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Arba Minch University

Numerical Method(Math-2073/53)
Lecture note: Chapter-VI

”If people do not believe that mathematics is simple, it is only because they do not realize how complicated life is.”

John von Neumann.

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Contents

Chapter 1

Numerical Differentiation and Integration

1.1 Differentiation

Objectives of the section

- Explain the definitions of forward, backward, and center divided methods for numerical differentiation
- Find approximate values of the first derivative of continuous functions reason about the accuracy of the numbers
- Find approximate values of the first derivative of discrete functions (given at discrete data points)

Often in Physics or Engineering it is necessary to use a calculus operation known as differentiation. Unlike textbook mathematics, the differentiated functions are data generated by an experiment or a computer code. In an elementary calculus course, the students learn the concept of the derivative of a function $y = f(x)$, denoted by $f'(x)$, $\frac{dy}{dx}$ or $\dfrac{d}{dx}f(x)$, along with various scientific and engineering applications. These applications include:

- Velocity and acceleration of a moving object
- Current, power, temperature, and velocity gradients
- Rates of growth and decay in a population
- Marginal cost and marginal profits in economics, etc.

The need for **numerical differentiation** arises from the fact that very often, either

- $f(x)$ is not explicitly given and only the values of $f(x)$ at certain discrete points are known or
- $f'(x)$ is difficult to compute analytically.

We will learn various ways to compute $f'(x)$ numerically in this Chapter. We start with the following biological application.

A Case Study on Numerical Differentiation

Velocity Gradient for Blood Flow:
Consider the blood flow through an artery or vein. It is known that the nature of viscosity dictates a flow profile, where the velocity v increases toward the center of the tube and is zero at the wall, as illustrated in the following diagram:
Let v be the velocity of blood that flows along a blood vessel which has radius R and length l at a distance r from the central axis. Let $\Delta P =$ Pressure difference between the ends of the tube and $\eta =$ Viscosity of blood.

From the law of laminar flow which gives the relationship between v and r, we have

$$v(r) = v_m(1 - \frac{r^2}{R^2})$$

where $v_m = \frac{1}{4\eta}\frac{4p}{l}R^2$ is the maximum velocity. Substituting the expression for v_m in above , we obtain

$$v(r) = \frac{1}{4\eta}\frac{\Delta p}{l}(R^2 - r^2)$$

Thus, if Δp and l are constant, then the velocity v of the blood flow is a function of r in $[0, R]$. In an experimental set up, one then can measure velocities at several different values of r, given $\eta, \Delta p$, l and R. The problem of interest is now to compute the velocity gradient (that is, $\frac{dv}{dr}$) from $r = r_1$ to $r = r_2$. We will consider this problem later with numerical values.

Numerical Differentiation Problem

Given the functional values, $f(x_0), f(x_1), \cdots, f(x_n)$, of a function $f(x)$ which is not explicitly known, at the points $x_0, x_1, \cdots, x_n \in [a, b]$ or a differentiable function $f(x)$ on $[a, b]$. Find an approximate value of $f'(x)$ for $a < x < b$.

1.1.1 Differentiation based on Newton's forward interpolation formula

We know that the Newton's forward and backward interpolation formulae are applicable only when the arguments are in equispaced. So, we assumed that the given arguments are equispaced.

Let the function $y = f(x)$ be known at the $(n+1)$ equispaced arguments $x_0, x_1, \cdots, x_n$ and $y_i = f(x_i)$ for $i = 0, 1, \cdots, n$. Since the arguments are in equispaced, therefore one $x - x_0$ can write $x_i = x_0 + ih$. Also, let $p = \frac{x - x_0}{h}$ where h is called the spacing. For this data set, the Newton's forward interpolation formula is

$$\begin{aligned}
P_n(x) &= y_0 + p \triangle y_0 + \frac{p(p-1)}{2!} \triangle^2 y_0 + \cdots + \frac{p(p-1)\cdots(p-n+1)}{n!} \triangle^n y_0 \\
&= y_0 + p \triangle y_0 + \frac{p^2 - p}{2!} \triangle^2 y_0 + \frac{p^3 - 3p^2 + 2p}{3!} \triangle^3 y_0 \\
&+ \frac{p^4 - 6p^3 + 11p^2 - 6p}{4!} \triangle^4 y_0 + \frac{p^5 - 10p^4 + 35p^3 - 50p^2 + 24p}{5!} \triangle^5 y_0 + \cdots
\end{aligned} \tag{1.1}$$

The error term of this interpolation formula is

$$E_(x) = \frac{p(p-1)(p-2)\cdots(p-n)}{(n+1)!} h^{n+1} f^{n+1}(\xi), \tag{1.2}$$

where $\min\{x, x_0, x_1, \cdots, x_n\} < \xi < \{x, x_0, x_1, \cdots, x_n\}$.

