Chapter 7 Numerical Differentiation

Baodong LIU
baodong@sdu.edu.cn

- The need often arises for evaluating the **definite integral** (定积分) of a function that has no explicit **antiderivative** （原函数）or whose antiderivative is not easy to obtain.
- The basic method involved in approximating

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

is called **numerical quadrature**—数值积分

Definition 7.1:

- The so called **numerical quadrature** is **using a sum of the type**

$$\sum_{i=0}^{n} a_i f(x_i)$$

to approximate

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

The methods of quadrature in this section are based on the **interpolation polynomials—-Lagrange Interpolation** given in chapter 3.

Steps To Construct The Numerical Quadrature

STEP 1:

We first select a set of distinct nodes $\{x_0, x_1, \cdots, x_n\}$ from the interval $[a, b]$, and then construct the Lagrange interpolation polynomial, such that

$$\begin{aligned} f(x) &= P_n(x) + R_n(x) \\ &= \sum_{i=0}^{n} f(x_i) L_i(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i), \end{aligned}$$

where

$$L_i(x) = \prod_{j=o, j \neq i}^{n} \frac{x - x_i}{x_i - x_j}, \quad i = 0, 1, \cdots, n$$

STEP 2

Then we integrate the equation over $[a, b]$ on each sides to obtain

$$\begin{aligned}
&\int_a^b f(x)\mathrm{d}x \\
&= \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x)dx + + \int_a^b \prod_{i=0}^{n}(x - x_i)\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\mathrm{d}x \\
&= \sum_{i=0}^{n} a_i f(x_i) + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x - x_i)f^{(n+1)}(\xi(x))\mathrm{d}x
\end{aligned}$$

where $\xi(x)$ is in $[a, b]$ for each x and

$$a_i = \int_a^b L_i(x)\mathrm{d}x,$$

for each $i = 0, 1, \cdots, n$.

The Numerical Quadrature Formula

- The Numerical Quadrature Formula is, therefore

$$I_n(f) = \sum_{i=0}^{n} a_i f(x_i),$$

with error given by

$$E_n(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i) f^{(n+1)}(\xi(x)) \mathrm{d}x.$$

- Next let us first consider formulas produced by using first and second Lagrange polynomials with equally spaced nodes.

Trapezoidal rule (n=1)—梯形公式

- To derive the Trapezoidal rule for approximating $\int_a^b f(x)dx$,
- Let $x_0 = a$, $x_1 = b$, $h = b - a$, and use the linear Lagrange polynomial:

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1).$$

- Then

$$\begin{aligned} \int_a^b f(x)\mathrm{d}x &= \int_{x_0}^{x_1} \Big[\frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)\Big]\mathrm{d}x \\ &\quad + \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\mathrm{d}x \end{aligned}$$

Trapezoidal rule

- Integrating each term, we have the known Trapezoidal Rule:

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

- **Trapezoidal rule:**

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

  where $x_0 = a, x_1 = b$, and $h = b - a, a < \xi < b$.

- **Notes:** since the Trapezoidal rule involves f'',the rule gives the exact result when applied to any function whose second derivative is identically zero, that is , **any polynomial of degree 1 or less.**

Simpson's rule (n=2)

- Let $x_0 = a, x_1 = a + h = \frac{a+b}{2}, x_2 = b$, where $h = \frac{(b-a)}{2}$.
- With the second Lagrange polynomial results from integrating over $[a, b]$, we have

$$\begin{aligned}\int_a^b f(x)\mathrm{d}x \;&=\; \int_{x_0}^{x_2} \Big[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0) \\ &+\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1) \\ &+\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)\Big]\mathrm{d}x \\ &+\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6}f^{(3)}(\xi(x))\mathrm{d}x\end{aligned}$$

Note:

- Deriving Simpson's rule in this manner, however, provides only an $O(h^4)$ error term involving $f^{(3)}$.
- By approaching the problem in another way, a higher-order term involving $f^{(4)}$ can be derived.
- To illustrate this alternative formula, suppose that f is expanded in the third Taylor polynomial about x_1.

- Then for each x in $[x_0, x_2]$, a number $\xi(x)$ in (x_0, x_2) exists with

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

- Integrate this equation on $[x_0, x_2]$, we get

$$
\begin{aligned}
\int_{x_0}^{x_2} f(x)\mathrm{d}x &= \Big[f(x_1)(x - x_1) + \frac{f'(x_1)}{2}(x - x_1)^2 \\
&\quad + \frac{f''(x_1)}{6}(x - x_1)^3 + \frac{f'''(x_1)}{24}(x - x_1)^4\Big]_{x_0}^{x_2} \\
&\quad + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4\mathrm{d}x \qquad (2)
\end{aligned}
$$

- Since $(x - x_1)^4$ is never negative on $[x_0, x_2]$,the Weighted Mean Value Theorem for Integrals implies that

$$
\begin{aligned}
\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4 dx &= \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4 \mathrm{d}x \\
&= \frac{f^{(4)}(\xi_1)}{120}(x-x_1)^5\Big|_{x_0}^{x_2}
\end{aligned}
$$

for some number ξ_1 in (x_0, x_2).

- However, $h = x_2 - x_1 = x_1 - x_0$, so

$$(x_2 - x_1)^2 - (x_0 - x_1)^2 = (x_2 - x_1)^4 - (x_0 - x_1)^4 = 0.$$

whereas

$$(x_2 - x_1)^3 - (x_0 - x_1)^3 = 2h^3$$

and

$$(x_2 - x_1)^5 - (x_0 - x_1)^5 = 2h^5.$$

- Consequently, Eq.(2) can be rewritten as

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{60}h^5.$$

If we now replace $f''(x_1)$ by the approximation given in Eq.(4.9) of Section 4.1, we have

$$\begin{aligned}\int_{x_0}^{x_2} f(x)\,dx &= 2hf(x_1) + \frac{h^3}{3}\Big\{\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] \\ &\quad - \frac{h^2}{12}f^{(4)}(\xi_2)\Big\} + \frac{f^{(4)}(\xi_1)}{60}h^5 \\ &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \\ &\quad - \frac{h^5}{12}\Big[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\Big]\end{aligned}$$

- It can be shown by alternative methods that the value ξ_1 and ξ_2 in this expression can be replaced by a common value ξ in (x_0, x_2).
- This gives Simpson's rule. **Simpson's rule**:

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

or

$$\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4f(\frac{a+b}{2}) + f(b)] - \frac{h^5}{90}f^{(4)}(\xi),$$

where $x_0 = a, x_2 = b, x_1 = a + h$,and $h = \frac{b-a}{2}, a < \xi < b$.

