left(x_{k+\frac{1}{2}}\right)+f\left(x_{k+1}\right)\right]=-\frac{h}{180}\left(\frac{h}{2}\right)^4 f^{(4)}\left(\eta_k\right),$$

where $\eta\in(x_k,x_{k+1})$. The error of composite Simpson's rule is

$$\begin{aligned}
I(f)-S_n(f) &=\sum_{k=0}^{n-1}\left\{\int_{x_k}^{x_{k+1}} f(x)\mathrm{d}x-\frac{h}{6}\left[f\left(x_k\right)+4f\left(x_{k+\frac{1}{2}}\right)+f\left(x_{k+1}\right)\right]\right\} \\
&=\sum_{k=0}^{n-1}\left(-\frac{h}{180}\right)\left(\frac{h}{2}\right)^4 f^{(4)}\left(\eta_k\right) \\
&=\left(-\frac{h}{180}\right)\left(\frac{h}{2}\right)^4 \sum_{k=0}^{n-1} f^{(4)}\left(\eta_k\right).
\end{aligned} \tag{6.26}$$

By Extreme Value Theorem, $\eta\in(a,b)$ exists with

$$\frac{1}{n}\sum_{k=0}^{n-1} f^{(4)}\left(\eta_k\right)=f^{(4)}(\eta).$$

Taking the above equation to Eq. (6.26), we have

$$\begin{aligned} I(f)-S_n(f) &= -\frac{h}{180}\left(\frac{h}{2}\right)^4 n f^{(4)}(\eta) \\ &= -\frac{b-a}{180}\left(\frac{h}{2}\right)^4 f^{(4)}(\eta), \quad \eta \in (a,b). \end{aligned} \tag{6.27}$$

Let $M_4 = \max\limits_{a \leqslant x \leqslant b} \left|f^{(4)}(x)\right|$. For given precision ε, we can choose h, such that

$$\frac{b-a}{180}\left(\frac{h}{2}\right)^4 M_4 \leqslant \varepsilon.$$

That is

$$|I(f)-S_n(f)| \leqslant \varepsilon.$$

Thus

$$I(f)-S_n(f) \approx \frac{1}{180}\left[f^{(3)}(a)-f^{(3)}(b)\right]\left(\frac{h}{2}\right)^4 \tag{6.28}$$

$$I(f)-S_{2n}(f) \approx \frac{1}{15}\left[S_{2n}(f)-S_n(f)\right]. \tag{6.29}$$

For given precision ε, if

$$\frac{1}{15}\left|S_{2n}(f)-S_n(f)\right| < \varepsilon,$$

we have

$$|I(f)-S_{2n}(f)| \approx \frac{1}{15}\left|S_{2n}(f)-S_n(f)\right| < \varepsilon. \tag{6.30}$$

Exercise 6.6. *Use composite Simpson's rule to approximate* $I(f) = \int_1^5 \frac{\sin x}{x}\,\mathrm{d}x$ *with seven significant figures.*

Solution Let $a=1, b=5, \varepsilon = \frac{1}{2}\times 10^{-7}, f(x)=\frac{\sin x}{x}$. The computed results by Eq. (6.25) are listed in Table 6.3.

Thus

$$I(f) \approx 0.6038482$$

and sixty-five nodes are used.

6.2.3 Composite Boole's rule

Let $x_{k+\frac{1}{4}} = x_k + \frac{1}{4}h, x_{k+\frac{1}{2}} = x_k + \frac{1}{2}h, x_{k+\frac{3}{4}} = x_k + \frac{3}{4}h$.The **composite Boole's rule** is

$$C_n(f) = \sum_{k=0}^{n-1} \frac{h}{90}\left[7f(x_k) + 32f\left(x_{k+\frac{1}{4}}\right) + 12f\left(x_{k+\frac{1}{2}}\right) + 32f\left(x_{k+\frac{3}{4}}\right) + 7f(x_{k+1})\right]. \tag{6.31}$$

TABLE 6.3
Example of composite Simpson's rule

k	2^k	S_{2^k}	$\frac{1}{15}\left(S_{2^k} - S_{2^{k-1}}\right)$
0	1	0.55856409	
1	2	0.60185283	0.00288592
2	4	0.60373227	0.00012530
3	8	0.60384106	0.00000725
4	16	0.60384773	0.00000044
5	32	0.60384815	0.00000003

The error can be obtained by the analysis of the error of composite Trapezoid rule and composite Simpson's rule similarly.

$$I(f) - C_n(f) = -\frac{2(b-a)}{945}\left(\frac{h}{4}\right)^6 f^{(6)}(\eta), \quad \eta \in (a,b). \tag{6.32}$$

For smaller h, there is

$$I(f) - C_n(f) \approx \frac{2}{945}\left[f^{(5)}(a) - f^{(5)}(b)\right]\left(\frac{h}{4}\right)^6, \tag{6.33}$$

and

$$I(f) - C_{2n}(f) \approx \frac{1}{63}\left[C_{2n}(f) - C_n(f)\right]. \tag{6.34}$$

For given precision ε, if

$$\frac{1}{63}\left|C_{2n}(f) - C_n(f)\right| < \varepsilon,$$

we have

$$|I(f) - C_{2n}(f)| \approx \frac{1}{63}\left|C_{2n}(f) - C_n(f)\right| < \varepsilon.$$

Exercise 6.7. *Use composite Boole's rule to approximate*

$$I(f) = \int_1^5 \frac{\sin x}{x}\,\mathrm{d}x$$

with seven significant figures.

Solution Take $a = 1, b = 5, \varepsilon = \frac{1}{2}\times 10^{-7}, f(x) = \frac{\sin x}{x}$. The computed results by Eq. (6.31) are listed in the Table 6.4. Thus

$$I(f) \approx 0.6038482$$

and thirty-three nodes are used.

TABLE 6.4
Example of composite Boole's Rule

k	2^k	C_{z^k}	$\frac{1}{63}\left(C_{z^k} - C_{2^{h-1}}\right)$
0	1	0.60473875	
1	2	0.60385756	-0.00001399
2	4	0.60384831	-0.00000015
3	8	0.60384818	0.00000000

6.3 Romberg Integration

In this section we will illustrate how Richardson extrapolation applied to results from the Composite Trapezoidal rule can be used to obtain high accuracy approximations with little computational cost.

