Numerical Differentiation and Integration

Introduction

Engineers are frequently confronted with the problem of differentiating functions which are defined in tabular or graphical form rather than as explicit functions. The interpretation of experimentally obtained data is a good example of this. A similar situation involves the integration of functions which have explicit forms that are difficult or impossible to integrate in terms of elementary functions.

Important Points of the Chapter 5

I. In this chapter we shall find the approximate solutions of derivative (first- and second-order) and antiderivative (definite integral only).

II. Given data points should be equally spaced only (length of each subinterval should be same). Smaller the length of the interval better the approximation.

III. Numerical methods for differentiation and integration can be derived using Lagrange interpolating polynomial at equally-spaced data points.

IV. Error term for each numerical method will be discuss

Numerical Differentiation

When a function is represented by a table of values, the most obvious approach is to differentiate

the Lagrange interpolation formula

$$f(x) = p_n(x) + \frac{f^{(n+1)}(\eta(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i), \tag{5.3}$$

First Derivative Numerical Formulas

To obtain general formula for approximation of the first derivative of a function $f(x)$, we consider that $\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ distinct equally spaced points in some interval I and function $f(x)$ is continuous and its $(n+1)th$ derivatives exist in the given interval, that is, $f \in C^{n+1}(I)$. Then by differentiating (5.3) with respect to x and at $x = x_k$, we have

$$f'(x_k) = \sum_{i=0}^{n} f(x_i) L_i'(x_k) + \frac{f^{(n+1)}(\eta(x_k))}{(n+1)!} \prod_{\substack{i=0 \\ i \neq k}}^{n} (x_k - x_i). \tag{5.4}$$

The formula (5.4) is called the *(n+1)-point formula* to approximate $f'(x_k)$.

Two-point Formula

Consider two distinct points x_0 and x_1, $x_1 = x_0 + h$ for some $h \neq 0$

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

By taking derivative with respect to x and at $x = x_0$, we obtain

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

$$f'(x_0) \approx -\frac{f(x_0)}{h} + \frac{f(x_0 + h)}{h}, \quad \Longleftrightarrow \quad f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h} = D_h f(x_0). \tag{5.6}$$

It is called the *two-point formula* for smaller values of h.

If $h < 0$, then the formula (5.6) is also called the *two-point backward-difference formula*, which can be written as

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}. \tag{5.7}$$

Example 5.1 *Let $f(x) = e^x$. Then use the two-point formula to approximate $f'(2)$, when $h = 0.1$ and $h = 0.01$.*

Solution. *Using the formula (5.6), with $x_0 = 2$, we have*

$$f'(2) \approx \frac{f(2+h) - f(2)}{h}.$$

Then for $h = 0.1$, we get

$$f'(2) \approx \frac{f(2.1) - f(2)}{0.1} \approx \frac{e^{2.1} - e^2}{0.1} = 7.7712.$$

Similarly, by using $h = 0.01$, we obtain

$$f'(2) \approx \frac{(e^{2.01} - e^2)}{0.01} = 7.4262.$$

Since the exact solution of $f'(2) = e^2$ is, 7.3891, so the corresponding actual errors with $h = 0.1$ and $h = 0.01$ are, -0.3821 and -0.0371 respectively. This shows that the approximation obtained with $h = 0.01$ is better than the approximation with $h = 0.1$. •

Similarly, by using the formula (5.7), with $x_0 = 2$, we have $$f'(2) \approx \frac{f(2) - f(2-h)}{h},$$

then for $h = 0.1$, we have $$f'(2) \approx \frac{f(2) - f(1.9)}{0.1} = \frac{e^2 - e^{1.9}}{0.1} = 7.0316.$$

For $h = 0.01$, we have $$f'(2) \approx \frac{e^2 - e^{1.99}}{0.01} = 7.3522.$$

Error Term of Two-point Formula

$$f(x) - p_1(x) = \frac{f''(\eta(x))}{2!} \prod_{i=0}^{1} (x - x_i), \qquad \eta(x) \in (x_0, x_1).$$

$$f'(x_0) \quad - \quad p_1'(x_0) = \left(\frac{d}{dx} f''(\eta(x)) \Big|_{x=x_0} \right) \frac{(x - x_0)(x - x_1)}{2}$$

$$+ \quad \frac{f''(\eta(x_0))}{2} \left(\frac{d}{dx} (x^2 - x(x_0 + h) - x x_0 + x_0(x_0 + h)) \Big|_{x=x_0} \right).$$

Since $\frac{d}{dx} f''(\eta(x)) = 0$ only if $x = x_0$, so error in the forward-difference formula (5.6) is

$$E_F(f, h) = f'(x_0) - D_h f(x_0) = -\frac{h}{2} f''(\eta(x)), \quad \text{where} \quad \eta(x) \in (x_0, x_1), \tag{5.8}$$

which is called the *error formula* of the two-point formula (5.6). Hence the formula (5.6) can be written as

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\eta(x)), \quad \text{where} \quad \eta \in (x_0, x_1). \tag{5.9}$$

Example 5.3 *Let* $f(x) = x^2 \cos x$. *Then*
(a) Compute the approximate value of $f'(x)$ *at* $x = 1$, *taking* $h = 0.1$ *using (5.6).*
(b) Compute the error bound for your approximation using the formula (5.8).
(c) Compute the absolute error.
(d) What best maximum value of stepsize h *required to obtain the approximate value of* $f'(1)$ *correct to two decimal places.*

Solution. *(a) Given* $x_0 = 1, h = 0.1$, *then by using the formula (5.6), we have*

$$f'(1) \approx \frac{f(1+0.1) - f(1)}{0.1} = \frac{f(1.1) - f(1)}{0.1} = D_h f(1).$$

Thus

$$f'(1) \approx \frac{(1.1)^2 \cos(1.1) - (1)^2 \cos(1)}{0.1} \approx \frac{0.5489 - 0.5403}{0.1} = 0.0860,$$

which is the required approximation of $f'(x)$ *at* $x = 1$.

(b) To find the error bound, we use the formula (5.8), which gives

$$E_F(f, h) = -\frac{0.1}{2} f''(\eta(x)), \quad \textit{where} \quad \eta(x) \in (1, 1.1),$$

or

$$|E_F(f, h)| = \left| -\frac{0.1}{2} \right| |f''(\eta(x))|, \quad \textit{for} \quad \eta \in (1, 1.1).$$

The second derivative $f''(x)$ *of the function can be found as*

$$f(x) = x^2 \cos x, \quad \textit{gives} \quad f''(x) = (2 - x^2) \cos x - 4x \sin x.$$

The value of the second derivative $f''(\eta(x))$ *cannot be computed exactly because* $\eta(x)$ *is not known. But one can bound the error by computing the largest possible value for* $|f''(\eta(x))|$*. So bound* $|f''|$ *on* $[1, 1.1]$ *can be obtain*

$$M = \max_{1 \leq x \leq 1.1} |(2 - x^2)\cos x - 4x \sin x| = 3.5630,$$

at $x = 1.1$*. Since* $|f''(\eta(x))| \leq M$*, therefore, for* $h = 0.1$*, we have*

$$|E_F(f, h)| \leq \frac{0.1}{2} M = 0.05(3.5630) = 0.1782,$$

which is the possible maximum error in our approximation.

