Numerical Differentiation and Integration

APM1137 - Numerical Analysis

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Numerical Differentiation

The derivative of f at x_0 is

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

An obvious way to generate an approximation to $f'(x_0)$ is to simply compute for

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

for small values of h but is not very successful due to roundoff error.

To approximate $f'(x_0)$, suppose $x_0 \in (a,b)$, where $f \in C^2[a,b]$ and $x_1 = x_0 + h$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a,b]$.

Construct the first Lagrange polynomial $P_{0,1}(x)$ of f determined by x_0 and x_1, with its error term:

$$\begin{aligned} f(x) &= P_{0,1}(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)) \\ &= \frac{f(x_0)(x-x_0-h)}{-h} + \frac{f(x_0+h)(x-x_0)}{h} \\ &\quad + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)) \end{aligned}$$

for some $\xi(x)$ between x_0 and x_1

Differentiating gives

$$\begin{aligned} f'(x) &= \frac{f(x_0+h)-f(x_0)}{h} + \frac{2(x-x_0)-h}{2} f''(\xi(x)) \\ &\quad + \frac{(x-x_0)(x-x_0-h)}{2} D_x(f''(\xi(x))) \end{aligned}$$

When $x = x_0$, the coefficient of $D_x(f''(\xi(x)))$ is 0, and the formula simplifies to

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} + \frac{h}{2} f''(\xi(x))$$

For small values of h, $[f(x_0+h)-f(x_0)]/h$ can be used to approximate $f'(x_0)$ with an error bounded by $M|h|/2$, where M is a bound on $|f''(x)|$ for $x_0 < x < x_0 + h$. This is the **forward-difference formula** if $h > 0$ and the **backward-difference formula** if $h < 0$.

Example

Use the forward-difference formula to approximate the derivative of $f(x) = lnx$ at $x_0 = 1.8$ using $h = 0.1$, and determine bounds for the approximation errors.

Solution

The forward-difference formula

$$\frac{f(1.8+h)-f(1.8)}{h}$$

with $h = 0.1$ gives 0.5406722.

because $f''(x) = -1/x^2$ and $1.8 < \xi < 1.9$, a bound for this approximation error is

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} < \frac{0.1}{2(1.8)^2} = 0.0154321$$

To obtain general derivative approximation formulas, suppose that $\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$. Then

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x - x_0)\cdots(x - x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$$

for some $\xi(x)$ in I, where $L_k(x)$ denotes the kth Lagrange coefficient polynomial for f at $x_0, x_1, \ldots, x_n$.

Differentiating this expression gives

$$\begin{aligned} f'(x) &= \sum_{k=0}^{n} f(x_k)L'_k(x) + D_x\left[\frac{(x-x_0)\cdots(x-x_n)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) \\ &\quad + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} D_x[f^{(n+1)}(\xi(x))] \end{aligned}$$

Thus, at any of the x_j, we have

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L'_k(x_j) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{\substack{k=0 \\ k\neq j}}^{n} (x_j - x_k)$$

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

Three-Point Formulas

Using the $(n+1)$-point formula with $x_j = x_0, x_1 = x_0 + h$ and $x_2 = x_0 + 2h$ gives

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_0)$$
$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$
$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, this gives three formulas for approximating $f'(x_0)$

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

$$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

$$f'(x_0) = \frac{1}{2h}\left[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

Three-Point Endpoint Formula

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

where $x_0 < \xi_0 < x_0 + 2h$

Three-Point Midpoint Formula

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

where $x_0 - h < \xi_0 < x_0 + h$

Five-Point Formulas

Five-Point Endpoint Formula

$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] + \frac{h^4}{5}f^{(5)}(\xi)$$

where $x_0 < x_0 + 4h$.Left-endpoint approximations are found using this formula with h > 0 and right-endpoint approximations with h < 0.

Five-Point Midpoint Formula

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30}f^{(5)}(\xi)$$

where $x_0 - 2h < x_0 + 2h$.

Example

Values for $f(x) = xe^x$ are given in the table. Use all applicable three-point and five-point formulas to approximate $f'(2.0)$.