From Eq. (6.23), the error of Composite Trapezoid rule can be estimated by

$$I(f) - T_{2n}(f) \approx \frac{1}{3}\left[T_{2n}(f) - T_n(f)\right].$$

Then

$$\begin{aligned}\widetilde{T}_n(f) &= T_{2n}(f) + \frac{1}{3}\left[T_{2n}(f) - T_n(f)\right]\\ &= \frac{4}{3}T_{2n}(f) - \frac{1}{3}T_n(f).\end{aligned}$$

From Eqs. (6.17) and (6.24), we have

$$\begin{aligned}\widetilde{T}_n(f) =&\frac{4}{3}\sum_{k=0}^{n-1}\left\{\frac{h}{4}\left[f\left(x_k\right) + f\left(x_{k+\frac{1}{2}}\right)\right] + \frac{h}{4}\left[f\left(x_{k+\frac{1}{2}}\right) + f\left(x_{k+1}\right)\right]\right\}\\ &-\frac{1}{3}\sum_{k=0}^{n-1}\frac{h}{2}\left[f\left(x_k\right) + f\left(x_{k+1}\right)\right]\\ =&\sum_{k=0}^{n-1}\left\{\frac{h}{3}\left[f\left(x_k\right) + 2f\left(x_{k+\frac{1}{2}}\right) + f\left(x_{k+1}\right)\right] - \frac{h}{6}\left[f\left(x_k\right) + f\left(x_{k+1}\right)\right]\right\}\\ =&\sum_{k=0}^{n-1}\frac{h}{6}\left[f\left(x_k\right) + 4f\left(x_{k+\frac{1}{2}}\right) + f\left(x_{k+1}\right)\right]\\ =&S_n(f),\end{aligned}$$

i.e.

$$S_n(f) = \frac{4}{3}T_{2n}(f) - \frac{1}{3}T_n(f). \tag{6.35}$$

Similarly, the error of Composite Simpson's rule can be estimated by

$$I(f) - S_{2n}(f) \approx \frac{1}{15}\left[S_{2n}(f) - S_n(f)\right].$$

Then

$$\begin{aligned}\widetilde{S}_n(f) &= S_{2n}(f) + \frac{1}{15}\left[S_{2n}(f) - S_n(f)\right] \\ &= \frac{16}{15}S_{2n}(f) - \frac{1}{15}S_n(f)\end{aligned}$$

It is easy to verify the righthand of the above equation is Boole's rule $C_n(f)$, i.e.

$$C_n(f) = \frac{16}{15}S_{2n}(f) - \frac{1}{15}S_n(f). \tag{6.36}$$

Repeatly, by Eq. (6.34) we have the estimation of the error of Composite Boole's rule

$$I(f) - C_{2n}(f) \approx \frac{1}{63}\left[C_{2n}(f) - C_n(f)\right]$$

Then let

$$\begin{aligned}R_n(f) &= C_{2n}(f) + \frac{1}{63}\left[C_{2n}(f) - C_n(f)\right] \\ &= \frac{64}{63}C_{2n}(f) - \frac{1}{63}C_n(f)\end{aligned} \tag{6.37}$$

which is said **Romberg Formula**.

It can be proved the degree of the precision of the Romberg formula is seven and the truncation error is about $O\left(h^8\right)$. For smaller h, the truncation error is

$$I(f) - R_n(f) \approx Ch^8 \tag{6.38}$$

and

$$I(f) - R_{2n}(f) \approx \frac{1}{255}\left[R_{2n}(f) - R_n(f)\right]. \tag{6.39}$$

The Romberg integration can be listed as follows

n	$T_n(f)$	$S_n(f)$	$C_n(f)$	$R_n(f)$
1	T_1	S_1	C_1	R_1
2	T_2	S_2	C_2	R_2
4	T_4	S_4	C_4	R_4
8	T_8	S_8	C_8	$\vdots$
16	T_{16}	S_{16}	$\vdots$	
32	T_{32}	$\vdots$		
$\vdots$	$\vdots$			

TABLE 6.5
Example of Romberg integration

n	T_n	S_n	C_n	R_n
1	1.29937226	0.55856409	0.60473875	0.60384358
2	0.74376614	0.60185283	0.60385756	0.60384816
4	0.63733116	0.60373227	0.60384831	
8	0.61213199	0.60384106		
16	0.60591379			

Exercise 6.8. *Use Romberg integration to approxiamate* $\int_1^5 \frac{\sin x}{x}\,\mathrm{d}x$ *with seven significant figures.*

Solution Take $a = 1, b = 5, \varepsilon = \frac{1}{2} \times 10^{-7}, f(x) = \frac{\sin x}{x}$, and the computed results are listed in the Table 6.5 . Since $\frac{1}{255}|R_2 - R_1| = 0.2 \times 10^{-7} < \frac{1}{2} \times 10^{-7}$,

$$I(f) \approx 0.6038482$$

and seventeen nodes are needed.

By an alternative method, that if $f \in C^\infty[a, b]$, the composite Trapezoidal rule can also be written with an error term in the form

$$T_n(f) = I(f) + \alpha_1 h^2 + \alpha_2 h^4 + \alpha_3 h^6 + \cdots + \alpha_k h^{2k} + \cdots \tag{6.40}$$

where $\alpha_k (k = 1, 2, \cdots)$ is independent on h. Eq. (6.40) is said Euler-Maclaurin expansion. Richardson extrapolation is applied to obtain high-order approximation. Since

$$T_{2n}(f) = I(f) + \alpha_1 \left(\frac{h}{2}\right)^2 + \alpha_2 \left(\frac{h}{2}\right)^4 + \alpha_3 \left(\frac{h}{2}\right)^6 + \cdots + \alpha_k \left(\frac{h}{2}\right)^{2k} + \cdots \tag{6.41}$$

then

$$\frac{4}{3} T_{2n}(f) - \frac{1}{3} T_n(f) = I(f) + \beta_1 h^4 + \beta_2 h^6 + \cdots$$

where $\beta_k(k=1,2,\cdots)$ is constant independent on h.