(c) Since the exact value of the derivative $f'(1)$ *is* 0.2392*, therefore the absolute error* $|E|$ *can be computed as follows:*

$$|E| = |f'(1) - D_h f(1)| = |0.2391 - 0.0860| = 0.1531.$$

(d) Since the given accuracy required is 10^{-2}*, so*

$$|E_F(f, h)| = |-\frac{h}{2} f''(\eta(x))| \leq 10^{-2},$$

for $\eta(x) \in (1, 1.1)$*. This gives*

$$\frac{h}{2} M \leq 10^{-2}, \quad or \quad h \leq \frac{(2 \times 10^{-2})}{M}.$$

Using $M = 3.5630$*, we obtain*

$$h \leq \frac{2}{356.3000} = 0.0056,$$

which is the best maximum value of h to get the required accuracy. •

Total Error

The total error, $E(h)$, $E(h) = E_{trunc} + E_{round} = \frac{h}{2}M + \frac{10^{-t}}{h}$,

where $M = \max_{x_0 \le x \le x_1} |f''(\eta(x_0))|$, t is the required decimal digits of accuracy,

the optimal value for h. Thus the minimum error is

$$E(h_{opt}) = \frac{M}{2}\sqrt{\frac{2}{M} \times 10^{-t}} + \frac{10^{-t}}{\sqrt{\frac{2}{M} \times 10^{-t}}} = \sqrt{2M \times 10^{-t}}$$

Example 5.4 *Consider $f(x) = x^2 \cos x$ and $x_0 = 1$. To show the effect of rounding error, the values $\tilde{f}_i$ are obtained by rounding $f(x_i)$ to seven significant digits, compute the total error for $h = 0.1$ and also, find the optimum h.*

Solution. $E(h) = \frac{h}{2}M + \frac{10^{-t}}{h}$ *where* $M = \max_{1 \le x \le 1.1} |(2 - x^2)\cos x - 4x \sin x| = 3.5630$

Then $E(h) = \frac{0.1}{2}(3.5630) + \frac{10^{-7}}{0.1} = 0.17815 + 0.000001 = 0.178151.$

Now to find the optimum h, we use

$$h = h_{opt} = \sqrt{\frac{2}{M} \times 10^{-t}} = \sqrt{\frac{2}{3.5630} \times 10^{-7}} = 0.00024,$$

which is the smallest value of h, below which the total error will begin to increase.

Note that for
$h = 0.00024$, $E(h) = 0.000844$,
$h = 0.00015$, $E(h) = 0.000934$,
$h = 0.00001$, $E(h) = 0.010018$.

Three-point Central Difference Formula

Consider the quadratic Lagrange interpolating polynomial $p_2(x)$ to the three distinct equally spaced points x_0, x_1, and x_2, with $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, for smaller value h, we have

$$f(x) \approx p_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2). \quad (5.11)$$

Now taking the derivative of the above expression with respect to x and then take $x = x_k$, for $k = 0, 1, 2$, we have

$$f'(x_k) \approx \frac{(2x_k - x_1 - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(2x_k - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(2x_k - x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2).$$

Firstly, we take $x_k = x_1$,

$$f'(x_1) \approx \frac{(2x_1 - x_1 - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(2x_1 - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(2x_1 - x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2).$$

$$\approx \frac{f(x_1 + h) - f(x_1 - h)}{2h} = D_h f(x_1).$$

It is called the *three-point central-difference formula*

Error Formula of Central Difference Formula

$$E_C(f, h) = f'(x_1) - D_h f(x_1) = -\frac{h^2}{6} f'''(\eta(x_1)), \qquad \text{where} \quad \eta(x_1) \in (x_1 - h, x_1 + h).$$

Three-point Forward Difference Formula

by taking $x_k = x_0$ in the formula (5.11),

$$f'(x_0) \approx \frac{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h} = D_h f(x_0),$$

which is called the *three-point forward-difference formula*

Error Formula

$$E_F(f,h) = \frac{h^2}{3} f'''(\eta(x_0)), \quad \text{where } \eta(x_0) \in (x_0, x_0 + 2h).$$

Three-point Backward Difference Formula:

Similarly, taking $x_k = x_2$ in the formula (5.11),

$$f'(x_2) \approx \frac{f(x_2 - 2h) - 4f(x_2 - h) + 3f(x_2)}{2h} = D_h f(x_2),$$

which is called the *three-point backward-difference formula*

Error Formula

$$E_B(f,h) = \frac{h^2}{3} f'''(\eta(x_2)), \qquad \text{where } \eta(x_2) \in (x_2 - 2h, x_2).$$

Example 5.5 *Let $f(x) = x^2 \cos x$. Then*
(a) Compute the approximate value of $f'(x)$ at $x = 1$, taking $h = 0.1$ using (5.12).
(b) Compute the error bound for your approximation using (5.13).
(c) Compute the absolute error.
(d) What is the best maximum value of stepsize h required to obtain the approximate value of $f'(1)$ correct to two decimal places.

Solution. *(a) Given $x_1 = 1, h = 0.1$, then using the formula (5.12), we have*

$$f'(1) \approx \frac{f(1+0.1) - f(1-0.1)}{2(0.1)} = \frac{f(1.1) - f(0.9)}{0.2} = D_h f(1).$$

Then

$$f'(1) \approx \frac{(1.1)^2 \cos(1.1) - (0.9)^2 \cos(0.9)}{0.2} \approx \frac{0.5489 - 0.5035}{0.2} = 0.2270.$$

(b) By using the error formula (5.13), we have

$$E_C(f,h) = -\frac{(0.1)^2}{6} f'''(\eta(x_1)), \quad \text{for} \quad \eta(x_1) \in (0.9, 1.1),$$

or

$$|E_C(f,h)| = \left| -\frac{(0.1)^2}{6} \right| |f'''(\eta(x_1))|, \quad \text{for} \quad \eta(x_1) \in (0.9, 1.1).$$

Since

$$f'''(\eta(x_1)) = -6\eta(x_1)\cos\eta(x_1) - (6 - \eta(x_1)^2)\sin\eta(x_1)$$

This formula cannot be computed exactly because $\eta(x_1)$ is not known. But one can bound the error by computing the largest possible value for $|f'''(\eta(x_1))|$. So bound $|f'''|$ on $[0.9, 1.1]$ is

$$M = \max_{0.9 \le x \le 1.1} |-6x\cos x - (6 - x^2)\sin x| = 7.4222,$$

at $x = 0.9$. *Thus, for* $|f'''(\eta(x_1))| \leq M$ *and* $h = 0.1$, *gives*

$$|E_C(f,h)| \leq \frac{0.01}{6} M = \frac{0.01}{6}(7.4222) = 0.0124,$$

which is the possible maximum error in our approximation.

(c) Since the exact value of the derivative $f'(1)$ *is,* 0.2391, *therefore, the absolute error* $|E|$ *can be computed as follows*

$$|E| = |f'(1) - D_h f(1)| = |0.2391 - 0.2270| = 0.0121.$$

(d) Since the given accuracy required is 10^{-2}, *so*

$$|E_C(f,h)| = \Big| -\frac{h^2}{6} f'''(\eta(x_1)) \Big| \leq 10^{-2},$$

for $\eta(x_1) \in (0.9, 1.1)$. *Then*

$$\frac{h^2}{6} M \leq 10^{-2}.$$

Solving for h *and taking* $M = 0.0121$, *we obtain*

$$h^2 \leq \frac{6}{742.22} = 0.01.$$

So the best maximum value of h is 0.1. •

Example 5.6 *Consider the following table for set of data points*

x	1	1.6	2	2.3	2.8	3	3.9	4	4.8	5
$f(x)$	0.00	0.47	0.69	0.83	1.03	1.10	1.36	1.39	1.57	1.61

(a) Use the best three-point formula to find approximation of $f'(3)$ and $f'(1.5)$.
(b) The function tabulated is $\ln x$, find error bound and absolute error for the approximation of $f'(3)$.
(c) What is the best maximum value of stepsize h required to obtain the approximate value of $f'(3)$ within the accuracy 10^{-4}.