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

We can use the three-point endpoint formula with $h = 0.1 or - 0.1$ and we can use the midpoint formula with $h = 0.1$ or $h = 0.2$. For the five-point formula, we can only use the midpoint formula with $h = 0.1$

$$f'(2.0) = \frac{1}{0.2}\left[-3f(2.0) + 4f(2.1) - f(2.2)\right] + \frac{h^2}{3}f^{(3)}(\xi_0) \approx 22.032310$$

$$f'(2.0) = \frac{1}{0.2}\left[-3f(2.0) + 4f(1.9) - f(1.8)\right] + \frac{h^2}{3}f^{(3)}(\xi_0) \approx 22.054525$$

$$f'(2.0) = \frac{1}{0.2}\left[f(2.1) - f(1.9)\right] - \frac{h^2}{6}f^{(3)}(\xi_1) \approx 22.228790$$

$$f'(2.0) = \frac{1}{0.4}\left[f(2.2) - f(1.8)\right] - \frac{h^2}{6}f^{(3)}(\xi_1) \approx 22.414163$$

$$f'(2.0) = \frac{1}{1.2}\left[f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)\right] + \frac{h^4}{30}f^{(5)}(\xi) \approx 22.166999$$

If we had no other information wewould accept the five-point midpoint approximation using $h = 0.1$ as the most accurate, and expect the true value to be between that approximation and the three-point mid-point approximation that is in the interval [22.166, 22.229].

Second Derivative Midpoint Formula

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0 - h) - 2f(x_0) + f(x_0 + h)\right] - \frac{h^2}{12} f^{(4)}(\xi)$$

for some $x_0 - h < \xi < x_0 + h$

Example

Using the same data from the previous example, we can approximate $f''(2.0)$ with $h = 0.1$ and $h = 0.2$

$$f''(2.0) = \frac{1}{0.01}\left[f(1.9) - 2f(2.0) + f(2.1)\right] - \frac{h^2}{12}f^{(4)}(\xi) \approx 29.593200$$

$$f''(2.0) = \frac{1}{0.02}\left[f(1.8) - 2f(2.0) + f(2.2)\right] - \frac{h^2}{12}f^{(4)}(\xi) \approx 29.704275$$

Roundoff Error Instability

It is particularly important to pay attention to round-off error when approximating derivatives.

Consider the three-point midpoint formula

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1)$$

Suppose that in evaluating $f(x_0+h) \& f(x_0-h)$, we encounter roundoff errors $e(x_0+h) \& e(x_0-h)$. The total error in approximation will be

$$f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} = \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1).$$

If we assume the roundoff errors $e(x_0 + h) \& e(x_0 - h)$ are each bounded by some $\varepsilon > 0$ and the third derivative is bounded by $M > 0$, then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M$$

To reduce the truncation error, $h2M/6$, we need to reduce h. But as h is reduced, the roundoff error ε/h grows. In practice, then, it is seldom advantageous to let h be too small, because in that case the round-off error will dominate the calculations.

Richardson Extrapolation

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 $N_1(h)$ that approximates an unknown constant M, and that the truncation error involved with the approximation has the form

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

for some collection of (unknown) constants $K_1, K_2, K_3, \ldots$

For small h, its higher orders are almost negligible so in general, $M - N_1(h) \approx K_1 h$.

The object of extrapolation is to find an easy way to combine these rather inaccurate $O(h)$ approximations in an appropriate way to produce formulas with a higher-order truncation error.

Suppose, for example, we can combine the $N_1(h)$ formulas to produce an $O(h^2)$ approximation formula, $N_2(h)$, for M with

$$M - N_2(h) = \hat{K}_2 h^2 + \hat{K}_3 h^3 + \cdots$$

for some collection of (unknown) constants $\hat{K}_2, \hat{K}_3, \ldots$. Then $M - N_2(h) \approx \hat{K}_2 h^2$.