Degree of Accuracy

Definition 7.2: degree of accuracy,or precision

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

Degree of Accuracy

- The Trapezoidal($n = 1$) rule:

$$\begin{aligned}\int_a^b f(x)\mathrm{d}x &= \frac{h}{2}[f(x_0)+f(x_1)] - \frac{h^3}{12}f''(\xi) \\ &= \frac{b-a}{2}[f(a)+f(b)] - \frac{h^3}{12}f''(\xi), \quad (3)\end{aligned}$$

  where $x_0 = a, x_1 = b$, and $h = b - a, a < \xi < b$, has degree or accuracy 1.

- The Simpson's($n = 2$) rules

$$\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4f(\frac{a+b}{2}) + f(b)] - \frac{h^5}{90}f^{(4)}(\xi),$$

  where $x_0 = a, x_2 = b, x_1 = a + h$,and $h = \frac{b-a}{2}, a < \xi < b$. have degree of precision 3.

Newton-Cotes formulas–牛顿-科斯特公式

- The **Trapezoidal** and **Simpson's rules** are examples of a class of methods known as **Newton-Cotes formulas–牛顿-科斯特公式**.
- There are two types of Newton-Cotes formulas,**open and closed**.
- The **(n+1)-point Newton-Cotes formula** uses nodes $x_i = x_0 + ih$, for $i = 0, 1, \cdots, n$.

General forms of Newton-Cotes Formula

- **Closed Newton- Cotes Formula:**

$$a = x_0 < x_1 < \cdots < x_n = b,$$

with

$$x_i = x_0 + ih, i = 1, 2, \cdots, n,$$

where $h = (b - a)/n$.

- Then

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

where

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

- **Open Newton- Cotes Formula:**

$$a = x_{-1} < x_0 < x_1 < \cdots < x_n < x_{n+1} = b,$$

with

$$x_i = x_0 + ih, i = 1, 2, \cdots, n,$$

where $h = (b-a)/(n+2)$.

- Then **Open Newton- Cotes Formula** assumes the form

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

where

$$a_i = \int_{x_{-1}}^{x_{n+1}} L_i(x)dx = \int_{x_{-1}}^{x_{n+1}} \prod_{j=0, j\neq i}^{n} \frac{(x-x_j)}{(x_i-x_j)} dx.$$

Theorem 7.3:Closed Newton-Cotes formula

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point closed Newton-Cotes formula with $x_0 = a, x_n = b$ and $h = (b-a)/n$.

- if n is even(– 偶数) and $f \in C^{n+2}[a,b]$, there exists $\xi \in (a,b)$ for which

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

- If n is odd (– 奇数) and $f \in C^{n+1}[a,b]$, there exists $\xi \in (a,b)$ for which

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

Notes:

- When n is an even integer, the degree of precision is $n+1$, although the interpolation polynomial is of degree at most n.
- In case n is odd, the second part of the theorem shows that the degree of precision is only n.

Some common Newton-Cotes formula

- Some of the common **closed Newton-Cotes formula** with their error terms are as follows.
- **Case:** $n = 1$:**Trapezoidal rule**

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

where $a = x_0 < \xi < x_1 = b, h = b - a$.

- **Case:** $n = 2$:**Simpson's rule**

$$\begin{aligned}
&\int_{x_0}^{x_2} f(x)\,dx \\
&= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi) \\
&= \frac{h}{3}[f(a) + 4f(\frac{a+b}{2}) + f(b)] - \frac{h^5}{90}f^{(4)}(\xi)
\end{aligned}$$

where $a = x_0 < \xi < x_2 = b, h = \frac{b-a}{2}$.

- **Case:** $n = 3$:**Simpson's Three-Eighths rule**

$$
\begin{aligned}
&\int_{x_0}^{x_3} f(x)dx \\
&= \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi) \\
&= \frac{3h}{8}[f(a) + 3f(a+h) + 3f(a+2h) + f(b)] \\
&- \frac{3h^5}{80} f^{(4)}(\xi)
\end{aligned}
$$

where $a = x_0 < \xi < x_3 = b, h = \frac{b-a}{3}$.

- **Case:** $n = 4$:

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

where $a = x_0 < \xi < x_4 = b, h = \frac{b-a}{4}$.

Open Newton-Cotes formula

- In the open Newton-Cotes formula, the nodes

$$x_i = x_0 + ih$$

  are used for each $i = 0, 1, \ldots, n$, where $h = (b - a)/(n + 2)$ and $x_0 = a + h$.
- This implies that

$$x_n = b - h,$$

  so we label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$.
- Open formula contain all the nodes used for approximation within the open interval (a, b).

The formula become

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

where again

$$a_i = \int_{x_{-1}}^{x_{n+1}} L_i(x)\mathrm{d}x = \int_a^b L_i(x)\mathrm{d}x.$$

Theorem 7.4: Open Newton-Cotes formula

- $(n+1)$-point open Newton-Cotes formula with $x_{-1} = a, x_{n+1} = b$ and $h = (b-a)/(n+2)$.
- If n is even and $f \in C^{n+2}[a,b]$, there exists $\xi \in (a,b)$ for which

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

- If n is odd and $f \in C^{n+1}[a,b]$. There exists $\xi \in (a,b)$ for which

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

Some common **open Newton-Cotes** formulas

- $n = 0$:**Midpoint Rule**

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

  where $x_{-1} < \xi < x_1$.

- **Case:** $n = 1$:

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

  where $x_{-1} < \xi < x_2$.

- **Case** $n = 2$:

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

  where $x_{-1} < \xi < x_3$.

- **Case:** $n = 3$:

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

where $x_{-1} < \xi < x_4$.