Solution. *(a) For the given table of data points, we can use all three-points formulas as for the central difference we can take*

$$x_0 = x_1 - h = 2, \quad x_1 = 3, \quad x_2 = x_1 + h = 4, \quad \textit{gives} \quad h = 1,$$

for the forward difference formula we can take

$$x_0 = 3, \quad x_1 = x_0 + h = 3.9, \quad x_2 = x_0 + 2h = 4.8, \quad \textit{gives} \quad h = 0.9,$$

and for the backward difference formula we can take

$$x_0 = x_2 - 2h = 1.6, \quad x_1 = x_2 - h = 2.3, \quad x_2 = 3, \quad \textit{gives} \quad h = 0.7.$$

Since we know that smaller the vale of h better the approximation of the derivative of the function, therefore, for the given problem, backward difference is the best formula to find approximation of $f'(3)$ as

$$f'(3) \approx \frac{f(1.6) - 4f(2.3) + 3f(3)}{2(0.7)} \approx \frac{[0.47 - 4(0.83) + 3(1.10)]}{1.4} = 0.3214.$$

(b) Using error term of backward difference formula, we have

$$E_B(f,h) = \frac{h^2}{3} f'''(\eta), \quad \text{or} \quad |E_B(f,h)| \leq \frac{h^2}{3}|f'''(\eta)|.$$

Taking $|f'''(\eta(x_2))| \leq M = \max_{1.6 \leq x \leq 3} |f'''(x)| = \max_{1.6 \leq x \leq 3} |2/x^3| = 0.4883$. *Thus using* $h = 0.7$, *we obtain*

$$|E_B(f,h)| \leq \frac{(0.7)^2}{3}(0.4883) = 0.0798,$$

the required error bounds for the approximations. To compute the absolute error we do as

$$|E| = |f'(3) - 0.3214| = |0.3333 - 0.3214| = 0.0119.$$

(c) Since the given accuracy required is 10^{-4}, *so*

$$|E_B(f,h)| = \left|\frac{h^2}{3} f'''(\eta)\right| \leq 10^{-4},$$

for $\eta \in (1.6, 3)$. *Then*

$$\frac{h^2}{3} M \leq 10^{-4}.$$

Solving for h *by taking* $M = 0.4883$, *we obtain*

$$h^2 \leq \frac{3 \times 10^{-4}}{0.4883} = 0.0248,$$

and so $h = 0.025$ *the best maximum value of* h. •

Second Derivative Numerical Formula

Three-point Central Difference Formula

$$f''(x_1) \approx \frac{f(x_1+h) - 2f(x_1) + f(x_1-h)}{h^2}$$

is called the *three-point central-difference formula* for the approximation of the second derivative of a function $f(x)$ at the given point $x = x_1$.

Error Formula

$$E_C(f,h) = -\frac{h^2}{12} f^{(4)}(\eta(x_1)), \quad \text{where} \quad \eta(x_1) \in (x_1 - h, x_1 + h).$$

Example 5.13 *Consider following set of data points*

x	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.9	1.0	1.1	1.2
$f(x)$	1.00	1.10	1.18	1.26	1.32	1.38	1.43	1.47	1.52	1.54	1.55	1.56

Use the table, find the best approximation of $f'(0.75)$ and the worst approximations of $f'(0.1)$ and $f''(0.6)$ by using three-point formulas.

Solution. *For the best approximation of* $f'(0.75)$, *we have to take small* $h = 0.15$, *so using the three-point formula (5.12), we get*

$$f'(0.75) \approx \frac{f(0.9) - f(0.6)}{2(0.15)} \approx \frac{1.52 - 1.43}{0.3} = 0.3,$$

while the exact value of $f'(0.75)$ *is* 0.3184. *For the worst approximation of* $f'(0.1)$, *we have to take big* $h = 0.5$, *so using again the three-point formula (5.15), we get*

$$f'(0.1) \approx \frac{-3f(0.1) + 4f(0.6) - f(1.1)}{2(0.5)} \approx \frac{-3(1.1) + 4(1.43) - 1.55}{1} = 0.87.$$

Similarly, for the worst approximation of $f''(0.6)$, *we have to take big* $h = 0.6$, *so using the three-point formula (5.19), we get*

$$\begin{aligned} f''(0.6) &\approx \frac{f(0.0) - 2f(0.6) + f(1.2)}{0.36} \\ &\approx \frac{[1.0 - 2(1.43) + 1.56]}{0.36} \approx -0.8333, \end{aligned}$$

the required approximation. •

Richardson's Extrapolation

Richardson's extrapolation is used to generate high-accuracy results while using low-order formulas.

Extrapolation can be applied whenever it is known that an approximation technique has an error term with a predictable form, one that depends on a parameter, usually the step size h. Suppose that for each number $h \neq 0$ we have a formula $N(h)$ that approximates an unknown value M and that the truncation error involved with the approximation has the form

$$M - N(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots,$$

$$M = N(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots. \tag{4.10}$$

Since the formula is assumed to hold for all positive h, consider the result when we replace the parameter h by half its value. Then we have the formula

$$M = N\left(\frac{h}{2}\right) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots.$$

Subtracting (4.10) from twice this equation eliminates the term involving K_1 and gives

$$M = \left[N\left(\frac{h}{2}\right) + \left(N\left(\frac{h}{2}\right) - N(h)\right)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots.$$

we define $N_1(h) \equiv N(h)$ and $\quad N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right].$

Then we have the $O(h^2)$ approximation formula for M:

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots . \tag{4.11}$$

If we now replace h by $h/2$ in this formula, we have

$$M = N_2\left(\frac{h}{2}\right) - \frac{K_2}{8}h^2 - \frac{3K_3}{32}h^3 - \cdots . \tag{4.12}$$

This can be combined with Eq. (4.11) to eliminate the h^2 term. Specifically, subtracting (4.11) from 4 times Eq. (4.12) gives

$$3M = 4N_2\left(\frac{h}{2}\right) - N_2(h) + \frac{3K_3}{8}h^3 + \cdots ,$$

and dividing by 3 gives an $O(h^3)$ formula for approximating M:

$$M = \left[N_2\left(\frac{h}{2}\right) + \frac{N_2(h/2) - N_2(h)}{3}\right] + \frac{K_3}{8}h^3 + \cdots .$$

By defining

$$N_3(h) \equiv N_2\left(\frac{h}{2}\right) + \frac{N_2(h/2) - N_2(h)}{3},$$

we have the $O(h^3)$ formula:

$$M = N_3(h) + \frac{K_3}{8}h^3 + \cdots.$$

The process is continued by constructing an $O(h^4)$ approximation

$$N_4(h) = N_3\left(\frac{h}{2}\right) + \frac{N_3(h/2) - N_3(h)}{7},$$

an $O(h^5)$ approximation

$$N_5(h) = N_4\left(\frac{h}{2}\right) + \frac{N_4(h/2) - N_4(h)}{15},$$

and so on. In general, if M can be written in the form

$$M = N(h) + \sum_{j=1}^{m-1} K_j h^j + O(h^m), \tag{4.13}$$

then for each $j = 2, 3, \ldots, m$, we have an $O(h^j)$ approximation of the form

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}. \tag{4.14}$$

These approximations are generated by rows in the order indicated by the numbered entries in Table 4.5. This is done to take best advantage of the highest-order formulas.