We obtain $O(h^4)$ approximations by

$$T_n^{(1)}(f) = \frac{4}{3}T_{2n}(f) - \frac{1}{3}T_n(f),$$

i.e.

$$T_n^{(1)}(f) = I(f) + \beta_1 h^4 + \beta_2 h^6 + \cdots . \tag{6.42}$$

It can be verified $T_n^{(1)}(f)$ is composite Simpson's rule. Similarly, repeating the above process, we can obtain $O(h^6)$ approximations by

$$T_n^{(2)}(f) = \frac{16}{15}T_{2n}^{(1)}(f) - \frac{1}{15}T_n^{(1)}(f)$$

which is composite Boole's rule.

Then $O(h^6)$ approximations by

$$T_n^{(3)}(f) = \frac{64}{63}T_{2n}^{(2)}(f) - \frac{1}{63}T_n^{(2)}(f)$$

which is Romberg rule and

$$T_n^{(3)}(f) = I(f) + \delta_1 h^8 + \delta_2 h^{10} + \cdots . \tag{6.43}$$

In general, after the appropriate $T_n^{(m-1)}(f)$ approximations have been obtained, we determine the $O(h^{2(m+1)})$ approximations from

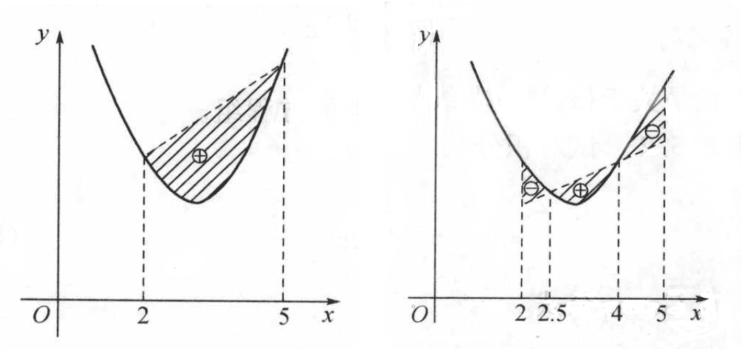
$$T_n^{(m)}(f) = \frac{4^m}{4^m-1}T_{2n}^{(m-1)}(f) - \frac{1}{4^m-1}T_n^{(m-1)}(f) \tag{6.44}$$

The order of the approximations can be improved theoretcally by Eq. (6.44). However, $m=3$ (Romberg formula) is appropriate since

$$\frac{4^m}{4^m-1} \approx 1, \quad \frac{1}{4^m-1} \leqslant \frac{1}{255}, m \geqslant 4.$$

6.4 Gaussian Quadrature

The Newton-Cotes formulas are derived by integrating interpolating polynomials. The error term in the interpolating polynomial of degree n involves the $(n+1)$st derivative of the function being approximated, so a Newton-Cotes formula is exact when approximating the integral of any polynomial of degree less than or equal to n. All the Newton-Cotes formulas use values of the function at equally-spaced points. This restriction is convenient when the formulas are combined to form the composite rules but it can significantly influence the accuracy of the approximation . Consider, for example, the Trapezoidal rule applied to determine the integrals of the functions.



(a) (b)

Exercise 6.9. *Use the Trapezoidal rule to approximate the integral*

$$\int_2^5 \left[2+(x-3)^2\right] \mathrm{d}x.$$

Solution

$$T=\frac{3}{2}[f(2)+f(5)]=13.5.$$

□

If we use linear interpolating polynomial on the nodes $x_0=2.5, x_1=4$, then $\widetilde{T}=8.3571$. Compared with $I=\int_2^5\left[2+(x-3)^2\right] \mathrm{d}x=9$, $\widetilde{T}$ is better for approximating the integral. The graphs are shown in the following figure.

Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally spaced way. The nodes $x_0, x_1, \cdots, x_n$ in the interval [a, b] and coefficients $A_1, A_1, \cdots, A_n$, are chosen to minimize the expected error obtained in the approximation

$$\int_a^b f(x) \mathrm{d}x \approx \sum_{k=0}^n A_k f\left(x_k\right).$$

Definition 37. *The quadrature* $I_n(f)=\sum_{k=0}^n A_k f\left(x_k\right)$ *is said* **Gaussian quadrature** *if the degree of precision is* $(2n+1)$.

According to the definition, $\left\{x_k\right\}_{k=0}^n$ and $\left\{A_k\right\}_{k=0}^n$ satisfy

$$\left\{\begin{array}{l}
\sum_{k=0}^n A_k=\int_a^b 1 \mathrm{~d} x \\
\sum_{k=0}^n x_k A_k=\int_a^b x \mathrm{~d} x \\
\sum_{k=0}^n x_k^2 A_k=\int_a^b x^2 \mathrm{~d} x \\
\vdots \\
\sum_{k=0}^n x_k^{2n+1} A_k=\int_a^b x^{2n+1} \mathrm{~d} x
\end{array}\right. \tag{6.45}$$

Exercise 6.10. *Determine* A_0, A_1, x_0, *and* x_1 *such that*

$$I_1(f) = A_0 f(x_0) + A_1 f(x_1) \tag{6.46}$$

is Gaussian quadrature to approximate

$$I(f) = \int_{-1}^{1} f(x)\mathrm{d}x \tag{6.47}$$

Solution From Eq. (6.46), x_0, x_1, A_0, A_1 satisfy

$$A_0 + A_1 = \int_{-1}^{1} 1 \, \mathrm{d}x = 2 \tag{6.48}$$

$$x_0 A_0 + x_1 A_1 = \int_{-1}^{1} x \, \mathrm{d}x = 0 \tag{6.49}$$

$$x_0^2 A_0 + x_1^2 A_1 = \int_{-1}^{1} x^2 \, \mathrm{d}x = \frac{2}{3} \tag{6.50}$$

$$x_0^3 A_0 + x_1^3 A_1 = \int_{-1}^{1} x^3 \, \mathrm{d}x = 0 \tag{6.51}$$

A little algebra shows that this system of equations has the unique solution

$$x_0 = -\frac{1}{\sqrt{3}}, \quad x_1 = \frac{1}{\sqrt{3}}, \quad A_0 = 1, \quad A_1 = 1.$$

□

When $n \geqslant 2$, Eqs. (6.45) is difficult to be solved directly, but an alternative method obtains them more easily.