7.2 Composite Numerical Integration

1. It is unsuitable for use over **large integration intervals**.
2. High-degree Newton-Cotes formulas require to evaluate the values of the coefficients in these formulas which are difficult to obtain.
3. The Newton-Cotes formulas are based on interpolatory polynomials that use equally spaced nodes, a procedure that inaccurate over large intervals because of the oscillatory nature of high-degree polynomials.

Example

- Consider finding an approximation to

$$\int_0^4 e^x\,dx = e^4 - e^0 = 53.59815.$$

- Simpson's rule with $h = 2$ gives

$$\int_0^4 e^x\,dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958$$

- In this case , the error is -3.17143 is far larger than we would normally accept.

- To apply a piecewise technique to this problem,divide $[0, 4]$ into $[0, 2] \cup [2, 4]$ and use Simpson's rule twice with $h = 1$;

$$\begin{aligned}\int_0^4 e^x\,dx &= \int_0^2 e^x\,dx + \int_2^4 e^x\,dx \\ &\approx \frac{1}{3}[e^0 + 4e + e^2] + \frac{1}{3}[e^2 + 4e^3 + e^4] \\ &= \frac{1}{3}[e^0 + 4e + 2e^2 + 4e^3 + e^4] = 53.86385.\end{aligned}$$

- The error has been reduced to -0.26570.

- Subdivide the intervals $[0,2]$ and $[2,4]$ into

$$[0,1] \cup [1,2] \cup [2,3] \cup [3,4],$$

- use Simpson's rule with $h = 1/2$ for each subintervals:

$$\begin{aligned}
\int_0^4 e^x\,dx &= \int_0^1 e^x\,dx + \int_1^2 e^x\,dx + \int_2^3 e^x\,dx + \int_3^4 e^x\,dx \\
&\approx \frac{1}{6}[e^0 + 4e^{1/2} + e] + \frac{1}{6}[e + 4e^{3/2} + e^2] + \\
&\quad + \frac{1}{6}[e^2 + 4e^{5/2} + e^3] + \frac{1}{6}[e^3 + 4e^{7/2} + e^4] \\
&= \frac{1}{6}[e^0 + 4e^{1/2} + 2e + 4e^{3/2} + 2e^2 \\
&\quad + 4e^{5/2} + 2e^3 + 4e^{7/2} + e^4] = 53.61622.
\end{aligned}$$

- The error for this approximation becomes -0.01807.

- To generalize this procedure,choose an even integer (偶数) n. Subdivide the interval $[a, b]$ into n subintervals:

$$[a, b] = [x_0, x_2] \cup [x_2, x_4] \cup \cdots \cup [x_{n-2}, x_n]$$

- Apply **Simpson's Rule** on each consecutive pair of subintervals $[x_{2j-2}, x_{2j}], j = 1, 2, \cdots, n/2$:

$$\int_{x_{2j-2}}^{x_{2j}} f(x)\,dx$$
$$= \frac{h}{3}[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90} f^{(4)}(\xi_j),$$

where $x_{2j-2} < \xi_j < x_{2j}, h = (b-a)/n$,and $x_j = a + jh$ for each $j = 0, 1, ..., n$.

Thus

$$\int_a^b f(x)\mathrm{d}x = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)\mathrm{d}x$$

$$= \sum_{j=1}^{n/2} \Big\{ \frac{h}{3}[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90} f^{(4)}(\xi_j) \Big\}$$

$$= \frac{h}{3}\Big[f(x_0) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\Big]$$

$$-\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

Error analysis

- The error associated with this approximation is

$$E(f) = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j),$$

  where $x_{2j-2} < \xi_j < x_{2j}$ for each $j = 1, 2, ..., n/2$.
- If $f \in C^4[a, b]$, the Extreme Value Theorem implies that $f^{(4)}$ assumes its maximum and minimum in $[a, b]$.
- Since

$$\min_{x\in[a,b]} f^{(4)}(x) \leq f^{(4)}(\xi_j) \leq \max_{x\in[a,b]} f^{(4)}(x).$$

we have

$$\frac{n}{2}\min_{x\in[a,b]} f^{(4)}(x) \le \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \frac{n}{2}\max_{x\in[a,b]} f^{(4)}(x)$$

and

$$\min_{x\in[a,b]} f^{(4)}(x) \le \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x).$$

- By the Intermediate Value Theorem,there is a $\mu \in (a, b)$ such that

$$f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

Thus

$$E(f) = -\frac{h^5}{180} n f^{(4)}(\mu).$$

- Since $n = (b - a)/h$, so

$$E(f) = -\frac{b-a}{180} h^4 f^{(4)}(\mu).$$

- These observations produce the following result.

Theorem 7.5

- Let $f \in C^4[a,b]$, n be even. $h = (b-a)/n$, and $x_j = a + jh$ for each $j = 0, 1, ..., n$.
- There exists a $\mu \in (a,b)$ for which the **Composite Simpson's rule** for n subintervals can be written with its error term as

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

ALGORITHM 7.1—The Composite Simpson's rule

To approximate the integer $I = \int_a^b f(x)dx$:

INPUT endpoints a,b;even positive integer n.

OUTPUT approximation XI to I.

Step 1 Set $h = (b-a)/n$.

Step 2 Set

$$\begin{aligned} XI0 &= f(a) + f(b); \\ XI1 &= 0; (\texttt{Summation of} f(x_{2j-1})); \\ XI2 &= 0. (\texttt{Summation of} f(x_{2j})). \end{aligned}$$

Step 3 For $i = 1, 2, \cdots, n-1$ do Step 4 and 5.

Step 4 Set $X = a + ih$.

Step 5 If i is even, then set $XI2 = XI2 + f(x)$, else set $XI1 = XI1 + f(x)$.

Step 6 Set $XI = h(XI0 + 2XI2 + 4XI1)/3$.

Step 7 OUTPUT(XI); STOP.

Composite Trapezoidal Rule

Since the Trapezoidal rule requires only one interval for each application,the integer n can be either odd or even .