$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^4)$
1: $N_1(h) \equiv N(h)$			
2: $N_1(\frac{h}{2}) \equiv N(\frac{h}{2})$	3: $N_2(h)$		
4: $N_1(\frac{h}{4}) \equiv N(\frac{h}{4})$	5: $N_2(\frac{h}{2})$	6: $N_3(h)$	
7: $N_1(\frac{h}{8}) \equiv N(\frac{h}{8})$	8: $N_2(\frac{h}{4})$	9: $N_3(\frac{h}{2})$	10: $N_4(h)$

EXAMPLE

The centered difference formula in Eq. (4.5) to approximate $f'(x_0)$ can be expressed with an error formula:

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots.$$

Since this error formula contains only even powers of h, extrapolation is more effective than as outlined in the opening discussion. In this case, we have the $O(h^2)$ approximation

$$f'(x_0) = N_1(h) - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots, \tag{4.15}$$

where $\quad N_1(h) \equiv N(h) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)].$

Replacing h by $h/2$ in this formula gives the approximation

$$f'(x_0) = N_1\left(\frac{h}{2}\right) - \frac{h^2}{24}f'''(x_0) - \frac{h^4}{1920}f^{(5)}(x_0) - \cdots.$$

Subtracting (4.15) from 4 times this equation eliminates the $O(h^2)$ term that involves $f'''(x_0)$ and gives

$$3f'(x_0) = 4N_1\left(\frac{h}{2}\right) - N_1(h) + \frac{h^4}{160}f^{(5)}(x_0) + \cdots.$$

Dividing by 3 provides an $O(h^4)$ formula

$$f'(x_0) = N_2(h) + \frac{h^4}{480}f^{(5)}(x_0) + \cdots,$$

where

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \frac{N_1(h/2) - N_1(h)}{3}.$$

Continuing this procedure gives, for each $j = 2, 3, \ldots,$ an $O(h^{2j})$ approximation

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}.$$

Notice that the denominator of the quotient is $4^{j-1} - 1$ instead of $2^{j-1} - 1$ because we are now eliminating powers of h^2 instead of powers of h. Since $(h/2)^2 = h^2/4$, the multipliers used to eliminate the powers of h^2 are powers of 4 instead of 2.

Suppose that $x_0 = 2.0$, $h = 0.2$, and $f(x) = xe^x$. Then

$$N_1(0.2) = N(0.2) = \frac{1}{0.4}[f(2.2) - f(1.8)] = 22.414160,$$

$$N_1(0.1) = N(0.1) = 22.228786,$$

and $$N_1(0.05) = N(0.05) = 22.182564.$$

The extrapolation table for these data is

$N_1(0.2) = 22.414160$		
$N_1(0.1) = 22.228786$	$N_2(0.2) = N_1(0.1) + \dfrac{N_1(0.1) - N_1(0.2)}{3} = 22.166995$	
$N_1(0.05) = 22.182564$	$N_2(0.1) = N_1(0.05) + \dfrac{N_1(0.05) - N_1(0.1)}{3} = 22.167157$	$N_3(0.2) = N_2(0.1) + \dfrac{N_2(0.1) - N_2(0.2)}{15} = 22.167168$

The exact value of $f'(x) = xe^x + e^x$ at $x_0 = 2.0$ to six decimal places is 22.167168, so all the digits of $N_3(0.2)$ are exact, even though the best original approximation, $N_1(0.05)$, has only one decimal place of accuracy.

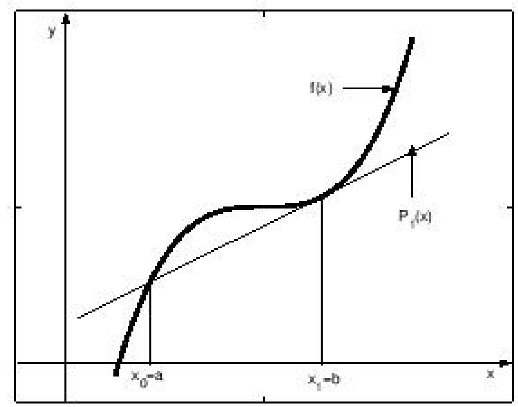
Numerical Integration

we wish to find an approximation to the *definite integral*

$$I(f) = \int_a^b f(x)dx,$$

An obvious approach is to replace a function $f(x)$ in the integral (5.21) by

$$I(f) = \int_a^b f(x)dx \approx \int_a^b p(x)dx.$$



Simple Trapezoidal Rule

$x_0 = a, x_1 = b$ and $h = x_1 - x_0$,

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

$$\int_{x_0}^{x_1} f(x)dx \approx \frac{f(x_0)}{x_0 - x_1} \int_{x_0}^{x_1} (x - x_1)dx + \frac{f(x_1)}{x_1 - x_0} \int_{x_0}^{x_1} (x - x_0)dx,$$

$$\approx \frac{f(x_0)}{x_0 - x_1} \left[\frac{(x - x_1)^2}{2} \bigg|_{x_0}^{x_1} \right] + \frac{f(x_1)}{x_1 - x_0} \left[\frac{(x - x_0)^2}{2} \bigg|_{x_0}^{x_1} \right] \approx \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)],$$

and by taking $h = x_1 - x_0$, we get

$$\int_a^b f(x)dx \approx T_1(f) = \frac{h}{2}[f(x_0) + f(x_1)].$$

Example 5.16 *Approximate the following integral*

$$\int_1^2 \frac{1}{x+1}dx,$$

using the Trapezoidal rule and compute the absolute error.

Solution. *Given* $f(x) = \dfrac{1}{x+1}$ *and* $h = 1$, *so using Trapezoidal rule (5.28), gives*

$$T_1(f) = \frac{1}{2}[f(1) + f(2)] = 0.4167.$$

The exact solution of the given integral is

$$I(f) = \ln(3/2) = 0.4055, \quad \text{so} \quad |E_{T_1}(f)| = |I(f) - T_1(f)| = |0.4055 - 0.4167| = 0.0112,$$

is the required absolute error. •

Composite Trapezoidal Rule

The interval $[a, b]$ is partitioned into n subintervals (x_{i-1}, x_i), $\quad i = 1, 2, \ldots, n$ with $a = x_0$ and $b = x_n$ of equal width $h = (b - a)/n$

Theorem 5.2 (Composite Trapezoidal Rule)

Let $f \in C^2[a, b]$, n may be odd or even, $h = (b - a)/n$, and $x_i = a + ih$ for each $i = 0, 1, 2, \ldots, n$. Then the composite Trapezoidal rule for n subintervals can be written as

$$\int_{a=x_0}^{b=x_n} f(x)dx \approx T_n(f) = \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right]. \tag{5.29}$$

Proof. *Since for the composite form of the Trapezoidal rule, the interval is divided into n equal subintervals of width h so that $h = \dfrac{b-a}{n}$, and (n+1) distinct points $a = x_0 < x_1 < x_2 \ldots < x_n = b$, then we have*

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx.$$

Applying the Trapezoidal rule (5.28) for one strip to each of these integral, we have

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(x_0) + f(x_1)] + \frac{h}{2}[f(x_1) + f(x_2)] + \cdots + \frac{h}{2}[f(x_{n-1}) + f(x_n)].$$

Note that each of the interior point is counted twice and therefore has a coefficient of two whereas the endpoints are counted once and therefore has a coefficient one. •

Example 5.17 *Evaluate the integral* $\int_0^1 e^{4x}dx$ *by using the Trapezoidal rule with* $n = 1, 2, 4, 8$. *Also compute the corresponding actual errors.*