Theorem 38. *Suppose*

$$I_n(f) = \sum_{k=0}^{n} A_k f(x_k), \tag{6.52}$$

is a quadrature to approximate $I(f) = \int_a^b f(x)\mathrm{d}x$ *where* $A_k = \int_a^b l_k(x)\mathrm{d}x \quad (k = 0, 1, \cdots, n)$. $I_n(f)$ *is Gaussian quadrature if and only if the polynomial* $W_{n+1}(x)$ *is orthogonal to any polynomial* $p(x)$ *of degree less than* n, *i.e.*

$$\int_a^b p(x) W_{n+1}(x)\mathrm{d}x = 0,$$

where $W_{n+1}(x) = (x - x_0)(x - x_1)\cdots(x - x_n)$.

Proof 1° **Necessity** Suppose $I_n(f)$ is Gaussian quadrature, then it is exact for any polynomial of degree less than $2n + 1$. Thus

$$\int_a^b p(x) W_{n+1}(x)\mathrm{d}x = \sum_{k=0}^{n} A_k p(x_k) W_{n+1}(x_k)$$

for any polynomial of degree at most n.

Noticing $W_{n+1}(x_k) = 0 (k = 0, 1, 2, \cdots, n)$, we have

$$\int_a^b p(x) W_{n+1}(x) \mathrm{d}x = 0.$$

2° **Sufficiency** Suppose

$$\int_a^b p(x) W_{n+1}(x) \mathrm{d}x = 0$$

holds for any polynomial of degree at most n. The polynomial $W_{n+1}(x)$ can be rewritten as

$$f(x) = p(x) W_{n+1}(x) + q(x),$$

where $p(x)$ and $q(x)$ are polynomial of degree $\leq n$. Then

$$\int_a^b f(x) \mathrm{d}x = \int_a^b p(x) W_{n+1}(x) \mathrm{d}x + \int_a^b q(x) \mathrm{d}x.$$

Since orthogonal condition,

$$\int_a^b f(x) \mathrm{d}x = \int_a^b q(x) \mathrm{d}x.$$

Because $I_n(f)$ has degree of precision at least n, then

$$\int_a^b q(x) \mathrm{d}x = \sum_{k=0}^n A_k q(x_k).$$

By

$$f(x_k) = p(x_k) W_{n+1}(x_k) + q(x_k) = q(x_k)$$

there is

$$\int_a^b f(x) \mathrm{d}x = \int_a^b q(x) \mathrm{d}x = \sum_{k=0}^n A_k q(x_k) = \sum_{k=0}^n A_k f(x_k)$$

i.e. $I_n(f)$ is exact for any polynomial of degree less than $2n+1$. Hence $I_n(f)$ is Gaussian quadrature.

6.4.1 Orthogonal Polynomials

Definition 38. *Let*

$$g_n(x) = a_{n,0} x^n + a_{n,1} x^{n-1} + \cdots + a_{n,n-1} x + a_{n,n} \quad (n = 0, 1, 2, \cdots)$$

where $a_{n,0} \neq 0$. $\{g_n(x)\}_{n=0}^\infty$ *is said to be an* **orthogonal set of functions** *for the interval* $[a, b]$ *if*

$$(g_l, g_k) = \int_a^b g_i(x) g_k(x) \mathrm{d}x = 0 \quad (l < k).$$

Theorem 39. *The orthogonal set of functions $\{g_n(x)\}_{n=0}^{\infty}$ is linearly independent on the interval $[a, b]$. and*

$$\int_a^b g_n(x)p_k(x)\mathrm{d}x = 0,$$

for any polynomial $p_k(x)$ of degree $k < n$.

Proof Suppose $C_0, C_1, \cdots, C_n$ are real numbers for which

$$C_0 g_0(x) + C_1 g_1(x) + \cdots + C_n g_n(x) = 0.$$

Then

$$C_k \int_a^b g_k^2(x)\mathrm{d}x = 0.$$

So

$$C_k = 0 \quad (k = 0, 1, \cdots, n).$$

Hence $g_0(x), g_1(x), \cdots, g_n(x)$ are linear independently and there exist numbers $c_0, \cdots, c_k$ such that

$$p_k(x) = c_0 g_0(x) + c_1 g_1(x) + \cdots + c_k g_k(x),$$

for any $p_k(x)$ be a polynomial of degree $k < n$.

Because g_n is orthogonal to g_j for each $j = 0, 1, \cdots, k$, we have

$$\int_a^b p_k(x)g_j(x)\mathrm{d}x = \sum_{j=0}^{k} \int_a^b g_j(x)g_k(x)\mathrm{d}x = 0.$$

□

Theorem 40. *Suppose $\{g_n(x)\}_{n=0}^{\infty}$ is an orthogonal set of polynomial functions on $[a, b]$. Then $g_n(x)$ have n distinct zeros on (a, b).*

Definition 39. *The polynomial of degree n*

$$P_n(t) = \frac{1}{2^n n!}\frac{\mathrm{d}^n \left(t^2-1\right)^n}{\mathrm{d}t^n} \quad (n = 0, 1, 2, \cdots) \tag{6.53}$$

is said **Legendre Polynomials** *and*

$$P_0(t) = 1, \quad P_1(t) = t$$
$$P_2(t) = \tfrac{1}{2}\left(3t^2 - 1\right), \quad P_3(t) = \tfrac{1}{2}\left(5t^3 - 3t\right)$$

$$P_4(t) = \frac{1}{8}\left(35t^4 - 30t^2 + 2\right), \quad P_5(t) = \frac{1}{8}\left(63t^5 - 70t^3 + 15t\right).$$

$\vdots$

Theorem 41. *The set of Legendre polynomials* $\{P_n(t)\}_{n=0}^{\infty}$ *is orthogonal on [-1,1].*

