

Chapter2: Numerical Integration

2.1 Introduction to Quadrature:

We now approach the subject of numerical integration. The goal is to approximate the definite integral of $f(x)$ over the interval $[a,b]$ by evaluating $f(x)$ at a finite number of sample points.

Definition(2.1): Suppose that $a=x_0 < x_1 < \dots < x_M = b$. A formula of the form:

$$Q[f] = \sum_{k=0}^M w_k f(x_k) = w_0 f(x_0) + w_1 f(x_1) + \dots + w_M f(x_M) \quad (2.1)$$

With the property that:

$$\int_a^b f(x) dx = Q[f] + E[f] \quad (2.2)$$

is called a numerical integration or **quadrature** formula. The term $E[f]$ is called the **truncation error** for integration. The values $\{x_k\}_{k=0}^M$ are called the **quadrature nodes** and $\{w_k\}_{k=0}^M$ are called **weights**.

Definition (2.2): The **degree of precision** of a quadrature formula is the positive integer n such that $E[P_i] = 0$ for all polynomials $P_i(x)$ of degree $i \leq n$, but for which $E[P_{n+1}] \neq 0$ for some polynomial $P_{n+1}(x)$ of degree $n+1$.

Theorem(2.1): (closed Newton-cotes Quadrature formula)

Assume that $x_k = x_0 + kh$ are equally spaced nodes and $f_k = f(x_k)$. The first four closed Newton-Cotes quadrature formulas are

$$\int_{x_0}^{x_1} f(x) dx \approx \frac{h}{2} (f_0 + f_1) \quad (2.3) \quad (\text{the trapezoidal rule})$$

$$\int_{x_0}^{x_2} f(x) dx \approx \frac{h}{3} (f_0 + 4f_1 + f_2) \quad (2.4) \quad (\text{Simpson rule})$$

$$\int_{x_0}^{x_3} f(x) dx \approx \frac{3h}{8} (f_0 + 3f_1 + 3f_2 + f_3) \quad (2.5) \quad (\text{Simpson's } \frac{3}{8} \text{ rule})$$

$$\int_{x_0}^{x_4} f(x)dx \approx \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) \quad (2.6) \quad (\text{Boole's rule})$$

Corollary(2.1): (Newton-Cotes precision)

Assume that $f(x)$ is sufficiently differentiable; then $E[f]$ for Newton-Cotes quadrature involves an approximate higher derivative. The trapezoidal rule has degree of precision $n=1$. If $f \in C^2[a, b]$, then:

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12}f^{(2)}(c) \quad (2.7)$$

Simpson's rule has degree of precision $n=3$. If $f \in C^4[a, b]$, then:

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90}f^{(4)}(c) \quad (2.8)$$

Simpson's $\frac{3}{8}$ rule has degree of precision $n=3$. If $f \in C^4[a, b]$, then:

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80}f^{(4)}(c) \quad (2.9)$$

Boole's rule has degree of precision $n=5$. If $f \in C^6[a, b]$, then:

$$\int_{x_0}^{x_4} f(x)dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) - \frac{8h^7}{945}f^{(6)}(c) \quad (2.10)$$

Proof of Theorem(2.1): Start with the Lagrange polynomial $P_M(x)$ based on x_0, x_1, \dots, x_M that can be used to approximate $f(x)$:

$$f(x) \approx P_M(x) = \sum_{k=0}^M f(x_k) \prod_{\substack{j=0 \\ j \neq k}}^M \frac{(x-x_j)}{(x_k-x_j)} \quad (2.11)$$

An approximate for the integral is obtained by replacing the integrand $f(x)$ with the polynomial $P_M(x)$. This is the general method for obtaining a Newton-Cotes integration formula:

$$\int_{x_0}^{x_M} f(x)dx \approx \int_{x_0}^{x_M} P_M(x)dx = \int_{x_0}^{x_M} \left(\sum_{k=0}^M f_k \prod_{\substack{j=0 \\ j \neq k}}^M \frac{(x-x_j)}{(x_k-x_j)} \right) dx \quad (2.12)$$