Solution. *For* $n = 1$, *we use the formula (5.28) for* $h = 1$, *as follows*

$$T_1(f) = \frac{1}{2}\Big[f(0) + f(1)\Big] = 27.7991.$$

For $n = 2$, *using the formula (5.29) and* $h = 0.5$, *we have*

$$T_2(f) = \frac{0.5}{2}\Big[f(0) + 2f(0.5) + f(1)\Big] = 17.5941.$$

For $n = 4$, *using the formula (5.29) and* $h = 0.25$, *we have*

$$T_4(f) = \frac{0.25}{2}\Big[f(0) + 2[f(0.25) + f(0.5) + f(0.75)] + f(1)\Big] = 14.4980.$$

Finally, for $n = 8$, *using (5.29) and* $h = 0.125$, *we have*

$$\begin{aligned} T_8(f) &= \frac{0.125}{2}\Big[f(0) + 2[f(0.125) + f(0.25) + f(0.375) + f(0.5) \\ &+ f(0.625) + f(0.75) + f(0.875)] + f(1)\Big] = 13.6776. \end{aligned}$$

Since the exact value of the given integral is

$$I(f) = \frac{1}{4}[e^4 - 1] = 13.4000.$$

So the corresponding actual errors are, $-14.3991, -4.1941, -1.0980$ and -0.2776, respectively, which decrease by a factor of about *four* at each stage. •

Error Terms for Trapezoidal Rule

Theorem 5.3 (Error term for Simple Trapezoidal Rule)

Let $f \in C^2[a,b]$, and $h = (b-a)$. The local error that the simple Trapezoidal rule (5.28) makes in estimating the definite integral (5.21) is

$$E_{T_1}(f) = -\frac{h^3}{12} f''(\eta(x)), \tag{5.30}$$

where $\eta(x) \in (a,b)$.

Error Term for Composite Trapezoidal Rule

The *global error* of the Trapezoidal rule (5.29) equals the sum of n local errors of the Trapezoidal rule (5.28), that is

$$\begin{aligned}
E_{T_n}(f) &= -\frac{h^3}{12} f''(\eta_1(x)) - \frac{h^3}{12} f''(\eta_2(x)) - \cdots - \frac{h^3}{12} f''(\eta_n(x)), \\
&= -\frac{h^3}{12} \sum_{i=1}^{n} f''(\eta_i(x)), \quad \text{for} \quad \eta_i(x) \in (x_{i-1}, x_i), \\
&= -\frac{h^3}{12} n f''(\eta(x)), \\
&= -\frac{h^2}{12} (b-a) f''(\eta(x)), \quad \eta(x) \in (a,b).
\end{aligned}$$

Example 5.20 *(a)Find approximation of* $\int_1^2 f(x)\,dx$ *taking* $h = 0.2$ *by using the following set of data points*

x	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0
$f(x)$	0.368	0.366	0.361	0.354	0.355	0.335	0.323	0.311	0.298	0.284	0.271

The function tabulated is xe^{-x}, *compute error bound and the absolute error for the approximation using Trapezoidal rule.*
(b) How many subintervals approximate the given integral to an accuracy of at least 10^{-6} *?*

Solution. *(a) Given* $h = 0.2$, *so we have the select following set of data points for Trapezoidal rule as*

x	1.0	1.2	1.4	1.6	1.8	2.0
$f(x)$	0.368	0.361	0.355	0.323	0.298	0.271

so the composite Trapezoidal rule (5.29) for six points can be written as

$$\int_1^2 f(x)\,dx \approx T_5(f) = \frac{h}{2}\Big[f(x_0) + 2\Big(f(x_1) + f(x_2) + f(x_3) + f(x_4)\Big) + f(x_5)\Big],$$

and by using the given values, we get

$$\int_1^2 f(x)\,dx \approx 0.1\Big[0.368 + 2(0.361 + 0.355 + 0.323 + 0.298) + 0.271\Big] = 0.3313.$$

The second derivative of the function $f(x) = xe^{-x}$ *can be obtain as*

$$f'(x) = (1-x)e^{-x} \quad \text{and} \quad f''(x) = (x-2)e^{-x}.$$

Since $\eta(x)$ *is unknown point in* $(1,2)$, *therefore, the bound* $|f''|$ *on* $[1,2]$ *is*

$$M = \max_{1\le x\le 2} |f''(x)| = \max_{1\le x\le 2} |(x-2)e^{-x}| = 0.3679,$$

at $x = 1$. *Thus the error formula (5.35) becomes*

$$|E_{T_5}(f)| \leq \frac{(0.2)^2(1)}{12}(0.3679) = 0.0012,$$

which is the possible maximum error in our approximation.
We can easily computed the exact value of the given integral as

$$\int_1^2 xe^{-x}\ dx = (-xe^{-x} - e^{-x})\Big|_1^2 = 0.3298.$$

Thus the absolute error $|E|$ *in our approximation is given as*

$$|E| = |0.3298 - T_5(f)| = |0.3298 - 0.3313| = 0.0015.$$

(b) To find the minimum subintervals for the given accuracy, we use the formula (5.35) such that

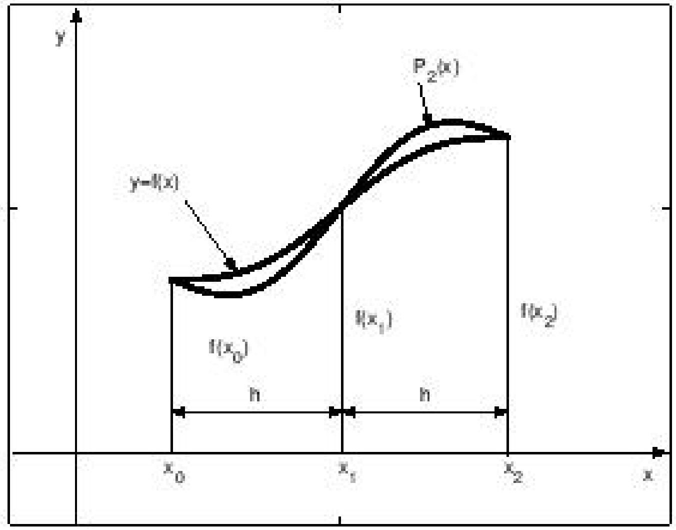
$$|E_{T_n}(f)| \leq \frac{|-(b-a)^3|}{12n^2} M \leq 10^{-6},$$

where $h = (b-a)/n$. *Since* $M = 0.3679$, *then solving for* n^2, *we obtain*

$$n^2 \geq 30658.3333, \quad \textit{gives} \quad n \geq 175.0952.$$

Hence to get the required accuracy, we need 176 *subintervals or* 177 *points.* •

Simple Simpson's Rule



Let us consider the second-degree Lagrange interpolating polynomial, with equally spaced base points, that is, $x_0 = a, x_1 = a + h$ and $x_2 = a + 2h$, with $h = (b - a)/2$, then

$$f(x) \approx p_2(x) \quad = \quad \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \quad + \quad \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2).$$

Taking integral on both sides of the above equation with respect to x between the limits x_0 and x_2, we have

$$\begin{aligned}\int_{x_0}^{x_2} f(x)dx \quad &\approx \quad \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} \int_{x_0}^{x_2} (x - x_1)(x - x_2)dx \quad + \quad \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} \int_{x_0}^{x_2} (x - x_0)(x - x_2)dx \\ &+ \quad \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)} \int_{x_0}^{x_2} (x - x_0)(x - x_1)dx, \\ &\approx \frac{f(x_0)}{2h^2} I_1 + \frac{f(x_1)}{-h^2} I_2 + \frac{f(x_2)}{2h^2} I_3,\end{aligned}$$

where

$$I_1 = \int_{x_0}^{x_2} (x - x_1)(x - x_2)dx \; = \frac{2h^3}{3},$$

$$I_2 = \int_{x_0}^{x_2} (x - x_0)(x - x_2)dx; \; = -\frac{4h^3}{3},$$

$$I_3 = \int_{x_0}^{x_2} (x - x_0)(x - x_1)dx = \frac{2h^3}{3}.$$

By using these values, we have

$$\int_a^b f(x)dx \approx \frac{f(x_0)}{2h^2}\left(\frac{2h^3}{3}\right) + \frac{f(x_1)}{-h^2}\left(\frac{-4h^3}{3}\right) + \frac{f(x_2)}{2h^2}\left(\frac{2h^3}{3}\right).$$

Simplifying, gives

$$\int_a^b f(x)dx \approx S_2(f) = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)].$$

which is called the *simple Simpson's rule* or Simpson's rule for two strips (or 3 points).