Differentiating Equation (1.1) thrice to get the first three derivatives of

$$\begin{aligned} P_n'(x) = \frac{1}{h}\Bigg[\triangle y_0 + \frac{2p-1}{2!}\triangle^2 y_0 + \frac{3p^2-6p+2)}{3!}\triangle^3 y_0 + \frac{4p^3-18p^2+22p-6}{4!}\triangle^4 y_0 \\ + \frac{5p^4-40p^3+105p^2-100p+24}{5!}\triangle^5 y_0 + \cdots\Bigg] \qquad \left(\because \frac{dp}{dx} = \frac{1}{h}\right) \end{aligned} \tag{1.3}$$

$$\begin{aligned} P_n''(x) = \frac{1}{h^2}\Bigg[\triangle^2 y_0 + \frac{6p-6}{3!}\triangle^3 y_0 + \frac{12p^2-36p+22}{4!}\triangle^4 y_0 \\ + \frac{20p^3-120p^2+210p-100}{5!}\triangle^5 y_0 + \cdots\Bigg] \end{aligned} \tag{1.4}$$

$$P_n'''(x) = \frac{1}{h^3}\left[\triangle^3 y_0 + \frac{24p-36}{4!}\triangle^4 y_0 + \frac{60p^2-240p+210}{5!}\triangle^5 y_0 + \cdots\right] \tag{1.5}$$

and so on.

In this way, we can find all other derivatives. It may be noted that $\triangle y_0, \triangle^2 y_0, \triangle^3 y_0, \cdots$ are constants.

The above three formulae give the first three (approximate) derivatives of $f(x)$ at any arbitrary argument x where $x = x_0 + ph$. The above formulae become simple when $x = x_0$, i.e. $p = 0$. That is,

$$P_n'(x_0) = \frac{1}{h}\left[\triangle y_0 - \frac{1}{2}\triangle^2 y_0 + \frac{1}{3}\triangle^3 y_0 - \frac{1}{4}\triangle^4 y_0 + \frac{1}{5}\triangle^5 y_0 - \cdots\right] \tag{1.6a}$$

$$P_n''(x_0) = \frac{1}{h}\left[\triangle^2 y_0 - \triangle^3 y_0 + \frac{11}{12}\triangle^4 y_0 - \frac{5}{6}\triangle^5 y_0 + \cdots\right] \tag{1.6b}$$

$$P_n'''(x_0) = \frac{1}{h}\left[\triangle^3 y_0 - \frac{3}{2}\triangle^4 y_0 + \frac{7}{5}\triangle^5 y_0 - \cdots\right] \tag{1.6c}$$

Error in Newton's forward differentiation formula

The error in Newton's forward differentiation formula is calculated from the expression of error in Newton's forward interpolation formula. The error in Newton's forward interpolation formula is given by

$$E_n(x) = p(p-1)(p-2)\cdots(p-n)h^{n+1}\frac{f^{(n+1)}(\xi)}{(n+1)!}$$

Differentiating this expression with respect to x, then we have

$$\begin{aligned} E_n'(x) &= h^{n+1}\frac{f^{(n+1)}(\xi)}{(n+1)!}\frac{d}{dp}\left[p(p-1)\cdots(p-n)\right]\frac{1}{h} + \frac{p(p-1)\cdots(p-n)}{(n+1)!}h^{n+1}\frac{d}{dx}\left[f^{(n+1)}(\xi)\right] \\ &= h^n\frac{f^{(n+1)}(\xi)}{(n+1)!}\frac{d}{dp}\left[p(p-1)\cdots(p-n)\right] + \frac{p(p-1)\cdots(p-n)}{(n+1)!}h^{n+1}f^{(n+2)}(\xi_1) \end{aligned}$$

where ξ and ξ_1 are two quantities depend on x and $\min\{x, x_0, \cdots, x_n\} < \xi, \xi_1 < \max\{x, x_0, \cdots, x_n\}$.