If the constants K_1 and $\hat{K}_2$ are roughly of the same magnitude, then the $N_2(h)$ approximations would be much better than the corresponding $N_1(h)$ approximations. The extrapolation continues by combining the $N_2(h)$ approximations in a manner that produces formulas with $O(h^3)$ truncation error, and so on.

To see specifically how we can generate the extrapolation formulas, consider the $O(h)$ formula for approximating M

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

The formula is assumed to hold for all positive h, so we replace the parameter h by half its value. Then we have a second $O(h)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + K_1\left(\frac{h}{2}\right) + K_2\left(\frac{h}{2}\right)^2 + K_3\left(\frac{h}{2}\right)^3 + \cdots$$

Subtracting the first and twice the second would eliminate K1

$$\begin{aligned} M \quad = \quad & N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] \\ & + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots \end{aligned} \qquad (**)$$

Define

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]$$

Then equation $(**)$ is an $O(h^2)$ approximation formula for M

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

$$M = N_1(h) + K_1h^2 + K_2h^4 + K_3h^6 + \cdots . \tag{4.14}$$

The extrapolation is much more effective than when all powers of h are present because the averaging process produces results with errors $O(h^2)$, $O(h^4)$, $O(h^6)$, ..., with essentially no increase in computation, over the results with errors, $O(h)$, $O(h^2)$, $O(h^3)$, ...

Assume that approximation has the form of Eq. (4.14). Replacing h with $h/2$ gives the $O(h^2)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h^2}{4} + K_2\frac{h^4}{16} + K_3\frac{h^6}{64} + \cdots .$$

Subtracting Eq. (4.14) from 4 times this equation eliminates the h^2 term,

$$3M = \left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^4}{4} - h^4\right) + K_3\left(\frac{h^6}{16} - h^6\right) + \cdots .$$

Dividing this equation by 3 produces an $O(h^4)$ formula

$$M = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + \frac{K_2}{3}\left(\frac{h^4}{4} - h^4\right) + \frac{K_3}{3}\left(\frac{h^6}{16} - h^6\right) + \cdots .$$

Defining

$$N_2(h) = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] = N_1\left(\frac{h}{2}\right) + \frac{1}{3}\left[N_1\left(\frac{h}{2}\right) - N_1(h)\right],$$

produces the approximation formula with truncation error $O(h^4)$:

$$M = N_2(h) - K_2\frac{h^4}{4} - K_3\frac{5h^6}{16} + \cdots . \tag{4.15}$$

Now replace h in Eq. (4.15) with $h/2$ to produce a second $O(h^4)$ formula

$$M = N_2\left(\frac{h}{2}\right) - K_2\frac{h^4}{64} - K_3\frac{5h^6}{1024} - \cdots .$$

Subtracting Eq. (4.15) from 16 times this equation eliminates the h^4 term and gives

$$15M = \left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] + K_3\frac{15h^6}{64} + \cdots .$$

Dividing this equation by 15 produces the new $O(h^6)$ formula

$$M = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] + K_3\frac{h^6}{64} + \cdots .$$

We now have the $O(h^6)$ approximation formula

$$N_3(h) = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] = N_2\left(\frac{h}{2}\right) + \frac{1}{15}\left[N_2\left(\frac{h}{2}\right) - N_2(h)\right].$$

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

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

Table 4.6 shows the order in which the approximations are generated when

$$M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots . \tag{4.16}$$

It is conservatively assumed that the true result is accurate at least to within the agreement of the bottom two results in the diagonal, in this case, to within $|N_3(h) - N_4(h)|$.

Table 4.6

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

Elements of Numerical Integration

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain. The basic method involved in approximating definite integrals $\int_a^b f(x)dx$ called numerical quadrature. It uses a sum $\sum_{i=0}^{n} a_i f(x_i)$ to approximate $\int_a^b f(x)dx$.

The methods of quadrature in this section are based on the interpolation polynomials given in Module 2. The basic idea is to select a set of distinct nodes $\{x_0, \ldots, x_n\}$ from the interval $[a, b]$.