Theorem 7.6—Composite Trapezoidal Rule

- Let $f \in C^2[a,b], h = (b-a)/n$,and $x_j = a + jh$ for each $j = 0, 1, ..., n$.
- There exists a $\mu \in (a,b)$ for which the **Composite trapezoidal rule** for n subintervals can be written with its error term as

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

Composite Midpoint rule

Theorem 7.7–Composite Midpoint Rule

- Let $f \in C^2[a, b]$, n be even.$h = (b - a)/(n + 2)$, and $x_j = a + (j + 1)h$ for each $j = -1, 0, 1, ..., n + 1$.
- There exists a $\mu \in (a, b)$ for which the **Composite trapezoidal rule**for $n + 2$ subintervals can be written with its error term as

$$\int_a^b f(x)dx = 2h \sum_{j=0}^{n/2} f(x_{2j}) + \frac{b-a}{6} h^2 f''(\mu).$$

EXAMPLE

- Consider approximating $\int_0^\pi \sin x dx$ with an absolute error less than 0.00002, using the Composite Simpson's rule.
- The Composite Simpson's rule gives

$$\int_0^\pi \sin x dx = \frac{h}{3}\left[2\sum_{j=1}^{(n/2)-1}\sin x_{2j} + 4\sum_{j=1}^{n/2}\sin x_{2j-1}\right] - \frac{\pi h^4}{180}\sin\mu$$

- Since the absolute error is to be less than 0.00002,the inequality

$$|\frac{\pi h^4}{180}\sin\mu| \leq \frac{\pi h^4}{180} = \frac{\pi^5}{180 n^4} < 0.00002$$

is used to determine n and h.Completing these calculations gives $n > 18$.
- If $n = 20$,then $h = \pi/20$, and the formula gives

$$\begin{aligned}\int_0^\pi \sin x dx &\approx \frac{\pi}{60}[2\sum_{j=1}^{9}\sin(\frac{j\pi}{10}) + 4\sum_{j=1}^{10}\sin(\frac{(2j-1)\pi}{20})] \\ &= 2.000006\end{aligned}$$

- To be assured of this degree of accuracy using the Composite Trapezoidal rule requires that

$$\left|\frac{\pi h^2}{12}\sin\mu\right| \leq \frac{\pi h^2}{12} = \frac{\pi^3}{12n^2} < 0.00002$$

or that $n > 360$.

- Since this is many more calculations than are needed for the Composite Simpson's rule.

- For comparison purposes,the Composite Trapezoidal's rule with $n = 20$ and $h = \pi/20$ gives

$$
\begin{aligned}
\int_0^{\pi} \sin x dx &\approx \frac{\pi}{40}\Big[\sin 0 + 2\sum_{j=1}^{19}\sin\Big(\frac{j\pi}{20}\Big) + \sin\pi\Big] \\
&= \frac{\pi}{40}\Big[2\sum_{j=1}^{19}\sin\Big(\frac{j\pi}{20}\Big)\Big] \\
&= 1.9958860
\end{aligned}
$$

- The exact answer is 2,so Simpson's rule with $n = 20$ gave an answer well within the required error bound,whereas the Trapezoidal rule with $n = 20$ clearly did not.

- **Romberg integration**:
  1. uses the Composite Trapezoidal rule to give **preliminary approximations**
  2. then applies the Richardson extrapolation process to obtain **improvements** of the approximations.

- To begin the presentation of the Romberg integration scheme,recall that the Composite Trapezoidal rule for approximating the Romberg integration scheme.
- Recall that the Composite Trapezoidal rule for approximating the integral of a function f on an interval $[a, b]$ using m subintervals is

$$\begin{aligned}\int_a^b f(x)dx &= \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{m-1} f(x_j) + f(b)\right] \\ &\quad -\frac{(b-a)}{12}h^2 f''(\mu).\end{aligned}$$

where $a < \mu < b, h = \frac{b-a}{m}$ and

$$x_j = a + jh,\ j = 0, 1, ..., m.$$

- We first obtain Composite Trapezoidal rule approximations with

$$m_1 = 1, m_2 = 2, m_3 = 4, ..., m_n = 2^{n-1},$$

where n is a positive integer.

- The values of the step size h_k corresponding to m_k are

$$h_k = \frac{b-a}{m_k} = \frac{b-a}{2^{k-1}}.$$

- With this notation the Trapezoidal rule becomes

$$\int_a^b f(x)dx = \frac{h_k}{2}\Big[f(a) + 2\Big(\sum_{i=1}^{2^{k-1}-1} f(a+ih_k)\Big) + f(b)\Big] - \frac{(b-a)}{12}h_k^2 f''(\mu_k). \quad (4)$$

where $\mu_k \in (a, b)$.

- If the notation $R_{k,1}$ is introduced to denote the portion of (4) used for the trapezoidal approximation.
- Then:

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

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

for each $k = 2, 3, ..., n$.

- If can be shown,although not easily, that if $f \in C^{\infty}[a, b]$, the Composite Trapezoidal rule can be written with an alternative error term in the form

$$\int_a^b f(x)\,dx - R_{k,1} = \sum_{i=1}^{\infty} K_i h_k^{2i} = K_1 h_k^2 + \sum_{i=2}^{\infty} K_i h_k^{2i}, \quad (5)$$

where K_i for each i is independent of h_k and depends only on $f^{(2i-1)}(a)$ and $f^{(2i-1)}(b)$.

- With the Composite Trapezoidal rule in this form,we can eliminate the term involving h_k^2 by combining this equation with its counterpart with h_k replaced by $h_{k+1} = h_k/2$:

$$\begin{aligned} \int_a^b f(x)\,dx - R_{k+1,1} &= \sum_{i=1}^{\infty} K_i h_{k+1}^{2i} = \sum_{i=1}^{\infty} \frac{K_i h_k^{2i}}{2^{2i}} \\ &= \frac{K_1 h_k^2}{4} + \sum_{i=2}^{\infty} \frac{K_i h_k^{2i}}{4^i} \qquad (6) \end{aligned}$$

Subtracting equation (6) from 4 times (5) and simplifying gives the $O(h_k^4)$ formula

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

- Extrapolation can not be applied to this formula to obtain an $O(h_k^6)$ result, and so on.
- To simplify the notation, we define

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

  for each $k = 2, 3, ..., n$,
- Apply the Richardson extrapolation procedure to these values.
- Continuing this notation, we have, for each $k = 2, 3, 4, ..., n$ and $j = 2, ..., k$, and $O(h_k^{2j})$ approximation formula defined by

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}. \tag{7}$$

ALGORITHM 5.2 Romberg

To approximate the integer

$$I = \int_a^b f(x)\mathrm{d}x,$$

select an integer $n > 0$.