Example 5.22 *Approximate the following integral*

$$\int_1^2 \frac{1}{x+1}dx,$$

using simple Simpson's rule. Compute the actual error.

Solution. *Since* $f(x) = \dfrac{1}{x+1}$ *and* $h = (2-1)/2 = 0.5$, *then by using Simpson's rule (5.37), we have*

$$S_2(f) = \frac{0.5}{3}\Big[f(1) + 4f(1.5) + f(2)\Big] = (0.1667)[0.5 + 1.6 + 0.3333] = 0.4056.$$

Hence

$$\int_1^2 \frac{1}{x+1}dx \approx S_2(f) = 0.4056.$$

Since the exact solution of the given integral is, 0.4055, *therefore, the actual error is*

$$E_{S_2} = I(f) - S_2(f) = -0.0001.$$

To compare this error with the error got by using the simple Trapezoidal rule, the error in Simpson's rule is much smaller than for the Trapezoidal rule by a factor of about 123, *a significant increase in accuracy.* •

Theorem 5.4 (Composite Simpson's Rule)

Let $f \in C^4[a,b]$, n be even, $h = (b-a)/n$, and $x_i = a + ih$ for each $i = 0, 1, 2, \ldots, n$. Then the composite Simpson's rule for n subintervals can be written as

$$\int_a^b f(x)dx \approx S_n(f) = \frac{h}{3}\left[f(a) + 2\sum_{i=1}^{n/2-1} f(x_{2i}) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + f(b)\right]. \tag{5.38}$$

Proof. *Since for the composite form of the Simpson's rule, the interval is divided into n equal subintervals of width h so that $h = \dfrac{b-a}{n}$. For this rule to work, n must be even number and the total number of (n+1) distinct points $a = x_0 < x_1 < x_2 \ldots < x_n = b$ should be odd. The total integral can be represented as*

$$\int_{x_0}^{x_n} f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx.$$

Substitute the simple Simpson's rule (5.37) for the individual integral yields

$$\begin{aligned}\int_{x_0}^{x_n} f(x)dx &\approx \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] + \frac{h}{3}[f(x_2) + 4f(x_3) + f(x_4)] \\ &+ \cdots + \frac{h}{3}[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)].\end{aligned}$$

To avoid repetition of terms, we summed them. Note that each of the odd interior point is counted four and so has a coefficient of four whereas each of the even interior point is counted two and so has a coefficient of two. Endpoints are counted once and so has a coefficient one. •

Example 5.27 *Evaluate the integral* $\int_0^1 e^{4x} dx$ *by using the Simpson's rule with* $n = 2, 4, 8$. *Also, compute the corresponding actual errors.*

Solution. *For* $n = 2$, *using the formula (5.37) and* $h = 0.5$, *we have*

$$S_2(f) = \frac{0.5}{3}\Big[f(0) + 4f(0.5) + f(1)\Big] = 14.1924.$$

For $n = 4$, *using the formula (5.38) and* $h = 0.25$, *we have*

$$S_4(f) = \frac{0.25}{3}\Big[f(0) + 4[f(0.25) + f(0.75)] + 2f(0.5) + f(1)\Big] = 13.4659.$$

For $n = 8$, *using the formula (5.38) and* $h = 0.125$, *we have*

$$\begin{aligned} S_8(f) = \frac{0.125}{3}\Big[f(0) &+ 4[f(0.125) + f(0.375) + f(0.625) + f(0.875)] \\ &+ 2[f(0.25) + f(0.5) + f(0.75)] + f(1)\Big] = 13.4041. \end{aligned}$$

Note that the exact value of the given integral is 13.39995, *and so the corresponding errors are,* $0.79245, 0.06595$, *and* 0.00411 *respectively, which decrease by a factor of about 16 at each stage.* •

Error Terms for Simpson's Rule

Now we discuss the local error and the global error formulas for Simpson's rule.

Theorem 5.5 (Error Term for Simple Simpson's Rule)

Let $f \in C^4[a,b]$, and $h = (b-a)/2$. The local error that the Simpson's rule makes in estimating the definite integral (5.21) is

$$E_{S_2}(f) = -\frac{h^5}{90} f^{(4)}(\eta(x)), \qquad \text{where } \eta(x) \in (a,b).$$

Example 5.28 *Compute the local error for the Simpson's rule using the following integral*

$$\int_1^2 \frac{1}{x+1} dx.$$

Solution. *Given $f(x) = \dfrac{1}{x+1}$, and $[a,b] = [1,2]$, then the fourth derivative of the function can be obtain as*

$$f' = \frac{-1}{(x+1)^2}, \quad f'' = \frac{2}{(x+1)^3}, \quad f''' = \frac{-6}{(x+1)^4}, \quad f^{(4)} = \frac{24}{(x+1)^5}.$$

$$|E_{S_2}(f)| = \left| -\frac{h^5}{90} \right| \left| f^{(4)}(\eta(x)) \right|, \quad \text{for} \quad \eta(x) \in (1,2).$$

$$M = \max_{1 \le x \le 2} = \left| \frac{24}{(x+1)^5} \right| = 0.75. \qquad \text{we get} \qquad |E_{S_2}(f)| \le \frac{(0.03125)}{90}(0.75) = 0.0003.$$

Comparing this with the actual error -0.0001, this bound is about 3 times the actual error.

Error Term for Composite Simpson's Rule

$$E_{S_n}(f) = -\frac{h^5}{90}f^{(4)}(\eta_1(x)) - \frac{h^5}{90}f^{(4)}(\eta_2(x)) - \cdots - \frac{h^5}{90}f^{(4)}(\eta_{n/2}(x)),$$

$$E_{S_n}(f) = -\frac{(b-a)}{180}h^4 f^{(4)}(\eta(x)), \quad \text{for } \eta(x) \in (a,b) \text{ and } nh = b-a.$$

is known as the *global error* of the Simpson's rule.