Then integrate the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i)L_i(x)$$

and its truncation error term over $[a, b]$ to obtain

$$\int_a^b f(x)\,dx = \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x)\,dx + \int_a^b \prod_{i=0}^{n}(x - x_i)\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,dx$$

$$= \sum_{i=0}^{n} a_i f(x_i) + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x - x_i) f^{(n+1)}(\xi(x))\,dx,$$

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

$$a_i = \int_a^b L_i(x)\,dx, \quad \text{for each } i = 0, 1, \ldots, n.$$

The quadrature formula is, therefore,

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

with error given by

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

Trapezoidal Rule

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

$$\begin{aligned}\int_a^b f(x)\,dx = &\int_{x_0}^{x_1} \left[\frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1)\right] dx \\ &+ \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)\,dx. \qquad (4.23)\end{aligned}$$

The product $(x-x_0)(x-x_1)$ does not change sign on $[x_0, x_1]$, so the Weighted Mean Value Theorem for Integrals 1.13 can be applied to the error term to give, for some ξ in (x_0, x_1),

$$\begin{aligned}\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)\,dx &= f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx \\ &= f''(\xi)\left[\frac{x^3}{3} - \frac{(x_1+x_0)}{2}x^2 + x_0x_1x\right]_{x_0}^{x_1} \\ &= -\frac{h^3}{6} f''(\xi).\end{aligned}$$

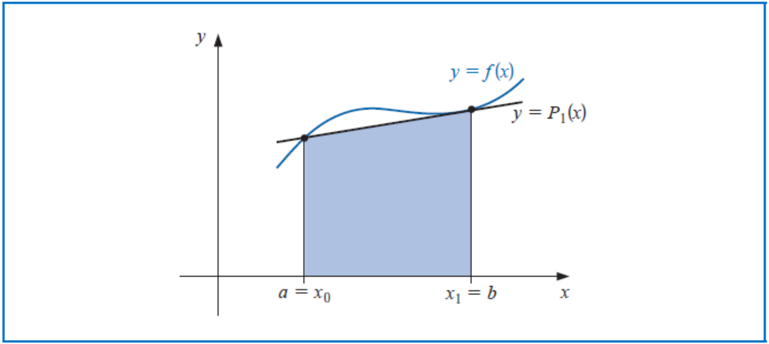
Consequently, Eq. (4.23) implies that

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

Using the notation $h = x_1 - x_0$ gives the following rule:

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

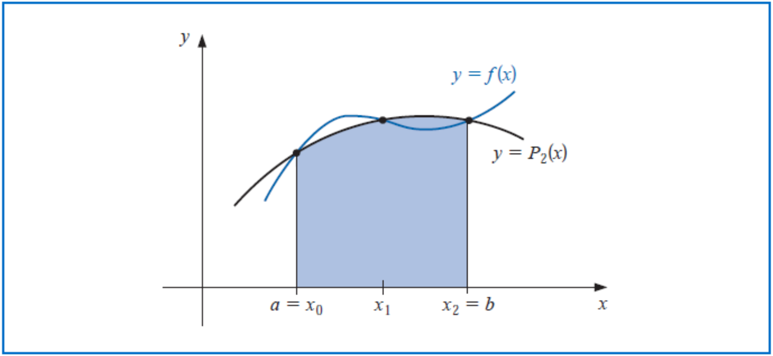
This is called the Trapezoidal rule because when f is a function with positive values, $\int_a^b f(x)\,dx$ is approximated by the area in a trapezoid, as shown in Figure 4.3.



The error term for the Trapezoidal rule involves f'', so the rule gives the exact result when applied to any function whose second derivative is identically zero, that is, any polynomial of degree one or less.

Simpson's Rule

Simpson's rule results from integrating over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a$, $x_2 = b$, and $x_1 = a + h$, where $h = (b - a)/2$. (See Figure 4.4.)