INPUT endpoints a,b; integer n.

OUTPUT an array R.(Complete R by rows;only the last 2 rows are saved in storage.)

Step 1 Set $h = b - a, R_{1,1} = \frac{h}{2}(f(a) + f(b))$.

Step 2 OUTPUT $(R_{1,1})$.

ALGORITHM 4.2 Romberg

Step 3 For $i = 2, \cdots, n$ do Step $4 - 8$.

Step 4 Set(Approximation from Trapezoidal method.)

$$R_{2,1} = \frac{1}{2}\big[R_{1,1} + h\sum_{k=1}^{2^{i-2}} f(a + (k - 0.5)h)\big].$$

Step 5 For $j = 2, \cdots, i$, set

$$R_{2,j} = R_{2,j-1} + \frac{R_{2,j-1} - R_{1,j-1}}{4^{j-1} - 1}.\ (\textit{Extrapolation.})$$

Step 6 OUTPUT($R_{2,j}$ for $j = 1, 2, \ldots, i$).

Step 7 Set $h = h/2$.

Step 8 For $j = 1, 2, \ldots, i$, set

$$R_{1,j} = R_{2,j}.(\texttt{Update row 1 Of R.})$$

Step 9 STOP.

- The method we discuss is based on the **Composite Simpson's rule**, but the technique is easily modified to use other composite procedures.
- Suppose that we want to approximate

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

to within a specified tolerance $\varepsilon > 0$.

First Step:

- Let $n = 2$, thus $h_1 = h = (b-a)/2$. This procedure by **Composite Simpson's rule** results in the following :

$$\int_a^b f(x)\mathrm{d}x = S(a,b) - \frac{h^5}{90} f^{(4)}(\mu),\ \ \mu \in (a,b). \tag{8}$$

where

$$S(a,b) = \frac{h}{3}[f(a) + 4f(a+h) + f(b)].$$

The Next Step:

Let $n = 4$ and step size $h_2 = (b-a)/4 = h/2$ giving

$$
\begin{aligned}
& \int_a^b f(x)\,dx \\
& = \frac{h_2}{3}\{f(a) + 2f(a+2h_2) + 4[f(a+h_2) \\
& +f(a+3h_2)] + f(b)\} - \frac{h_2^4(b-a)}{180} f^{(4)}(\tilde{\mu}) \\
= \;\; & \frac{h}{6}\Bigg[f(a) + 2f(a+h) + 4f(a+\frac{h}{2}) \\
& +4f(a+\frac{3h}{2}) + f(b)\Bigg] - \left(\frac{h}{2}\right)^4 \frac{(b-a)}{180} f^{(4)}(\tilde{\mu})
\end{aligned} \tag{9}
$$

for some $\tilde{\mu} \in (a, b)$.

- To simplify notation, let

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

and

$$S\left(\frac{a+b}{2}, b\right) = \frac{h}{6}\left[f(a+h) + 4f\left(a + \frac{3h}{2}\right) + f(b)\right]$$

- Then Equation (9) can be rewritten as

$$\int_a^b f(x)dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\mu}). \tag{10}$$

- The error estimation is derived by assuming that $\mu \approx \tilde{\mu}$ or, more precisely, that

$$f^{(4)}(\mu) \approx f^{(4)}(\tilde{\mu}).$$

- The success of the technique depends on the accuracy of this assumption.
- If it is accurate, then equating the integrals in Equations (8) and (10) implies that

$$S\big(a, \frac{a+b}{2}\big) + S\big(a, \frac{a+b}{2}\big) - \frac{1}{16}\big(\frac{h^5}{90}\big) f^{(4)}(\mu)$$
$$\approx S(a, b) - \frac{h^5}{90} f^{(4)}(\mu).$$

so

$$\frac{h^5}{90} f^{(4)}(\mu) \approx \frac{16}{15}\big[S(a, b) - S\big(a, \frac{a+b}{2}\big) - S\big(\frac{a+b}{2}, b\big)\big].$$

- Using this estimate in Eq.(10) produces the error estimation

$$
\begin{aligned}
&\left|\int_a^b f(x)dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \\
&\approx \frac{1}{15}\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right|.
\end{aligned}
$$

- This result means that

$$
S(a, (a+b)/2) + S((a+b)/2, b)
$$

approximates $\int_a^b f(x)$ about 15 times better than it agrees with the known value $S(a,b)$.

- Thus, if

$$
\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < 15\varepsilon, \qquad (11)
$$

- we expect to have

$$\left|\int_a^b f(x)dx - S\big(a, \frac{a+b}{2}\big) - S\big(\frac{a+b}{2}, b\big)\right| < \varepsilon. \quad (12)$$

- So if ε is an acceptable error tolerance.

$$S\big(a, \frac{a+b}{2}\big) + S\big(\frac{a+b}{2}, b\big)$$

is assumed to a sufficiently accurate approximation to

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

General Case with Composite Simpson's Rule:

- Let n be even, thus $h_n = (b-a)/n$.
- By the Composite Simpson's Rule, we have

$$\begin{aligned}\int_a^b f(x)\mathrm{d}x &= \frac{h_n}{3}\left[f(a) + 2\sum_{j=1}^{\frac{n}{2}-1} f(x_{2j}) + 4\sum_{j=1}^{\frac{n}{2}} f(x_{2j-1}) + f(b)\right] \\ &\quad -\frac{b-a}{180} h_n^4 f^{(4)}(\mu) \\ &= S_n - \frac{b-a}{180} h_n^4 f^{(4)}(\mu), \end{aligned} \tag{13}$$

where

$$S_n = \frac{h_n}{3}\left[f(a) + 2S_n^{(1)} + 4S_n^{(2)} + f(b)\right], \tag{14}$$

$$S_n^{(1)} = \sum_{j=1}^{\frac{n}{2}-1} f(x_{2j}) = f(x_2) + f(x_4) + \cdots + f(x_{n-2})$$

$$S_n^{(2)} = \sum_{j=1}^{\frac{n}{2}} f(x_{2j-1}) = f(x_1) + f(x_3) + \cdots + f(x_{n-1})$$