Proof

$$
\begin{aligned}
(P_m, P_n) =& \frac{1}{2^{m+n} m! n!} \int_{-1}^{1} \frac{\mathrm{d}^m \left(t^2-1\right)^m}{\mathrm{d}t^m} \cdot \frac{\mathrm{d}^n \left(t^2-1\right)^n}{\mathrm{d}t^n}\ \mathrm{d}t \\
=& \frac{1}{2^{m+n} m! n!} \int_{-1}^{1} \frac{\mathrm{d}^m \left(t^2-1\right)^m}{\mathrm{d}t^m}\ \mathrm{d}\frac{\mathrm{d}^{n-1} \left(t^2-1\right)^n}{\mathrm{d}t^{n-1}} \\
=& \frac{1}{2^{m+n} m! n!} \left[\left. \frac{\mathrm{d}^m \left(t^2-1\right)^m}{\mathrm{d}t^m} \frac{\mathrm{d}^{n-1} \left(t^2-1\right)^n}{\mathrm{d}t^{n-1}} \right|_{-1}^{1} \right. \\
& \left. - \int_{-1}^{1} \frac{\mathrm{d}^{m+1} \left(t^2-1\right)^m}{\mathrm{d}t^{m+1}} \frac{\mathrm{d}^{n-1} \left(t^2-1\right)^n}{\mathrm{d}t^{n-1}}\ \mathrm{d}t \right] \\
=& \frac{(-1)^1}{2^{m+n} m! n!} \int_{-1}^{1} \frac{\mathrm{d}^{m+1} \left(t^2-1\right)^m}{\mathrm{d}t^{m+1}} \frac{\mathrm{d}^{n-1} \left(t^2-1\right)^n}{\mathrm{d}t^{n-1}}\ \mathrm{d}t \\
=& \dots \\
=& \frac{(-1)^n}{2^{m+n} m! n!} \int_{-1}^{1} \frac{\mathrm{d}^{m+n} \left(t^2-1\right)^m}{\mathrm{d}t^{m+n}} \cdot \left(t^2-1\right)^n\ \mathrm{d}t
\end{aligned}
$$

If $m < n$, there is $\dfrac{\mathrm{d}^{m+n} \left(t^2-1\right)^m}{\mathrm{d}t^{m+n}} = 0$. So $(P_m, P_n) = 0$.

□

Consider

$$
I(g) = \int_{-1}^{1} g(t)\mathrm{d}t. \tag{6.54}
$$

From Th. 40, Legendre polynomial $P_{n+1}(t)$ of degree $(n+1)$ have $n+1$ distinct zeros $t_0, t_1, \cdots, t_n$ on (-1,1). And Th. 39 tells us $P_{n+1}(t)$ is orthogonal to any polynomial of degree at most n on [-1,1]. Then

$$
\widetilde{A}_k = \int_{-1}^{1} \prod_{\substack{j=0 \\ j \neq k}}^{n} \frac{t - t_j}{t_k - t_j}\ \mathrm{d}t \quad (k = 0, 1, \cdots, n). \tag{6.55}
$$

From Th. 38, the Gaussian quadrature is

$$
I_n(g) = \sum_{k=0}^{n} \widetilde{A}_k g\left(t_k\right) \tag{6.56}
$$

(1) If $n = 0$, $t_0 = 0$, $\widetilde{A}_k = 2$, and the Gaussian quadrature is

$$
\int_{-1}^{1} g(t)\mathrm{d}t \approx 2g(0).
$$

TABLE 6.6
t_k and A_k of Gaussian quadrature on $[-1,1]$

	t_k	$\widetilde{A}_k$
1	0	2.000 000 0
2	$\pm$0.577 350 3	1.000 000 0
3	$\pm$0.774 596 7	0.555 555 6
	0	0.888 888 9
4	$\pm$0.861 136 3	0.347 854 8
	$\pm$0.339 982 0	0.652 145 2
5	$\pm$0.9061798	0.236 926 9
	$\pm$0.538 469 3	0.478 628 7
	0	0.568 888 9

(2) If $n = 1$, $t_0 = -\frac{1}{\sqrt{3}}, t_1 = \frac{1}{\sqrt{3}}, \widetilde{A}_0 = 1, \widetilde{A}_1 = 1$, and the Gaussian quadrature is

$$\int_{-1}^{1} g(t)\mathrm{d}t \approx g\left(-\frac{1}{\sqrt{3}}\right) + g\left(\frac{1}{\sqrt{3}}\right)$$

(3)If $n = 2$, $t_0 = -\sqrt{\frac{3}{5}}, t_1 = 0, t_2 = \sqrt{\frac{3}{5}}, \widetilde{A}_0 = \frac{5}{9}, \widetilde{A}_1 = \frac{8}{9}, \widetilde{A}_2 = \frac{5}{9}$, and we have

$$\int_{-1}^{1} g(t)\mathrm{d}t \approx \frac{5}{9}g\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9}g(0) + \frac{5}{9}g\left(\sqrt{\frac{3}{5}}\right).$$

The nodes $\{t_k\}_{k=0}^{n}$ and the coefficients $\left\{\widetilde{A}_k\right\}_{k=0}^{n}$ are independent on the function g. So they can be listed in Table 6.6.

In general, consider

$$I(f) = \int_a^b f(x)\mathrm{d}x. \tag{6.57}$$

Take the transformation $x = \frac{a+b}{2} + \frac{b-a}{2}t$, and we have

$$I(f) = \int_{-1}^{1} \frac{b-a}{2} f\left(\frac{a+b}{2} + \frac{b-a}{2}t\right)\mathrm{d}t. \tag{6.58}$$

Let

$$g(t) = \frac{b-a}{2} f\left(\frac{a+b}{2} + \frac{b-a}{2}t\right) \tag{6.59}$$

By Eq. (6.56), the quadrature is

$$I_n(f) = \sum_{k=0}^{n} \frac{b-a}{2}\widetilde{A}_k f\left(\frac{a+b}{2} + \frac{b-a}{2}t_k\right) \tag{6.60}$$

Let

$$x_k = \frac{a+b}{2} + \frac{b-a}{2}t_k, \quad A_k = \frac{b-a}{2}\widetilde{A}_k \quad (k = 0, 1, 2, \cdots, n). \tag{6.61}$$

Then

$$I_n(f) = \sum_{k=0}^{n} A_k f(x_k). \tag{6.62}$$

If the function $f(x)$ is the polynomial of degree of $(2n+1)$, the function $g(t)$ is also a polynomial of degree $(2n+1)$ by Eq. (6.59). Thus

$$\begin{aligned} I(f) &= \int_a^b f(x)\mathrm{d}x = \int_{-1}^{1} \frac{b-a}{2} f\left(\frac{a+b}{2} + \frac{b-a}{2}t\right)\mathrm{d}t \\ &= \sum_{k=0}^{n} \widetilde{A}_k \left[\frac{b-a}{2} f\left(\frac{a+b}{2} + \frac{b-a}{2}t_k\right)\right] \\ &= \sum_{k=0}^{n} A_k f(x_k) = I_n(f). \end{aligned}$$

That is Eq. (6.62) is exact for the polynomial of degree of $2n+1$. Eq. (6.62) is Gaussian quadrature to approximate to (6.57).