Example 5.30 *Consider the integral* $I(f) = \int_1^2 \ln(x+1)dx; \qquad n = 6.$

(a) Find the approximation of the give integral using the composite Simpson's rule.
(b) Compute the error bound for the approximation using the formula (5.57).
(c) Compute the absolute error.
(d) How many subintervals approximate the given integral to an accuracy of at least 10^{-4} *using the composite Simpson's rule ?*

Solution. *(a) Given* $f(x) = \ln(x+1), n = 6$*, and so* $h = \frac{2-1}{6} = \frac{1}{6}$*, then the composite Simpson's rule (5.38) for n = 6, can be written as*

$$\begin{aligned}\int_1^2 \ln(x+1)dx \approx S_6(f) &= \frac{1/6}{3}\Big[\ln(1+1) + 4(\ln\Big(\frac{7}{6}+1\Big) + \ln\Big(\frac{9}{6}+1\Big) + \ln\Big(\frac{11}{6}+1\Big)\Big)\Big] \\ &+ \Big[2\Big(\ln\Big(\frac{8}{6}+1\Big) + \ln\Big(\frac{10}{6}+1\Big)\Big) + \ln(2+1)\Big]. \\ &= \frac{1}{18}\Big[0.6932 + 4(2.7309) + 2(1.8281) + 1.0986\Big] = 0.9095.\end{aligned}$$

(b) Since the fourth derivative of the function is

$$f^{(4)}(x) = \frac{-6}{(x+1)^4}.$$

Since $\eta(x)$ *is unknown point in* $(1,2)$*, therefore, the bound* $|f^{(4)}|$ *on* $[1,2]$ *is*

$$M = \max_{1 \leq x \leq 2} |f^{(4)}(x)| = \left| \frac{-6}{(x+1)^4} \right| = 6/16 = 0.375.$$

Thus the error formula (5.57) becomes

$$|E_{T_6}(f)| \leq \frac{(1/6)^4}{180}(0.375) = 0.000002,$$

which is the possible maximum error in our approximation in part (a).
(c) The absolute error $|E|$ *in our approximation is given as*

$$|E| = |3\ln 3 - 2\ln 2 - 1 - S_6(f)| == 0.0000003.$$

(d) To find the minimum subintervals for the given accuracy, we use the error formula (5.57) which is

$$|E_{S_n}(f)| \leq \frac{(b-a)^5}{180n^4} M \leq 10^{-4}.$$

Since we know $M = 0.375$*, then we have*

$$n^4 \geq 20.83333, \quad \textit{gives} \quad n \geq 2.136435032.$$

Hence to get the required accuracy, we need 4 subintervals (because n *should be even) that ensures the stipulated accuracy.* •

EXAMPLE

The Trapezoidal rule for a function f on the interval [0, 2] is

$$\int_0^2 f(x)\,dx \approx f(0) + f(2),$$

and Simpson's rule for f on [0,2] is

$$\int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

The results to three places for some elementary functions are summarized in Table 4.7. Notice that in each instance Simpson's Rule is significantly better. ■

$f(x)$	x^2	x^4	$1/(x+1)$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

The standard derivation of quadrature error formulas is based on determining the class of polynomials for which these formulas produce exact results. The next definition is used to facilitate the discussion of this derivation.

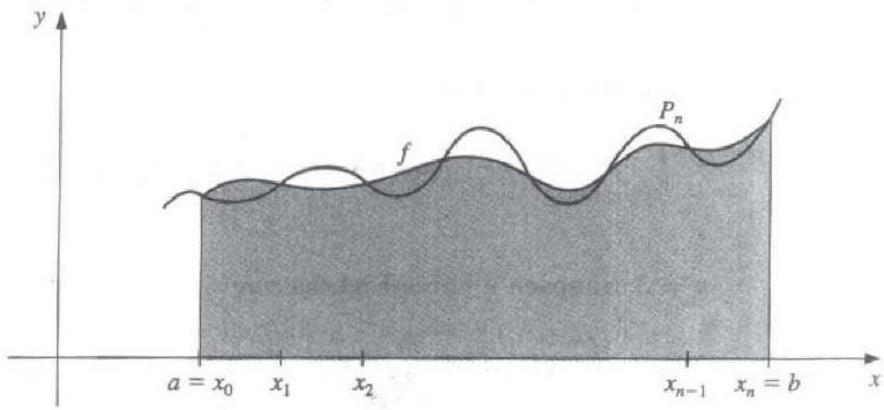
Definition The **degree of accuracy**, or **precision**, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$. ■

Definition implies that the Trapezoidal and Simpson's rules have degrees of precision one and three, respectively.

Newton-Cotes formulas.

The Trapezoidal and Simpson's rules are examples of a class of methods known as Newton-Cotes formulas. There are two types of Newton-Cotes formulas, open and closed.

The $(n+1)$-*point closed Newton-Cotes formula* uses nodes $x_i = x_0 + ih$, for $i = 0, 1, \ldots, n$, where $x_0 = a$, $x_n = b$ and $h = (b-a)/n$. (See Figure 4.5.) It is called closed because the endpoints of the closed interval $[a, b]$ are included as nodes. The formula



assumes the form

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

where

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

Theorem

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 $h = (b-a)/n$. 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 even and $f \in C^{n+2}[a, b]$, and

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

if n is odd and $f \in C^{n+1}[a, b]$. ■

Some of the common **closed Newton-Cotes formulas** with their error terms are as follows:

$n = 1$: Trapezoidal rule

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

$n = 2$: Simpson's rule

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

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

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

$n = 4$:

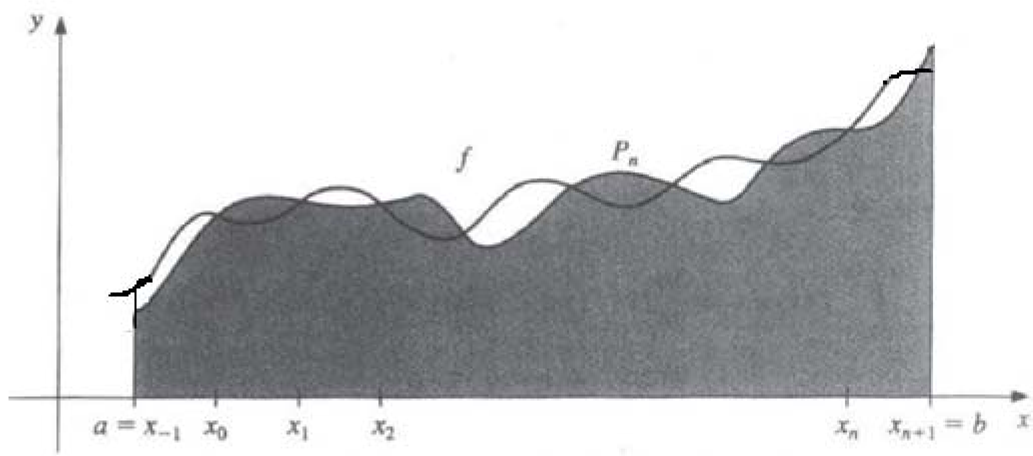
$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] - \frac{8h^7}{945}f^{(6)}(\xi),$$

where $\quad x_0 < \xi < x_4.$

The *open Newton-Cotes formulas* use the nodes $x_i = x_0 + ih$, 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 $x_{n+1} = b$, as shown in Figure 4.6. Open formulas contain all the nodes used for the approximation within the open interval (a, b). The formulas 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 $\qquad a_i = \int_a^b L_i(x)\,dx.$



Theorem

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

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

if n is even and $f \in C^{n+2}[a, b]$, and

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

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

Some of the common **open Newton-Cotes** formulas with their error terms are

$n = 0$: Midpoint rule $$\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_1.$$

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

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

$n = 3$: $$\int_{x_{-1}}^{x_4} f(x)\,dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95}{144} h^5 f^{(4)}(\xi), \quad \text{where} \quad x_{-1} < \xi < x_4.$$

EXAMPLE

Using the closed and open Newton-Cotes formulas listed as (4.23)–(4.26) and (4.27)–(4.30) to approximate $\int_0^{\pi/4} \sin x \, dx = 1 - \sqrt{2}/2 \approx 0.29289322$ gives the results in Table 4.8. ■

n	0	1	2	3	4
Closed formulas		0.27768018	0.29293264	0.29291070	0.29289318
Error		0.01521303	0.00003942	0.00001748	0.00000004
Open formulas	0.30055887	0.29798754	0.29285866	0.29286923	
Error	0.00766565	0.00509432	0.00003456	0.00002399	

Romberg Integration

Romberg integration uses the Composite Trapezoidal rule to give preliminary approximations and then applies the Richardson extrapolation process to improve the approximations.