- Next let $h_{2n} = (b-a)/2n = h_n/2$
- Again uses the Composite Simpson's Rule, we can drive

$$\begin{aligned}\int_a^b f(x)\mathrm{d}x &= \frac{h_{2n}}{3}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_{2j}) + 4\sum_{j=1}^{n} f(x_{2j-1}) + f(b)\right] \\ &\quad -\frac{b-a}{180}h_{2n}^4 f^{(4)}(\tilde{\mu}) \\ &= S_{2n} - \frac{b-a}{180}\frac{h_n^4}{16}f^{(4)}(\tilde{\mu}), \end{aligned} \tag{15}$$

where

$$S_{2n} = \frac{h_{2n}}{3}\left[f(a) + 2S_{2n}^{(1)} + 4S_{2n}^{(2)} + f(b)\right], n = 2, 4, 8, 16, 32, \cdots . \tag{16}$$

- Let

$$S_{2n}^{(1)} = \sum_{j=1}^{n-1} f(x_{2j}) = f(x_2) + f(x_4) + \cdots + f(x_{2n-2})$$

be the summarization of values of function $f(x)$ at the original inner nodes,

- $$S_{2n}^{(2)} = \sum_{j=1}^{n} f(x_{2j-1}) = f(x_1) + f(x_3) + \cdots + f(x_{2n-1})$$

be the summarization of values of function $f(x)$ at the new additional inner nodes.

- Similarly, we assume that $\mu \approx \tilde{\mu}$,or,more precisely,that $f^{(4)}(\mu) \approx f^{(4)}(\tilde{\mu})$. ,
- then use equations (13) and (16), we have

$$S_n - \frac{b-a}{180} h_n^4 f^{(4)}(\mu) = S_{2n} - \frac{b-a}{180} \frac{h_n^4}{16} f^{(4)}(\tilde{\mu}) \qquad (17)$$

or

$$\frac{b-a}{180} h_n^4 f^{(4)}(\mu) \approx \frac{16}{15}[S_n - S_{2n}].$$

- Substitute this inequality into equation (15), we get

$$\int_a^b f(x)\mathrm{d}x - S_{2n} \approx \frac{1}{15}[S_n - S_{2n}], \tag{18}$$

- Thus, for given required tolerance ε, if

$$\left|S_n - S_{2n}\right| < 15\varepsilon, \tag{19}$$

- Then we have

$$\left|\int_a^b f(x)\mathrm{d}x - S_{2n}\right| < \varepsilon. \tag{20}$$

- That is S_{2n} be the required accurate numerical approximation to $\int_a^b f(x)\mathrm{d}x$.
- **One can easily extend this procedure to composite Trapezoidal Rule.**

5.5 Gaussian Quadrature

- Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally spaced,way.
- The nodes

$$x_1, x_2, \ldots, x_n$$

in the interval $[a, b]$ and coefficients

$$c_1, c_2, \ldots, c_n,$$

are chosen to minimize the expected error obtained in performing the approximation

$$\int_a^b f(x)\mathrm{d}x \approx \sum_{i=1}^{n} c_i f(x_i). \tag{21}$$

for an arbitrary function f.

- To measure this accuracy, we assume that the best choice of these values

$$x_1, x_2, \ldots, x_n; c_1, c_2, \ldots, c_n$$

is that producing the exact result for the largest class of polynomials.

- Consideration: The coefficients

$$c_1, c_2, \ldots, c_n$$

in the approximation formula are arbitrary, and the nodes

$$x_1, x_2, \ldots, x_n$$

are restricted only by the specification that they lie in $[a, b]$, the interval of integration.

- This gives us $2n$ parameters to choose.

- If the coefficients of a polynomial are considered parameters, the class of polynomial of degree at most $(2n-1)$ also contains $2n$ parameters.
- This, then, is the largest class of polynomials for which it is possible to polynomials for which it is possible to expect the formula to be exact.
- For the proper choice of the values and constants exactness on this set can be obtained.

- To illustrate the procedure for choosing the appropriate parameters,we will show how to select the coefficients and nodes when $n = 2$ and the interval of integration is $[-1, 1]$.
- Suppose we want to determine c_1, c_2, x_1, x_2, so that the integration formula

$$\int_{-1}^{1} f(x)\mathrm{d}x \approx c_1 f(x_1) + c_2 f(x_2)$$

gives the exact result whenever $f(x)$ is a polynomial of degree $2 \times 2 - 1 = 3$ or less, that is, when

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3,$$

for some collection of constants, a_0, a_1, a_2 and a_3.

- Because

$$\int (a_0 + a_1 x + a_2 x^2 + a_3 x^3)\mathrm{d}x$$
$$= a_0 \int 1\mathrm{d}x + a_1 \int x\mathrm{d}x + a_2 \int x^2\mathrm{d}x + a_3 \int x^3\mathrm{d}x$$

this is equivalent to showing that the formula gives exact result when $f(x)$ is $1, x, x^2$,and x^3 .
- Hence, we need c_1, c_2, x_1, x_2, so that

$$c_1 \cdot 1 + c_2 \cdot 1 = \int_{-1}^{1} 1\mathrm{d}x = 2,$$

$$c_1 \cdot x_1 + c_2 \cdot x_2 = \int_{-1}^{1} x\mathrm{d}x = 0,$$

$$c_1 \cdot x_1^2 + c_2 \cdot x_2^2 = \int_{-1}^{1} x^2\mathrm{d}x = \frac{2}{3},$$

$$c_1 \cdot x_1^3 + c_2 \cdot x_2^3 = \int_{-1}^{1} x^3\mathrm{d}x = 0,$$

- Solving this system of equations gets the unique solution

$$c_1 = 1, \;\; c_2 = 1, \;\; x_1 = -\frac{\sqrt{3}}{3}, \;\; x_2 = \frac{\sqrt{3}}{3}$$

- This gives the approximation formula

$$\int_{-1}^{1} f(x)\mathrm{d}x \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right). \tag{22}$$

- This formula has **degree of precision three**,that is,**it produces the exact result for every polynomial of degree three or less**.
- This technique could be used to determine the nodes and coefficients for formulas that give exact results for higher-degree polynomials.