Exercise 6.11. *Construct a Gaussian quadrature for* $\int_0^{10} f(x)\mathrm{d}x$ *with degree of precision seven.*

Solution Let $a = 0, b = 10$. Since $2n+1 = 7$, then $n = 3$. The coefficients can be obtained in the Table 6.6

$$\begin{aligned} t_0 &= -0.8611363, \quad t_1 = -0.3399810 \\ t_2 &= 0.3399810, \quad t_3 = 0.8611363 \\ \widetilde{A}_0 &= 0.3478548, \quad \widetilde{A}_1 = 0.6521452 \\ \widetilde{A}_2 &= 0.6521452, \quad \widetilde{A}_3 = 0.3478548 \end{aligned}$$

By $x_k = \frac{a+b}{2} + \frac{b-a}{2}t_k = 5(1+t_k)$, there is

$$\begin{aligned} x_0 &= 0.6943185, \quad x_1 = 3.300095 \\ x_2 &= 6.699905, \quad x_3 = 9.3056815 \end{aligned}$$

By $A_k = \dfrac{b-a}{2}\widetilde{A}_k = 5\widetilde{A}_k$, we have

$$\begin{aligned} A_0 &= 1.739274, \quad A_1 = 3.260726 \\ A_2 &= 3.260726, \quad A_3 = 1.739274 \end{aligned}$$

The Gaussian quadrature is

$$\begin{aligned} \int_0^{10} f(x)\mathrm{d}x \approx & 1.739274 f(0.6943185) + 3.260726 f(3.300095) \\ & + 3.260726 f(6.699905) + 1.739274 f(9.3056815). \end{aligned}$$

6.4.2 Truncation Error of Gaussian Quadrature

Theorem 42. *Suppose $f(x) \in C^{2n+2}[a,b]$. The truncation error of Gaussian quadrature*

$$\int_a^b f(x)\mathrm{d}x \approx \sum_{k=0}^{n} A_k f(x_k)$$

is

$$\begin{aligned} R(f) &= \int_a^b f(x)\mathrm{d}x - \sum_{k=0}^{n} A_k f(x_k) \\ &= \frac{f^{(2n+2)}(\xi)}{(2n+2)!}\int_a^b W_{n+1}^2(x)\mathrm{d}x \end{aligned}$$

where $W_{n+1}(x) = (x-x_0)(x-x_1)\cdots(x-x_n), \xi \in (a,b)$.

Proof Construct a polynomial $H(x)$ of degree $2n+1$ satisfying

$$H(x_k) = f(x_k), \quad H'(x_k) = f'(x_k) \quad (k = 0, 1, \cdots, n).$$

Then the error is

$$f(x) - H(x) = \frac{f^{(2n+2)}(\eta)}{(2n+2)!}W_{n+1}^2(x), \quad \eta \in (a,b).$$

Since the degree of precision of Gaussian quadrature is $(2n+1)$, there is

$$\int_a^b H(x)\mathrm{d}x = \sum_{k=0}^{n} A_k H(x_k) = \sum_{k=0}^{n} A_k f(x_k)$$

So

$$\begin{aligned} R(f) &= \int_a^b f(x)\mathrm{d}x - \sum_{k=0}^{n} A_k f(x_k) \\ &= \int_a^b f(x)\mathrm{d}x - \int_a^b H(x)\mathrm{d}x = \int_a^b [f(x) - H(x)]\mathrm{d}x \\ &= \int_a^b \frac{f^{(2n+2)}(\eta)}{(2n+2)!}W_{n+1}^2(x)\mathrm{d}x, \quad \eta \in (a,b) \end{aligned}$$

Since $W_{n+1}^2(x)$ keeps sign in $[\ a,b]$, applying Weighted Mean Value Theorem for Integrals, we have

$$R(f) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}\int_a^b W_{n+1}^2(x)\mathrm{d}x, \quad \xi \in [a,b]$$

□

6.4.3 Stability and Convergence

Theorem 43. *The coefficients $A_k (k = 0, 1, \cdots, n)$ of Gaussian formula are positive.*

Proof Let

$$L_k(x) = \prod_{\substack{j=0 \\ j \neq k}}^{n} \frac{x - x_j}{x_k - x_j} \quad (k = 0, 1, \cdots, n)$$

which is polynomial of degree n. Then the Gaussian quadrature is exact for the polynomial $l_k^2(x)$ of degree $2n$, i.e.

$$\int_a^b l_k^2(x)\mathrm{d}x = \sum_{i=0}^{n} A_i l_k^2\left(x_i\right).$$

Since

$$l_k\left(x_i\right) = \delta_{ki} = \begin{cases} 1 & (i = k) \\ 0 & (i \neq k), \end{cases}$$

then

$$\int_a^b l_k^2(x)\mathrm{d}x = A_k.$$

So $A_k > 0 (k = 0, 1, \cdots, n)$.

□

Theorem 44. *The Gaussian quadrature $\int_a^b f(x)\mathrm{d}x \approx \sum\limits_{k=0}^{n} A_k f\left(x_k\right)$ is stable.*

Proof By

$$\begin{aligned} \left|I_n(f) - I_n(\tilde{f})\right| &= \left|\sum_{k=0}^{n} A_k \left[f\left(x_k\right) - \tilde{f}_k\right]\right| \\ &\leqslant \sum_{k=0}^{n} \left|A_k\right| \cdot \left|f\left(x_k\right) - \tilde{f}_k\right|, \end{aligned}$$

and Th. 43, we have

$$\begin{aligned} \left|I_n(f) - I_n(\tilde{f})\right| &\leqslant \sum_{k=0}^{n} A_k \left|f\left(x_k\right) - \tilde{f}_k\right| \\ &\leqslant \left(\max_{0 \leqslant k \leqslant n} \left|f\left(x_k\right) - \tilde{f}_k\right|\right) \sum_{k=0}^{n} A_k. \end{aligned}$$