To begin the presentation of 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

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

where $a < \mu < b$, $h = (b-a)/m$ and $x_j = a + jh$, for each $j = 0, 1, \ldots, m$.

We first obtain Composite Trapezoidal rule approximations with $m_1 = 1$, $m_2 = 2$, $m_3 = 4, \ldots$, and $m_n = 2^{n-1}$, where n is a positive integer.

If the notation $R_{k,1}$ is introduced to denote the portion used for the trapezoidal approximation, then

$$R_{1,1} = \frac{h_1}{2}[f(a) + f(b)] = \frac{(b-a)}{2}[f(a) + f(b)];$$

$$R_{2,1} = \frac{h_2}{2}[f(a) + f(b) + 2f(a + h_2)] = \frac{1}{2}[R_{1,1} + h_1 f(a + h_2)];$$

$$R_{3,1} = \frac{1}{2}\{R_{2,1} + h_2[f(a + h_3) + f(a + 3h_3)]\};$$

$$R_{k,1} = \frac{1}{2}\left[R_{k-1,1} + h_{k-1}\sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k)\right] \qquad \text{for each } k = 2, 3, \ldots, n.$$

Richardson extrapolation will be used to speed the convergence.

To simplify the notation we define

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

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

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

The results that are generated from these formulas are shown in Table

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

EXAMPLE

Using Eq. (4.32) to perform the first step of the Romberg integration scheme for approximating $\int_0^\pi \sin x\, dx$ with $n = 6$ leads to the equations

$$R_{1,1} = \frac{\pi}{2}[\sin 0 + \sin \pi] = 0;$$

$$R_{2,1} = \frac{1}{2}\left[R_{1,1} + \pi \sin \frac{\pi}{2}\right] = 1.57079633;$$

$$R_{3,1} = \frac{1}{2}\left[R_{2,1} + \frac{\pi}{2}\left(\sin \frac{\pi}{4} + \sin \frac{3\pi}{4}\right)\right] = 1.89611890;$$

$$R_{4,1} = \frac{1}{2}\left[R_{3,1} + \frac{\pi}{4}\left(\sin \frac{\pi}{8} + \sin \frac{3\pi}{8} + \sin \frac{5\pi}{8} + \sin \frac{7\pi}{8}\right)\right] = 1.97423160;$$

$$R_{5,1} = 1.99357034, \quad \text{and} \quad R_{6,1} = 1.99839336.$$

Since the correct value for the integral in Example 1 is 2, the convergence is quite slow. Romberg technique will be used to speed the convergence.

0					
1.57079633	2.09439511				
1.89611890	2.00455976	1.99857073			
1.97423160	2.00026917	1.99998313	2.00000555		
1.99357034	2.00001659	1.99999975	2.00000001	1.99999999	
1.99839336	2.00000103	2.00000000	2.00000000	2.00000000	2.00000000

Gaussian Quadrature

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 decrease the accuracy of the approximation.

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 the approximation

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} c_i f(x_i).$$

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 fact that they must 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 polynomials of degree at most $2n - 1$ also contains $2n$ parameters. This, then, is the largest class of polynomials for which it is reasonable to expect the formula to be exact. With 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, and x_2 so that the integration formula

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

gives the exact result whenever $f(x)$ is a polynomial of degree $2(2) - 1 = 3$ 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

$$\int (a_0 + a_1 x + a_2 x^2 + a_3 x^3)\,dx = a_0 \int 1\,dx + a_1 \int x\,dx + a_2 \int x^2\,dx + a_3 \int x^3\,dx,$$

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

$$c_1 \cdot 1 + c_2 \cdot 1 = \int_{-1}^{1} 1\,dx = 2, \qquad c_1 \cdot x_1 + c_2 \cdot x_2 = \int_{-1}^{1} x\,dx = 0,$$

$$c_1 \cdot x_1^2 + c_2 \cdot x_2^2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3}, \quad \text{and} \quad c_1 \cdot x_1^3 + c_2 \cdot x_2^3 = \int_{-1}^{1} x^3\,dx = 0.$$

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

$$c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3}, \quad \text{and} \quad x_2 = \frac{\sqrt{3}}{3},$$

which gives the approximation formula

$$\int_{-1}^{1} f(x)\,dx \approx f\left(\frac{-\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right). \tag{4.41}$$

This formula has degree of precision 3, that is, it produces the exact result for every polynomial of degree 3 or less.

This technique could be used to determine the nodes and coefficients for formulas that give exact results for higher-degree polynomials, but an alternative method obtains them more easily.

The constants c_i needed for the quadrature rule are extensively tabulated. Table 4.11 lists these values for $n = 2, 3, 4$, and 5.

n	Roots $r_{n,i}$	Coefficients $c_{n,i}$
2	0.5773502692	1.0000000000
	−0.5773502692	1.0000000000
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	−0.7745966692	0.5555555556
4	0.8611363116	0.3478548451
	0.3399810436	0.6521451549
	−0.3399810436	0.6521451549
	−0.8611363116	0.3478548451
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286705
	0.0000000000	0.5688888889
	−0.5384693101	0.4786286705
	−0.9061798459	0.2369268850

An integral $\int_a^b f(x)\,dx$ over an arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using the change of variables

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

This permits Gaussian quadrature to be applied to any interval $[a, b]$, since

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b - a)t + (b + a)}{2}\right)\frac{(b - a)}{2}\,dt.$$

EXAMPLE

Consider the problem of finding approximations to $\int_1^{1.5} e^{-x^2}\,dx$. Table 4.12 lists the values for the Newton-Cotes formulas given in Section 4.3. The exact value of the integral to seven decimal places is 0.1093643.

n	0	1	2	3	4
Closed formulas		0.1183197	0.1093104	0.1093404	0.1093643
Open formulas	0.1048057	0.1063473	0.1094116	0.1093971	

The Gaussian quadrature procedure applied to this problem requires that the integral first be transformed into a problem whose interval of integration is $[-1, 1]$. Using Eq. (4.42), we have

$$\int_1^{1.5} e^{-x^2}\,dx = \frac{1}{4}\int_{-1}^{1} e^{(-(t+5)^2/16)}\,dt.$$

The values in Table 4.11 give the following Gaussian quadrature approximations for this problem:

$n = 2$:

$$\int_1^{1.5} e^{-x^2}\,dx \approx \frac{1}{4}[e^{-(5+0.5773502692)^2/16} + e^{-(5-0.5773502692)^2/16}] = 0.1094003;$$

$n = 3$:

$$\int_1^{1.5} e^{-x^2}\,dx \approx \frac{1}{4}[(0.5555555556)e^{-(5+0.7745966692)^2/16} + (0.8888888889)e^{-(5)^2/16}$$
$$+ (0.5555555556)e^{-(5-0.7745966692)^2/16}] = 0.1093642.$$

For further comparison, the values obtained using the Romberg procedure with $n = 4$ are listed in Table 4.13. ■

0.1183197			
0.1115627	0.1093104		
0.1099114	0.1093610	0.1093643	
0.1095009	0.1093641	0.1093643	0.1093643