- consider various collections of **orthogonal polynomials**, functions that have the property that a particular definite integral of the product or any two of them is zero.
- The set that is relevant to our problem is the set of **Legendre polynomials**.

Definition:

Legendre polynomials are a collection

$$\{P_0, P_1(x), ..., P_n(x), ...,\}$$

with properties:

1. For each n, $P_n(x)$is a polynomial of degree n.
2. $\int_{-1}^{1} P(x)P_n(x)dx = 0$ whenever $P(x)$ is a polynomial of degree less than n.

The first few **Legendre polynomials** are

$$\begin{aligned}
P_0(x) &= 1, \\
P_1(x) &= x, \\
P_2(x) &= x^2 - \frac{1}{3}, \\
P_3(x) &= x^3 - \frac{3}{5}x, \\
P_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{35}. \\
\dots &\quad \dots
\end{aligned}$$

Remarks:

1. The roots of these polynomials are distinct,lie in the interval$(-1, 1)$.
2. Each of them have a symmetry with respect to the origin.
3. It is important that the roots of these polynomials are the correct choice for determining the parameters that solve our problem.
4. The nodes $x_1, x_2, ..., x_n$ needed to produce an integral approximation formula that gives exact results for any polynomial of degree less than $2n$ are the roots of the nth-degree Legendre polynomial.

Theorem 5.7

Suppose that

$$x_1, x_2, ..., x_n$$

are the roots of the nth Legendre polynomial $P_n(x)$, and that for each $i = 1, 2, ..., n$, the numbers c_i are defined by

$$c_i = \int_{-1}^{1} \prod_{j=1, j\neq i}^{n} \frac{x - x_j}{x_i - x_j} \mathrm{d}x.$$

If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^{1} P(x)\mathrm{d}x = \sum_{i=1}^{n} c_i P(x_i).$$

Proof of Theorem 5.7

- Let us first consider the situation for a polynomial $R(x)$ as an $(n-1)$st **Lagrange polynomial** with nodes at the roots $x_1, x_2, ..., x_n$ of the nth **Legendre polynomial** $P_n(x)$.
- This representation of $R(x)$ is exact, since the error term involves the nth derivative of $R(x)$, and the nth derivative of $R(x)$ is zero.
- Hence,

$$\begin{aligned}
\int_{-1}^{1} R(x)\mathrm{d}x &= \int_{-1}^{1} [\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} \frac{x-x_j}{x_i-x_j} R(x_i)]\mathrm{d}x \\
&= \sum_{i=1}^{n} [\prod_{j=1, j\neq i} \int_{-1}^{1} \prod_{j=1, j\neq i}^{n} \frac{x-x_j}{x_i-x_j}\mathrm{d}x] R(x_i) \\
&= \sum_{i=1}^{n} c_i R(x_i)
\end{aligned}$$

- This verifies the result for polynomials of degree less than n.
- If the polynomial $P(x)$ of degree less than $2n$ is divided by the nth Legendre polynomial $P_n(x)$,then two polynomials $Q(x)$ and $R(x)$ of degree less than n are produced with

$$P(x) = Q(x)P_n(x) + R(x).$$

- We now invoke the unique power of the Legendre polynomials. First, the degree of the polynomial $Q(x)$ is less than n,so (by property 2).
- That is

$$\int_{-1}^{1} Q(x)P_n(x)dx = 0.$$

- Next, since x_i is a root of $P_n(x)$ for each $i = 1, 2, ..., n$, we have

$$P(x_i) = Q(x_i)P_n(x_i) + R(x_i) = R(x_i).$$

- Finally, since $R(x)$ is a polynomial of degree less than n,the opening argument implies that

$$\int_{-1}^{1} R(x)dx = \sum_{i=1}^{n} c_i R(x_i).$$

- Putting these facts together verifies that the formula is exact for the polynomial $P(x)$:

$$\begin{aligned}\int_{-1}^{1} P(x)dx &= \int_{-1}^{1} [Q(x)P_n(x) + R(x)]dx \\ &= \int_{-1}^{1} R(x)dx = \sum_{i=1}^{n} c_i R(x_i) \\ &= \sum_{i=1}^{n} c_i P(x_i), \blacksquare\blacksquare\blacksquare.\end{aligned}$$

Remarks:

1. The constants c_i needed for the quadrature rule can be generated from the equation in Theorem 4.7 but both these constants and the roots of the Legendre polynomials are extensively tabulated.
2. An integral $\int_a^b f(x)\mathrm{d}x$ over arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using the change of variables:

$$t = \frac{2x - a - b}{b - a} \Leftrightarrow x = \frac{1}{2}[(b-a)t + a + b].$$

3. This permits the Gaussian Quadrature to be applied to

$$\int_a^b f(x)\mathrm{d}x = \int_{-1}^{1} f\left(\frac{(b-a)t + (b+a)}{2}\right)\frac{b-a}{2}\mathrm{d}t \tag{23}$$

5.6 Multiple Integrals

- The techniques discussed in the previous sections can be modified in a straightforward manner for use in the approximation of multiple integrals.Consider the double integral

$$\int\int_R f(x,y)\mathrm{d}A$$

where R is a rectangular region in the plane;

$$R = \{(x,y)|a \leq x \leq b, c \leq y \leq d\}.$$

for some constants a, b, c and$d$.

- To illustrate the approximation technique,we employ the Composite Simpson's rule,although any other composite formula could be used in its place.
- To apply the Composite Simpson's rule we divide the region R by partitioning both $[a, b]$ and $[c, d]$ into an even number of subintervals.