The details for the general proof of the theorem are tedious. We shall give a Simpson's rule, which is the case $M=2$. This case involves the approximation polynomial

$$P_2(x) = f_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \quad (2.13)$$

Since f_0, f_1 and f_2 are constant with respect to integration, the relations in (2.12) lead to:

$$\begin{aligned} \int_{x_0}^{x_2} f(x)dx &\approx \int_{x_0}^{x_2} f_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} dx + \int_{x_0}^{x_2} f_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} dx \\ &+ \int_{x_0}^{x_2} f_2 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} dx \end{aligned} \quad (2.14)$$

We introduce the change of variable $x=x_0+th$ with $dx=hdt$ to assist with the evaluation of the integrals in (2.14). The new limits of integration are from $t=0$ to $t=2$. The equal spacing of the nodes $x_k=x_0+kh$ leads to $x_k-x_j=(k-j)h$ and $x-x_k=(t-k)h$, which are used to simplify (2.14), and get:

$$\begin{aligned} \int_{x_0}^{x_2} f(x)dx &\approx f_0 \int_0^2 \frac{h(t-1)h(t-2)}{(-h)(-2h)} hdt + f_1 \int_0^2 \frac{h(t-0)h(t-2)}{(h)(-h)} hdt \\ &+ f_2 \int_0^2 \frac{h(t-0)h(t-1)}{(2h)(h)} hdt \\ &= f_0 \frac{h}{2} \int_0^2 (t^2 - 3t + 2) dt + f_1 h \int_0^2 (t^2 - 2t) dt + f_2 \frac{h}{2} \int_0^2 (t^2 - t) dt \\ &= f_0 \frac{h}{2} \left(\frac{t^3}{3} - \frac{3t^2}{2} + 2t \right) \Big|_{t=0}^{t=2} - f_1 h \left(\frac{t^3}{3} - \frac{2t^2}{2} \right) \Big|_{t=0}^{t=2} + f_2 \frac{h}{2} \left(\frac{t^3}{3} - \frac{t^2}{2} \right) \Big|_{t=0}^{t=2} \end{aligned}$$

$$\begin{aligned}
 &= f_0 \frac{h}{2} \left(\frac{2}{3} \right) - f_1 h \left(\frac{-4}{3} \right) + f_2 \frac{h}{2} \left(\frac{2}{3} \right) \\
 &= \frac{h}{3} (f_0 + 4f_1 + f_2)
 \end{aligned}$$

and the proof is complete.

Example(2.1): Consider the function $f(x)=1+e^{-x}\sin(4x)$, the equally spaced quadrature nodes $x_0 = 0$, $x_1 = 0.5$, $x_2 = 1$, $x_3 = 1.5$, $x_4 = 2$ and the corresponding function values $f_0 = 1$, $f_1 = 1.55152$, $f_2 = 0.72159$, $f_3 = 0.93765$ and $f_4 = 1.13390$. Apply the various quadrature formulas (2.3) through (2.6).

The step size is $h=0.5$, and the computations are:

$$\int_0^{0.5} f(x)dx \approx \frac{0.5}{2} (1 + 1.55152) = 0.63788$$

$$\int_0^1 f(x)dx \approx \frac{0.5}{3} (1 + 4(1.55152) + 0.72159) = 1.32128$$

$$\int_0^{1.5} f(x)dx \approx \frac{3(0.5)}{8} (1 + 3(1.55152) + 3(0.72159) + 0.93765) = 1.64193$$

$$\begin{aligned}
 \int_0^2 f(x)dx &\approx \frac{2(0.5)}{45} (7(1) + 32(1.55152) + 12(0.72159) + 32(0.93765) + 7(1.1339)) \\
 &= 2.29444
 \end{aligned}$$

Examples (2.2): Consider the integration of the function $f(x)=1+e^{-x}\sin(4x)$ over the fixed interval $[a,b]=[0,1]$. Apply the various formulas (2.3) through (2.6).