Therefore

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))\,dx.$$

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 method, 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

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

and

$$\int_{x_0}^{x_2} f(x)\,dx = \left[f(x_1)(x-x_1) + \frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 + \frac{f'''(x_1)}{24}(x-x_1)^4 \right]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx. \quad (4.24)$$

Because $(x-x_1)^4$ is never negative on $[x_0, x_2]$, the Weighted Mean Value Theorem for Integrals 1.13 implies that

$$\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{120}(x-x_1)^5\Big]_{x_0}^{x_2},$$

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

$$(x_2-x_1)^3-(x_0-x_1)^3=2h^3 \quad \text{and} \quad (x_2-x_1)^5-(x_0-x_1)^5=2h^5.$$

Consequently, Eq. (4.24) 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

$$\int_{x_0}^{x_2} f(x)\,dx = 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2)\right\} + \frac{f^{(4)}(\xi_1)}{60}h^5$$
$$= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12}\left[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\right].$$

It can be shown by alternative methods (see Exercise 24) that the values 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:

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

The error term in Simpson's rule involves the fourth derivative of f, so it gives exact results when applied to any polynomial of degree three or less.

Example

Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)\,dx$ when $f(x)$ is

(a) x^2 **(b)** x^4 **(c)** $(x+1)^{-1}$
(d) $\sqrt{1+x^2}$ **(e)** $\sin x$ **(f)** e^x

Solution On $[0, 2]$ the Trapezoidal and Simpson's rule have the forms

$$\text{Trapezoid:} \quad \int_0^2 f(x)\,dx \approx f(0) + f(2) \quad \text{and}$$

$$\text{Simpson's:} \quad \int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

When $f(x) = x^2$ they give

$$\text{Trapezoid:} \quad \int_0^2 f(x)\,dx \approx 0^2 + 2^2 = 4 \quad \text{and}$$

$$\text{Simpson's:} \quad \int_0^2 f(x)\,dx \approx \frac{1}{3}[(0^2) + 4 \cdot 1^2 + 2^2] = \frac{8}{3}.$$

The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^2$.

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

	(a)	(b)	(c)	(d)	(e)	(f)
$f(x)$	x^2	x^4	$(x+1)^{-1}$	$\sqrt{1+x^2}$	$\sin x$	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

Measure of Precision

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.

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

Integration and summation are linear operations; that is,

$$\int_a^b (\alpha f(x) + \beta g(x))\, dx = \alpha \int_a^b f(x)\, dx + \beta \int_a^b g(x)\, dx$$

and

$$\sum_{i=0}^{n} (\alpha f(x_i) + \beta g(x_i)) = \alpha \sum_{i=0}^{n} f(x_i) + \beta \sum_{i=0}^{n} g(x_i),$$

for each pair of integrable functions f and g and each pair of real constants α and β. This

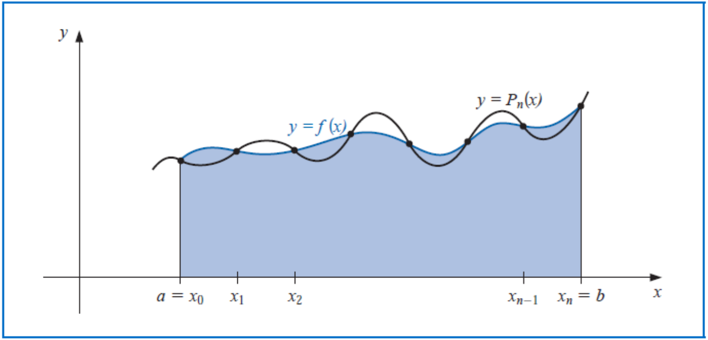
The degree of precision of a quadrature formula is n if and only if the error is zero for all polynomials of degree $k = 0, 1, ..., n$, but is not zero for some polynomial of degree $n + 1$.

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.

Closed Newton-Cotes Formula

Closed Newton-Cotes Formulas

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

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

The following theorem details the error analysis associated with the closed Newton-Cotes formulas. For a proof of this theorem, see [IK], p. 313.

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 $f \in C^{n+1}[a,b]$. ■

Examples

$n = 1$: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi), \quad \text{where} \quad x_0 < \xi < x_1. \tag{4.25}$$

$n = 2$: Simpson's rule

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi), \quad \text{where} \quad x_0 < \xi < x_2. \tag{4.26}$$

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

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi), \tag{4.27}$$

where $x_0 < \xi < x_3$.