Since $\sum\limits_{k=0}^{n} A_k = b - a$, we have

$$|I_n(f) - I_n(\tilde{f})\Big| \leqslant (b - a) \max_{0 \leqslant k \leqslant n}\Big| f\left(x_k\right) - \tilde{f}_k \mid.$$

For any $\varepsilon > 0$, if

$$\max_{0 \leq k < n} \left| f(x_k) - \widetilde{f}_k \right| < \frac{\varepsilon}{b-a}$$

there is $\left| I_n(f) - I_n(\widetilde{f}) \right| \leqslant \varepsilon$. $\square$

Let

$$I_n(f) = \sum_{k=0}^{n} A_k^{(n)} f\left(x_k^{(n)}\right).$$

Definition 40. *The quadrature is said to be* **stable** *if for any* $\varepsilon > 0$, *the positive integer* N *exists in which* $|I(f) - I_n(f)| < \varepsilon$, *for* $n \geqslant N$.

Theorem 45. *The Gaussian quadrature is stable for any continuous function on* $[a, b]$.

6.5 Numerical Differentiation

The derivative of the function f at x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

This formula gives an obvious way to generate an approximation to $f'(x_0)$; simply compute

$$\frac{f(x_0 + h) - f(x_0)}{h}$$

for small values of h. Although this may be obvious, it is not very successful, due to our old nemesis round-off error. But it is certainly a place to start. A simple way to approximate $f'(x_0)$ to use divided difference:

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h} \tag{6.63}$$

which is called **forward-difference formula**. Similarly, there are two another formulas called **backward-difference formula** and **centered-difference formula**

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}, \tag{6.64}$$

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0 - h)}{2h}, \tag{6.65}$$

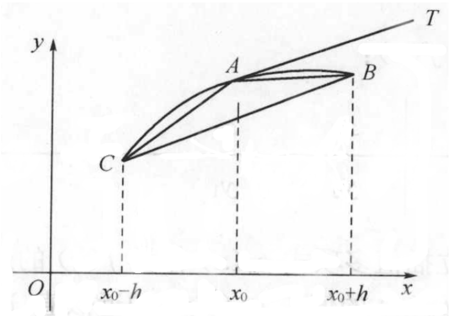


FIGURE 6.1
Numerical Differentiation

or

$$D(h) = \frac{f(x_0+h) - f(x_0-h)}{2h}. \tag{6.66}$$

From the figure, we can see the centered-difference is better. Next we will use Taylor's expansion to analyze the error. From the Taylor expansion, we have

$$\begin{aligned} f(x_0 \pm h) =& f(x_0) \pm hf'(x_0) + \frac{h^2}{2!}f''(x_0) \pm \frac{h^3}{3!}f'''(x_0) + \frac{h^4}{4!}f^{(4)}(x_0) \\ & \pm \frac{h^5}{5!}f^{(5)}(x_0) + \cdots \end{aligned}$$

Taking it to Eq. (6.66), there is

$$D(h) = f'(x_0) + \frac{h^2}{3!}f'''(x_0) + \frac{h^4}{5!}f^{(5)}(x_0) + \cdots$$

So the error

$$f'(x_0) - D(h) = -\frac{h^2}{3!}f'''(x_0) - \frac{h^4}{5!}f^{(5)}(x_0) - \cdots \tag{6.67}$$

In general, if the error is $O(h^n)$, we call the formula an **order** n approximation. The forward-difference formula and backward-difference formula are first-order methods for approximating the first derivative and the centered-difference formula is a second-order method.

To obtain general derivative approximation formulas, suppose that $x_0, x_1, ..., x_n$ are $(n+1)$ distinct numbers in some interval [a,b] and $f \in C^{n+1}[a,b]$. We can use interpolating polynomial to approximate the function f, and differentiating this expression gives

$$f'(x) \approx p_n'(x), \tag{6.68}$$

which is called an **(n+1)-point formula** to approximate $f'(x)$. The error is

$$f'(x) - p_n'(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} W_{n+1}'(x) + \frac{W_{n+1}(x)}{(n+1)!} \frac{\mathrm{d}}{\mathrm{d}x} f^{(n+1)}(\xi), \tag{6.69}$$

where $\xi = \xi(x) \in (\min\{x, x_0, \cdots, x_n\}, \max\{x, x_0, \cdots, x_n\})$, $W_{n+1}(x) = (x - x_0)(x - x_1) \cdots (x - x_n)$.

We again have a problem estimating the truncation error unless x is one of the numbers x_k. In this case, $\frac{\mathrm{d}}{\mathrm{d}x} f^{(n+1)}(\xi) = 0$ and the error becomes

$$f'(x_k) - p_n'(x_k) = \frac{f^{(n+1)}(\xi)}{(n+1)!} W_{n+1}'(x_k) \tag{6.70}$$

We first derive some useful formulas and consider aspects of their errors.

(1)**Two-point Formula**

For the given data

x	x_0	x_1
y	$f(x_0)$	$f(x_1)$

the linear interpolating polynomial at x_0, x_1 is

$$p_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1).$$

Let $h = x_1 - x_0$, and

$$p_1'(x) = \frac{1}{h}[-f(x_0) + f(x_1)].$$

These formulas can also be expressed as

$$p_1'(x_0) = \frac{1}{h}[f(x_1) - f(x_0)], \tag{6.71}$$

$$p_1'(x_1) = \frac{1}{h}[f(x_1) - f(x_0)], \tag{6.72}$$

which are forward and backward formulas.