For the trapezoidal rule, $h=1$ and

$$\int_0^1 f(x)dx \approx \frac{1}{2}(f(0) + f(1)) = \frac{1}{2}(1 + 0.72159) = 0.86079$$

For Simpson's rule, $h=1/2$, and we get:

$$\int_0^1 f(x)dx \approx \frac{1/2}{3}(f(0) + 4f\left(\frac{1}{2}\right) + f(1)) = \frac{1}{6}(1 + 4(1.55152) + 0.72159) = 1.32128$$

For Simpson's $\frac{3}{8}$ rule, $h=1/3$, and we obtain:

$$\begin{aligned} \int_0^1 f(x)dx &\approx \frac{3\left(\frac{1}{3}\right)}{8}(f(0) + 3f\left(\frac{1}{3}\right) + 3f\left(\frac{2}{3}\right) + f(1)) \\ &= \frac{1}{8}(1 + 3(1.69642) + 3(1.23447) + 0.72159) = 1.31440 \end{aligned}$$

For Boole's rule, $h=1/4$, and the result is:

$$\begin{aligned} \int_0^1 f(x)dx &\approx \frac{2\left(\frac{1}{4}\right)}{45}(7f(0) + 32f\left(\frac{1}{4}\right) + 12f\left(\frac{1}{2}\right) + 32f\left(\frac{3}{4}\right) + 7f(1)) \\ &= \frac{1}{90}(7(1) + 32(1.65534) + 12(1.55152) + 32(1.06666) + 7(0.72159)) \\ &= 1.30859 \end{aligned}$$

The true value of the definite integral is:

$$\int_0^1 f(x)dx = 1.308\ 250\ 604$$

To make a fair comparison of quadrature methods, we must use the same number of function evaluations in each method. Our final example is concerned with comparing integration over a fixed interval $[a,b]$ using exactly five function evaluation $f_k=f(x_k)$, for

$k=0,1,\dots,4$ for each method. When the trapezoidal rule is applied on the four subintervals $[x_0, x_1]$, $[x_1, x_2]$, $[x_2, x_3]$ and $[x_3, x_4]$, it is called a **composite trapezoidal rule**:

$$\begin{aligned}
 \int_{x_0}^{x_4} f(x)dx &= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \int_{x_2}^{x_3} f(x)dx + \int_{x_3}^{x_4} f(x)dx \\
 &\approx \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \frac{h}{2}(f_2 + f_3) + \frac{h}{2}(f_3 + f_4) \\
 &= \frac{h}{2}(f_0 + 2f_1 + 2f_2 + 2f_3 + f_4)
 \end{aligned} \tag{2.15}$$

Simpson's rule can also be used in this manner. When Simpson's rule is applied on the two subintervals $[x_0, x_2]$ and $[x_2, x_4]$, it is called a **composite Simpson's rule**:

$$\begin{aligned}
 \int_{x_0}^{x_4} f(x)dx &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx \\
 &\approx \frac{h}{3}(f_0 + 4f_1 + f_2) + \frac{h}{3}(f_2 + 4f_3 + f_4) \\
 &= \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4)
 \end{aligned} \tag{2.16}$$

Example(2.3): Consider the integration of the function $f(x)=1+e^{-x}\sin(4x)$ over $[a,b]=[0,1]$. Use exactly five function evaluations and compare the results from the composite trapezoidal rule and composite Simpson's rule.

The uniform step size is $h=1/4$. The composite trapezoidal rule (2.15) produces:

$$\begin{aligned}
 \int_0^1 f(x)dx &\approx \frac{1/4}{2} \left(f(0) + 2f\left(\frac{1}{4}\right) + 2f\left(\frac{1}{2}\right) + 2f\left(\frac{3}{4}\right) + f(1) \right) \\
 &= \frac{1}{8}(1 + 2(1.65534) + 2(1.55152) + 2(1.06666) + 0.72159) \\
 &= 1.28358
 \end{aligned}$$

Using the composite Simpson's rule (2.16), we get:

$$\begin{aligned} \int_0^1 f(x)dx &\approx \frac{1/4}{3} \left(f(0) + 4f\left(\frac{1}{4}\right) + 2f\left(\frac{1}{2}\right) + 4f\left(\frac{3}{4}\right) + f(1) \right) \\ &= \frac{1}{12} (1 + 4(1.65534) + 2(1.55152) + 4(1.06666) + 0.72159) \\ &= 1.30938 \end{aligned}$$

Example(2.4): Determine the degree of precision of Simpson's $\frac{3}{8}$ rule.