$n = 4$:

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

where $x_0 < \xi < x_4$. (4.28)

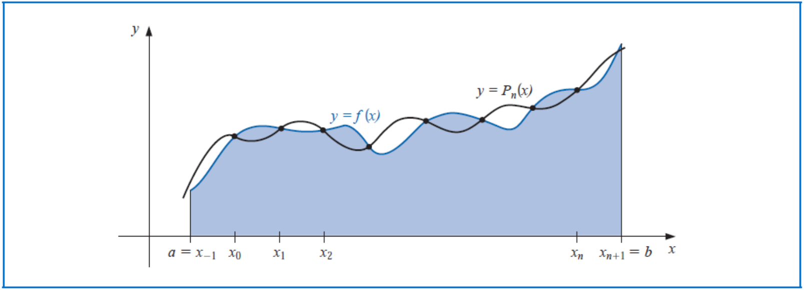
Open Newton-Cotes Formula

The *open Newton-Cotes formulas* do not include the endpoints of $[a, b]$ as nodes. They 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 on page 200. 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

$$a_i = \int_a^b L_i(x)\,dx.$$


y
x
$y = P_n(x)$
$y = f(x)$
$a = x_{-1}$
x_0
x_1
x_2
x_n
$x_{n+1} = b$

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 $f \in C^{n+1}[a,b]$. ■

Examples

$n = 0$: Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_1. \tag{4.29}$$

$n = 1$:

$$\int_{x_{-1}}^{x_2} f(x)\,dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4}f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_2. \tag{4.30}$$

$n = 2$:

$$\int_{x_{-1}}^{x_3} f(x)\,dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45} f^{(4)}(\xi), \tag{4.31}$$

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

$n = 3$:

$$\int_{x_{-1}}^{x_4} f(x)\,dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95}{144} h^5 f^{(4)}(\xi), \tag{4.32}$$

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

Compare the results of the closed and open Newton-Cotes formulas listed as (4.25)–(4.28) and (4.29)–(4.32) when approximating

$$\int_0^{\pi/4} \sin x\, dx = 1 - \sqrt{2}/2 \approx 0.29289322.$$

Solution For the closed formulas we have

$$n = 1: \quad \frac{(\pi/4)}{2}\left[\sin 0 + \sin\frac{\pi}{4}\right] \approx 0.27768018$$

$$n = 2: \quad \frac{(\pi/8)}{3}\left[\sin 0 + 4\sin\frac{\pi}{8} + \sin\frac{\pi}{4}\right] \approx 0.29293264$$

$$n = 3: \quad \frac{3(\pi/12)}{8}\left[\sin 0 + 3\sin\frac{\pi}{12} + 3\sin\frac{\pi}{6} + \sin\frac{\pi}{4}\right] \approx 0.29291070$$

$$n = 4: \quad \frac{2(\pi/16)}{45}\left[7\sin 0 + 32\sin\frac{\pi}{16} + 12\sin\frac{\pi}{8} + 32\sin\frac{3\pi}{16} + 7\sin\frac{\pi}{4}\right] \approx 0.29289318$$

and for the open formulas we have

$$n=0: \quad 2(\pi/8)\left[\sin\frac{\pi}{8}\right] \approx 0.30055887$$

$$n=1: \quad \frac{3(\pi/12)}{2}\left[\sin\frac{\pi}{12}+\sin\frac{\pi}{6}\right] \approx 0.29798754$$

$$n=2: \quad \frac{4(\pi/16)}{3}\left[2\sin\frac{\pi}{16}-\sin\frac{\pi}{8}+2\sin\frac{3\pi}{16}\right] \approx 0.29285866$$

$$n=3: \quad \frac{5(\pi/20)}{24}\left[11\sin\frac{\pi}{20}+\sin\frac{\pi}{10}+\sin\frac{3\pi}{20}+11\sin\frac{\pi}{5}\right] \approx 0.29286923$$

Table 4.8 summarizes these results and shows the approximation errors. ■

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	