The errors are

$$f'(x_0) - p_1'(x_0) = \frac{f''(\xi_0)}{2!} W_2'(x_0) = \frac{f''(\xi_0)}{2}(x_0 - x_1) = -\frac{h}{2} f''(\xi_0),$$

$$f'(x_1) - p_1'(x_1) = \frac{f''(\xi_1)}{2!} W_2'(x_1) = \frac{f'(\xi_1)}{2}(x_1 - x_0) = \frac{h}{2} f''(\xi_1).$$

So the two-point formulas are expressed

$$f'(x_0) = \frac{1}{h}[f(x_1) - f(x_0)] - \frac{h}{2} f''(\xi_0) \quad (x_0 < \xi_0 < x_1) \tag{6.73}$$

$$f'(x_1) = \frac{1}{h}[f(x_1) - f(x_0)] + \frac{h}{2} f''(\xi_1) \quad (x_0 < \xi_1 < x_1) \tag{6.74}$$

(2) **Three-point formula**
For the given data

x	x_0	x_1	x_2
y	$f(x_0)$	$f(x_1)$	$f(x_2)$

the interpolating polynomial of degree 2 at x_0, x_1, x_2 is

$$\begin{aligned} p_2(x) =& \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \\ &+ \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) . \end{aligned}$$

Then

$$\begin{aligned} p_2'(x) =& \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)} f(x_1) \\ &+ \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)} f(x_2) . \end{aligned}$$

If the nodes are equally spaced, that is $x_2 - x_1 = x_1 - x_0 = h$.

$$\begin{cases} p_2'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_1) - f(x_2)\right] \\ p_2'(x_1) = \frac{1}{2h}\left[-f(x_0) + f(x_2)\right] \\ p_2'(x_2) = \frac{1}{2h}\left[f(x_0) - 4f(x_1) + 3f(x_2)\right] \end{cases} \tag{6.75}$$

$$\begin{cases} f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_1) - f(x_2)\right] + \dfrac{h^2}{3} f''(\xi_0) \quad (x_0 < \xi_0 < x_2) \\ f'(x_1) = \frac{1}{2h}\left[-f(x_0) + f(x_2)\right] - \dfrac{h^2}{6} f'''(\xi_1) \\ f'(x_2) = \frac{1}{2h}\left[f(x_0) - 4f(x_1) + 3f(x_2)\right] + \dfrac{h^2}{3} f'''(\xi_2) \quad\ (x_0 < \xi_1 < x_2) \end{cases} \tag{6.76}$$

By the interpolating polynomial $p_n(x)$ to approximate to $f(x)$, numerical methods for high-order derivative can be obtained

$$f^{(k)}(x) \approx p_n^{(k)}(x) \quad (k = 1, 2, \cdots).$$

Theorem 46. *Suppose $f(x) \in C^{n+1}[a,b]$, and $p_n(x)$ is an interpolating polynomial of the function f about $a \leqslant x_0 < x_1 < \cdots < x_n \leqslant b$. For any $x \in [a,b]$, there is*

$$f^{(k)}(x) - p_n^{(k)}(x) = \frac{f^{(n+1)}(\xi)}{(n-k+1)!}\left(x - x_0^{(k)}\right)\left(x - x_1^{(k)}\right)\cdots\left(x - x_{n-k}^{(k)}\right) \\ (k = 0, 1, 2, \cdots) \tag{6.77}$$

where $\xi \in (a,b)$ dependent on k and x, and $x_i < x_i^{(k)} < x_{i+k} (i = 0, 1, \cdots, n - k)$.

6.6 Exercise

1. Derive the following quadrature formulas and give the truncation errors:

   (1) **Left-side Rectangle Rule** : $\int_a^b f(x)\mathrm{d}x \approx f(a)(b-a)$;

   (2) **Right-side Rectangle Rule**: $\int_a^b f(x)\mathrm{d}x \approx f(b)(b-a)$;

   (3) **Midpoint Rule**: $\int_a^b f(x)\mathrm{d}x \approx f\left(\frac{a+b}{2}\right)(b-a)$.

2. Find the degree of precision of the following quadrature formulas:

   (1) $\int_0^1 f(x)\mathrm{d}x \approx \frac{1}{4}f(0)+\frac{3}{4}f\left(\frac{2}{3}\right)$;

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

3. Find the constants so that the following quadrature formulas have the highest possible degree of precision.

   (1) $\int_{-1}^1 f(x)\mathrm{d}x \approx \frac{1}{3}[f(-1)+2f(\alpha)+3f(\beta)]$;

   (2) $\int_a^b f(x)\mathrm{d}x \approx \frac{b-a}{2}[f(a)+f(b)]+\alpha(b-a)^2\left[f'(a)-f'(b)\right]$;

   (3) $\int_{-1}^1 f(x)\mathrm{d}x \approx Af(-x_0)+Bf(0)+Af(x_0)$.

4. Given the function f at the following values,

x	1.6	1.8	2.0	2.2	2.4	2.6
$f(x)$	4.953	6.050	7.389	9.025	11.023	13.464
x	2.8	3.0	3.2	3.4	3.6	3.8
$f(x)$	16.445	20.086	24.533	29.964	36.598	44.701

   approximate $\int_{1.8}^{3.4} f(x)\mathrm{d}x$ by Composite Trapezoid rule and Composite Simpson's rule.

5. Determine the values of n and h required to approximate $\int_2^8 \frac{1}{x}\,\mathrm{d}x = \ln 4$ to within $\frac{1}{2}\times 10^{-5}$ using Composite Trapezoid rule.

6. Determine the values of n required to approximate $\int_2^8 \frac{1}{x}\,\mathrm{d}x$ to within $\frac{1}{2}\times 10^{-5}$ by Romberg integration method.

7. Suppose $I=\int_0^1 \frac{\sin x}{2\sqrt{x}}\,\mathrm{d}x$.

   (1) Can Romberg integration method be applied to approximate I?

   (2) Let $x=t^2$, then $I=\int_0^1 \sin t^2\,\mathrm{d}t$. Why we can use Romberg integration method to approximate I?

8. Use three-point Gaussian formula to approximate $I=\int_0^1 \mathrm{e}^{-x}\,\mathrm{d}x$.

9. Suppose $f(x) = \tan x$ and

x	1.20	1.24	1.28	1.32	1.36
$f(x)$	2.57215	2.91193	3.34135	3.90335	4.67344

   Use centered-difference formula to approximate $f'(1.28)$ and determine bound for the approximation errors.

10. Suppose the interpolating polynomial $L_4(x)$ of degree 4 to approximate the function f about $x_0 - 2h, x_0 - h, x_0, x_0 + h, x_0 + 2h$. Prove

    (1) $L_4'(x_0) = \frac{4}{3} D(x_0, h) - \frac{1}{3} D(x_0, 2h)$;

    (2) $f'(x_0) - L_4'(x_0) = \frac{4}{5!} f^{(5)}(\xi) h^4, \quad \xi \in (x_0 - 2h, x_0 + 2h)$.