It will suffice to apply Simpson's $\frac{3}{8}$ rule over the interval $[0,3]$ with the five test functions $f(x)=1, x, x^2, x^3$, and x^4 . For the first four functions. Simpson's $\frac{3}{8}$ rule is exact.

$$\int_0^3 1 dx = \frac{3}{8} (1 + 3(1) + 3(1) + 1) = 3$$

$$\int_0^3 x dx = \frac{3}{8} (0 + 3(1) + 3(2) + 3) = \frac{9}{2}$$

$$\int_0^3 x^2 dx = \frac{3}{8} (0 + 3(1) + 3(4) + 9) = 9$$

$$\int_0^3 x^3 dx = \frac{3}{8} (0 + 3(1) + 3(8) + 27) = \frac{81}{4}$$

the function $f(x)=x^4$ is the lowest power of x for which the rule is not exact.

$$\int_0^3 x^4 dx = \frac{3}{8} (0 + 3(1) + 3(16) + 81) = \frac{99}{2}$$

Therefore, the degree of precision of Simpson's $\frac{3}{8}$ rule is n=3.

Exercises:

1. Consider a general interval [a,b]. Show that Simpson's rule produces exact results for the function $f(x)=x^2$ and $f(x)=x^3$, that is

$$\text{a. } \int_a^b x^2 dx = \frac{b^3}{3} - \frac{a^3}{3} \quad \text{b. } \int_a^b x^3 dx = \frac{b^4}{4} - \frac{a^4}{4}$$

2. Integrate the Lagrange interpolation polynomial

$$P_1(x) = f_0 \frac{(x - x_1)}{(x_0 - x_1)} + f_1 \frac{(x - x_0)}{(x_1 - x_0)}$$

over the interval $[x_0, x_1]$ and establish the trapezoidal rule.

3. Determine the degree of precision of the trapezoidal rule.

2.2 Other Ways to Derive Integration Formulas Using Newton Forward Polynomial:

During the integration we will need to change the variable of integration from x to t since our polynomials are expressed in terms of t . Observe that $dx=hdt$.

$$\begin{aligned} \int_{x_0}^{x_1} f(x) dx &= h \int_{t=0}^{t=1} \left[f_0 + t\Delta f_0 + \frac{t(t-1)}{2!} \Delta^2 f_0 + \frac{t(t-1)(t-2)}{3!} \Delta^3 f_0 + \dots \right] dt \\ &= h \int_0^1 \left[f_0 + t\Delta f_0 + \frac{t^2-t}{2} \Delta^2 f_0 + \frac{t^3-3t^2+2t}{6} \Delta^3 f_0 + \dots \right] dt \\ &= h \left[f_0 t + \frac{t^2}{2} \Delta f_0 + \left(\frac{t^3}{6} - \frac{t^2}{4} \right) \Delta^2 f_0 + \left(\frac{t^4}{24} - \frac{t^3}{6} + \frac{t^2}{6} \right) \Delta^3 f_0 + \dots \right]_{t=0}^{t=1} \\ &= h \left[f_0 + \frac{1}{2} \Delta f_0 - \frac{1}{12} \Delta^2 f_0 + \frac{1}{24} \Delta^3 f_0 + \dots \right] \end{aligned}$$

using first two terms only, we get:

$$\int_{x_0}^{x_1} f(x) dx = h \left[f_0 + \frac{1}{2} \Delta f_0 \right] = h \left[f_0 + \frac{1}{2} (f_1 - f_0) \right] = \frac{h}{2} [f_0 + f_1]$$

Exercise:

Derive Simpson's formula using Newton Forward polynomial.

2.3 Composite Trapezoidal and Simpson's Rule:

Theorem(2.2): (Composite Trapezoidal Rule)

Suppose that the interval $[a,b]$ is subdivided into subinterval $[x_k, x_{k+1}]$ of width $h=(b-a)/M$ by using equally spaced nodes $x_k=a+kh$, for $k=0,1,\dots,M$. The **composite trapezoidal rule for M subintervals** can be expressed in:

$$\begin{aligned} \int_a^b f(x)dx &\approx T(f, h) = \frac{h}{2} [f_0 + 2(f_1 + \dots + f_{M-1}) + f_M] \\ &= \frac{h}{2} [f(a) + f(b)] + h \sum_{k=1}^{M-1} f(x_k) \end{aligned} \quad (2.17)$$