- To simplify the notation we choose integers n and m and partition $[a, b]$ and $[c, d]$ with the evenly spaced mesh points $x_0, x_1, ..., x_{2n}$ and $y_0, y_1, ..., y_{2m}$ respectively.
- These subdivisions determine step sizes $h = (b - a)/2n$ and $k = (d - c)/2m$.
- Writing the double integral as the iterated integral

$$\int\int_R f(x, y)\mathrm{d}A = \int_a^b \Big(\int_c^d f(x, y)dy\Big)\mathrm{d}x,$$

- We first use the Composite Simpson's rule to approximate

$$\int_c^d f(x, y)\mathrm{d}y$$

treating x as a constant.

- Let $y_j = c + jk$ for each $j = 1, 2, ..., 2m$.
- Then

$$\begin{aligned}\int_c^d f(x,y)\mathrm{d}y &= \frac{k}{3}\Big[f(x,y_0) + 2\sum_{j=1}^{m-1} f(x,y_{2j}) + 4\sum_{j=1}^{m} f(x,y_{2j-1}) \\ &\quad + f(x,y_{2m})\Big] - \frac{(d-c)k^4}{180}\frac{\partial^4 f(x,\mu)}{\partial y^4}\end{aligned}$$

for some μ in (c, d).

- Thus

$$\begin{aligned}\int_a^b\int_c^d f(x,y)\mathrm{d}y\mathrm{d}x &= \frac{k}{3}\Big[\int_a^b f(x,y_0)\mathrm{d}x + 2\sum_{j=1}^{m-1}\int_a^b f(x,y_{2j})\mathrm{d}x \\ &\quad + 4\sum_{j=1}^{m}\int_a^b f(x,y_{2j-1})\mathrm{d}x + \int_a^b f(x,y_{2m})\mathrm{d}x\Big] \\ &\quad - \frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f(x,\mu)}{\partial y^4}dx\end{aligned}$$

for some ε_j in (a, b).

The resulting approximation has the form

$$
\begin{aligned}
&\int_a^b \int_c^d f(x, y_j)\,dy \\
= \quad & \frac{hk}{9}\Big\{\Big[f(x_0, y_0) + 2\sum_{i=1}^{n-1} f(x_{2i}, y_0) + 4\sum_{i=1}^{n} f(x_{2i-1}, y_0) + f(x_{2n}, y_0)\Big] \\
&+2\Big[\sum_{j=1}^{m-1} f(x_0, y_{2j}) + 2\sum_{j=1}^{m-1}\sum_{i=1}^{n-1} f(x_{2i}, y_{2j}) \\
&+4\sum_{j=1}^{m-1}\sum_{i=1}^{n} f(x_{2i-1}, y_{2j}) + \sum_{j=1}^{m-1} f(x_{2n}, y_{2j})\Big] \\
&+4\Big[\sum_{j=1}^{m} f(x_0, y_{2j-1}) + 2\sum_{j=1}^{m}\sum_{i=1}^{n-1} f(x_{2i}, y_{2j-1}) \\
&+4\sum_{j=1}^{m}\sum_{i=1}^{n} f(x_{2i-1}, y_{2j-1}) + \sum_{j=1}^{m} f(x_{2n}, y_{2j-1})\Big] \\
&+\Big[f(x_0, y_{2m}) + 2\sum_{i=1}^{n-1} f(x_{2i}, y_{2m}) + 4\sum_{i=1}^{n} f(x_{2i-1}, y_{2m}) + f(x_{2n}, y_{2m})\Big]\Big\}
\end{aligned}
$$

The error term E is given by

$$
\begin{aligned}
E \;\; = \;\; & \frac{-k(b-a)h^4}{540}\Big[\frac{\partial^4 f(\xi_0, y_0)}{\partial x^4} + 2\sum_{j=1}^{m-1}\frac{\partial^4 f(\xi_{2j}, y_{2j})}{\partial x^4} \\
& +4\sum_{j=1}^{m}\frac{\partial^4 f(\xi_{2j-1}, y_{2j-1})}{\partial x^4} \\
& +\frac{\partial^4 f(\xi_{2m}, y_{2m})}{\partial x^4} - \frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f(x,\mu)}{\partial y^4}\,dx\Big]
\end{aligned}
$$

If $\frac{\partial^4 f}{\partial x^4}$ is continuous, the Intermediate Value Theorem can be repeatedly applied to show that the evaluation of the partial derivatives with respect to x can be replaced by a common value and that

$$\begin{aligned} E &= \frac{-k(b-a)h^4}{540}\left[6m\frac{\partial^4 f}{\partial x^4}(\bar{\eta},\bar{\mu})\right] \\ &\quad -\frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f(x,\mu)}{\partial y^4}\mathrm{d}x \end{aligned}$$

for some $(\bar{\eta},\bar{\mu})$ in R .

If $\frac{\partial^4 f}{\partial y^4}$ is also contimuous.the Weighted Mean Value Theorem for Integrals implies that

$$\int_a^b \frac{\partial^4 f(x,\mu)}{\partial y^4}\mathrm{d}x = (b-a)\frac{\partial^4 f}{\partial y^4}(\hat{\eta},\hat{\mu})$$

for some $(\hat{\eta},\hat{\mu})$ in R.

Since $2m = (d-c)/k$,the error term has the form

$$\begin{aligned} E &= \frac{-k(b-a)h^4}{540}\left[6m\frac{\partial^4 f}{\partial x^4}(\bar{\eta},\bar{\mu})\right] \\ &\quad -\frac{(d-c)(b-a)}{180}k^4\frac{\partial^4 f}{\partial y^4}(\hat{\eta},\hat{\mu})\right] \end{aligned}$$

for some $(\bar{\eta},\bar{\mu})$ and $(\hat{\eta},\hat{\mu})$ in R.

- The use of approximation methods for double integrals is not limited to integrals with rectangular regions of integration.The techniques previously discussed can be modified to approximate double integrals of the form
- In fact, integrals on regions not of this type can also be approximated by performing appropriate partitions of the region.
- To describe the technique involved with approximating an integral in the form we will use the basic Simpson's rule to integrate with respect to both variables.The step size for the variable x is $h = (b - a)/2$,but the step size for y varies with x and is written