Proof: Apply the trapezoidal rule over each subinterval $[x_{k-1}, x_k]$. Use the additive property of the integral for subintervals:

$$\begin{aligned} \int_a^b f(x)dx &= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \dots + \int_{x_{M-1}}^{x_M} f(x)dx \\ &= \frac{h}{2} [f_0 + f_1] + \frac{h}{2} [f_1 + f_2] + \dots + \frac{h}{2} [f_{M-1} + f_M] \\ &= \frac{h}{2} [f_0 + 2(f_1 + f_2 + \dots + f_{M-1}) + f_M]. \end{aligned}$$

Example(2.5): Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite trapezoidal rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1,6]$.

To generate 11 sample points, we use $M=10$ and $h=(6-1)/10=1/2$.

x	1	1.5	2	2.5	3	3.5	4	4.5	5	5.5	6
$f(x)$	2.909297	2.638157	2.308071	1.979316	1.683052	1.4353041	1.243197	1.108317	1.028722	1.000241	1.017357

$$\int_1^6 f(x)dx = \frac{\frac{1}{2}}{2} [f(1) + 2(f(1.5) + f(2) + f(2.5) + f(3) + f(3.5) + f(4) + f(4.5) + f(5) + f(5.5)) + f(6)] = 8.193854.$$

Theorem(2.3): (Composite Simpson Rule)

Suppose that $[a,b]$ is subdivided into $2M$ subintervals $[x_k, x_{k+1}]$ of equal width with $h=(b-a)/(2M)$ by using $x_k=a+kh$ for $k=0,1,\dots,2M$. The **composite Simpson rule for $2M$ subintervals** can be expressed in:

$$\begin{aligned} \int_a^b f(x)dx &\approx S(f, h) = \frac{h}{3} [f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + 2f_{2M-2} + 4f_{2M-1} + f_{2M}] \\ &= \frac{h}{3} [f(a) + f(b)] + \frac{2h}{3} \sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3} \sum_{k=1}^M f(x_{2k-1}) \quad (2.18) \end{aligned}$$

proof: (EXC)

Example(2.6): Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite Simpson rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1,6]$.

$$\int_a^b f(x)dx = \frac{1/2}{3} [f(1) + f(6)] + \frac{1}{3} [f(2) + f(3) + f(4) + f(5)] + \frac{2}{3} [f(1.5) + f(2.5) + f(3.5) + f(4.5) + f(5.5)] = 8.1830155$$

Error Analysis:

Corollary(2.2): (Trapezoidal Rule: Error Analysis)

Suppose that $[a,b]$ is subdivided into M subintervals $[x_k, x_{k+1}]$ of width $h=(b-a)/M$. The composite trapezoidal rule:

$$T(f, h) = \frac{h}{2} [f(a) + f(b)] + h \sum_{k=1}^{M-1} f(x_k) \quad (2.19)$$

is an approximation to the integral:

$$\int_a^b f(x)dx = T(f, h) + E_T(f, h) \quad (2.20)$$

Furthermore, if $f \in C^2[a, b]$, there exists a value c with $a < c < b$ so that the error term $E_T(f, h)$ has the form:

$$E_T(f, h) = \frac{-(b-a)f^{(2)}(c)h^2}{12} = O(h^2) \quad (2.21)$$

Proof: We first determine the error term when the rule is applied over $[x_0, x_1]$. Integrating the Lagrange polynomial $P_1(x)$ and its remainder yields:

$$\int_{x_0}^{x_1} f(x)dx = \int_{x_0}^{x_1} P_1(x)dx + \int_{x_0}^{x_1} \frac{(x-x_0)(x-x_1)f^{(2)}(c(x))}{2!} dx \quad (2.22)$$

The term $(x-x_0)(x-x_1)$ does not change sign on $[x_0, x_1]$, and $f^{(2)}(c(x))$ is continuous. Hence the second Mean value Theorem for integrals implies that there exists a value c_1 so that:

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2} [f_0 + f_1] + f^{(2)}(c_1) \int_{x_0}^{x_1} \frac{(x-x_0)(x-x_1)}{2!} dx \quad (2.23)$$

Use the change of variable $x=x_0+ht$ in the integral on the right side of (2.23)

$$\begin{aligned} \int_{x_0}^{x_1} f(x)dx &= \frac{h}{2} [f_0 + f_1] + \frac{f^{(2)}(c_1)}{2} \int_0^1 h(t-0)h(t-1)hdt \\ &= \frac{h}{2} [f_0 + f_1] + \frac{f^{(2)}(c_1)h^3}{2} \int_0^1 (t^2 - t)dt \\ &= \frac{h}{2} [f_0 + f_1] - \frac{f^{(2)}(c_1)h^3}{12} \end{aligned} \quad (2.24)$$

Now we are ready to add up the error terms for all of the intervals $[x_k, x_{k+1}]$:

$$\int_a^b f(x)dx = \sum_{k=1}^M \int_{x_{k-1}}^{x_k} f(x)dx = \sum_{k=1}^M \frac{h}{2} [f(x_{k-1}) + f(x_k)] - \frac{h^3}{12} \sum_{k=1}^M f^{(2)}(c_k) \quad (2.25)$$

The first sum is the composite trapezoidal rule $T(f, h)$. In the second term, one factor of h is replaced with its equivalent $h=(b-a)/M$, and the result is:

$$\int_a^b f(x)dx = T(f, h) - \frac{(b-a)h^2}{12} \left(\frac{1}{M} \sum_{k=1}^M f^{(2)}(c_k) \right)$$

The term in parentheses can be recognized as an average of values for the second derivative and hence is replaced by $f^{(2)}(c)$. Therefore, we have established that:

$$\int_a^b f(x)dx = T(f, h) - \frac{(b-a)f^{(2)}(c)h^2}{12}$$

and the proof is complete.

Corollary(2.3): (Simpson's rule: Error analysis)

Suppose that $[a,b]$ is subdivided into $2M$ subintervals $[x_k, x_{k+1}]$ of equal width $h=(b-a)/(2M)$. The composite Simpson rule

$$S(f, h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3} \sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3} \sum_{k=1}^M f(x_{2k-1}) \quad (2.26)$$

is an approximation to the integral:

$$\int_a^b f(x)dx = S(f, h) + E_S(f, h) \quad (2.27)$$

Furthermore, if $f \in C^4[a, b]$, there exists a value c with $a < c < b$ so that the error term $E_S(f, h)$ has the form:

$$E_S(f, h) = \frac{-(b-a)f^{(4)}(c)h^4}{180} = O(h^4) \quad (2.28)$$

Example(2.7): Consider $f(x) = \frac{1}{x}$. Investigate the error when the composite trapezoidal rule is used over $[1,6]$ and the number of subintervals is 10.

$h=(6-1)/10=0.5$, since:

$$E_T(f, h) = \frac{-(b-a)f^{(2)}(c)h^2}{12} = O(h^2)$$

we first compute $f'(x) = \frac{-1}{x^2}$ and $f''(x) = \frac{2}{x^3}$, therefore:

$$f''(1) = 2, f''(2) = \frac{1}{4}, f''(6) = \frac{2}{6^3} = 0.009\ 259$$

and hence $f''(c)=2$ and $E_T(f,h)=\frac{-(6-1)(2)(0.5)^2}{12}=\frac{-2.5}{12}=-0.208333$

Example(2.8): Find the number M and the step size h so that the error $E_S(f,h)$ for the Simpson's rule is less than 5×10^{-9} for the approximation $\int_2^7 dx/x \approx S(f,h)$.

$$f(x) = \frac{1}{x} \xrightarrow{\text{yields}} f'(x) = \frac{-1}{x^2} \xrightarrow{\text{yields}} f''(x) = \frac{2}{x^3} \xrightarrow{\text{yields}} f^{(3)}(x) = \frac{-6}{x^4} \xrightarrow{\text{yields}} f^{(4)}(x) = \frac{24}{x^5}$$

the maximum value of $|f^{(4)}(x)|$ taken over $[2,7]$ occurs at the end point $x=2$ and $f^{(4)}(2)=3/4$, then:

$$|E_S(f,h)| = \frac{|-(b-a)f^{(4)}(c)h^4|}{180} \leq \frac{(7-2)\frac{3}{4}h^4}{180} = \frac{h^4}{48}$$

The step size h and number M satisfy the relation $h=5/(2M)$, and this is used in the above equation to get the relation

$$|E_S(f,h)| \leq \frac{625}{768M^4} \leq 5 \times 10^{-9}$$

$$\xrightarrow{\text{yields}} \frac{125}{768} \times 10^9 \leq M^4 \xrightarrow{\text{yields}} 112.95 \leq M$$

since M must be integer, we chose $M=113$

and the corresponding step size $h=5/226=0.022123$

Exercises:

1. Approximate the integral $\int_{-1}^1 \frac{dx}{1+x^2}$ using the composite trapezoidal rule with $M=10$.
2. The length of the curve $y=f(x)$ over the interval $a \leq x \leq b$ is $L=\int_a^b \sqrt{1+(f'(x))^2} dx$
approximate the length of the function $f(x)=x^3$ over $[0,1]$ using composite Simpsons rule with $M=5$.

3. Verify that the trapezoidal rule ($M=1$, $h=1$) is exact for polynomials of degree ≤ 1 of the form $f(x)=c_1x+c_0$ over $[0,1]$.
4. Determine the number M and the interval width h so that the composite trapezoidal rule for M subintervals can be used to compute the integral $\int_0^2 xe^{-x}dx$ with an accuracy of 5×10^{-9} .

2.4 Romberg Integration:

The discussion here is based upon the trapezium rule. Let the integration domain $[a,b]$ be divided by three equispaced nodes $x_0=a$, $x_1=(a+b)/2$ and $x_2=b$ at interval of size h . Two successive trapezium estimates using one and two subintervals respectively are:

$$T_1 = \frac{2h}{2} [f(x_0) + f(x_1)] \text{ and } T_2 = \frac{h}{2} [f(x_0) + 2f(x_1) + f(x_2)]$$

On including the truncation error for this estimate we can write:

$$I = T_1 - \frac{(2h)^2}{12} f''(x_0) - G(2h)^4 - \dots$$

$$I = T_2 - \frac{h^2}{12} f''(x_0) - Gh^4 - \dots$$

where G is independent of the step size h . Four times the second estimate minus the first estimate gives:

$$I = \frac{1}{3} [4T_2 - T_1] + 4Gh^4 + O(h^6) \quad (2.29)$$

Taken as an estimate to I , the values $(4T_2 - T_1)/3$ has leading error of $O(h^4)$. Expand this estimate:

$$I \approx \frac{1}{3} [4T_2 - T_1] = \frac{1}{3} \left[4 \left\{ \frac{h}{2} (f_0 + 2f_1 + f_2) \right\} - \frac{2h}{2} (f_0 + f_2) \right]$$

$$= \frac{h}{3} [f_0 + 4f_1 + f_2]$$

Shows it to be the Simpson estimate S_2 using two sub-intervals of size $h=(b-a)/2$.

This process can be carried out for any two trapezium estimates T_N and T_{2N} to give the more accuracy Simpson's estimate S_{2N} .

Trapezoidal	Simpson	
T_1		
T_2	S_2	
T_4	S_4	In general $S_{2N}=1/3\{4T_{2N}-T_N\}$
T_8	S_8	

In the same way we get:

$$I \approx \frac{1}{15} [16S_4 - S_2] + O(h^6) \quad (2.30)$$

known as Boole's rule.

Trapezoidal	Simpson	Boole's	
T_1			
T_2	S_2		
T_4	S_4	B_4	In general $S_{2N}=1/3\{4T_{2N}-T_N\}$
T_8	S_8	B_8	In general $B_{4N}=1/15\{16S_{4N}-S_{2N}\}$

Example(2.9): Estimate the value of $\int_0^1 e^{\sin x} dx$ using Romberg integration

N	Trapezium $k=1$	Simpson $k=2$	Boole $k=3$	$k=4$
1	1.659 888			
2	1.637 517	1.630 060		
4	1.633 211	1.631 776	1.631 891	
8	1.632 201	1.631 864	1.631 869	1.631 869

Exercises:

1. Use Romberg integration to estimate $\int_0^2 x^2 e^{-x^2} dx$ as accurately as possible, working to four decimal places.