The expression for error at the starting argument $x = x_0$, i.e., $p = 0$ is evaluated as

$$\begin{aligned}
E_n'(x_0) &= h^n \frac{f^{(n+1)}(\xi)}{(n+1)!} \frac{d}{dp}\left[p(p-1)\cdots(p-n)\right]_{p=0} + 0 \\
&= \frac{h^n(-1)^n n! f^{(n+1)}(\xi)}{(n+1)!} \qquad \left[\text{as } \frac{d}{dp}\left[p(p-1)\cdots(p-n)\right]_{p=0} = (-1)^n n!\right] \\
&= \frac{(-1)^n h^n f^{(n+1)}(\xi)}{n+1},
\end{aligned}$$

where ξ lies between $\min\{x, x_0, \cdots, x_n\}$ and $\max\{x, x_0, \cdots, x_n\}$.

Example 1.1

Consider the following table

x	:	1.0	1.5	2.0	2.5	3.0	3.5
y	:	1.234	2.453	7.625	12.321	18.892	23.327

Find the value of splaystyle $\frac{dy}{dx}$, $\frac{d^2y}{dx^2}$ *at* $x = 1$ *and* $\frac{dy}{dx}$ *when* $x = 1.2$

Solution: *The forward difference table is*

x	y	$\triangle y$	$\triangle^2 y$	$\triangle^3 y$	$\triangle^4 y$	$\triangle^5 y$
1.0	1.234					
		3.425				
1.5	2.453		3.095			
		6.520		0.36		
2.0	7.625		3.455		0.71	
		9.975		1.07		-0.680
2.5	12.321		4.525		0.03	
		14.500		1.10		
3.0	18.892		5.625			
		20.125				
3.5	23.327					

Here $x = x_0 = 1$ *and* $h = 0.5$. *Then* $p = 0$ *hence we can use Equation* (1.6a) *to find the first derivative at* $x = 1$. *Thus,*

$$\begin{aligned}
y'(1) &\approx \frac{1}{h}\left[\triangle y_0 - \frac{1}{2}\triangle^2 y_0 + \frac{1}{3}\triangle^3 y_0 - \frac{1}{4}\triangle^4 y_0 + \frac{1}{5}\triangle^5 y_0\right] \\
&= \frac{1}{0.5}\left[3.425 - \frac{1}{2}\times 3.095 + \frac{1}{3}\times 0.36 - \frac{1}{4}\times 0.71 + \frac{1}{5}\times(-0.680)\right] \\
&= 3.36800.
\end{aligned}$$

Similarly, using Equation (1.6b) *we can compute the second derivative at* $x = 1$*:*

$$\begin{aligned}
y''(1) &\approx \frac{1}{0.5}\left[\triangle^2 y_0 - \triangle^3 y_0 + \frac{11}{12}\triangle^4 y_0 - \frac{5}{6}\triangle^5 y_0\right] \\
&= 4.0 \times \left[3.095 - \times 0.36 + \frac{11}{12}\times 0.71 + \frac{5}{6}\times(-0.680)\right] \\
&= 15.8100.
\end{aligned}$$

Now, at $x = 1.2, h = 0.5, p = \frac{x - x_0}{h} = \frac{1.2 - 1}{0.5} = 0.4$

Example

Therefore, using Equation (1.3) *we have:*

$$y'(1.2) = \frac{1}{0.5}\left[\triangle y_0 + \frac{2p-1}{2!}\triangle^2 y_0 + \frac{3p^2-6p-2)}{3!}\triangle^3 y_0 + \frac{4p^3-18p^2+22p-6}{2!}\triangle^4 y_0 + \frac{5p^4-40p^3+105p^2-100p+24}{2!}\triangle^5 y_0\right]$$
$$= \frac{1}{0.5}\left[3.425 + \frac{2\times 0.4-1}{2!}\times 3.095 + \frac{3(0.4)^2-6(0.4)-2)}{3!}0.36 + \frac{4(0.4)^3-18(0.4)^2+22(0.4)-6}{4!}\times 0.71 + \frac{5(0.4)^4-40(0.4)^3+105(0.4)^2-100(0.4)+24}{5!}\times(-0.68)\right]$$
$$= 6.26948.$$

1.1.2 Differentiation based on Newton's backward interpolation formula

Like Newton's forward differentiation formula one can derive **Newton's backward differentiation formula** based on Newton's backward interpolation formula.
Suppose the function $y = f(x)$ is not know explicitly, but it is known at $(n+1)$ arguments $x_0, x_1, \cdots, x_n$. That is, $y_i = f(x_i), i = 0, 1, 2, \cdots, n$ are given. Since the Newton's backward interpolation formula is applicable only when the arguments are equispaced, therefore, $x_i = x_0 + ih, i = 0, 1, 2, \cdots, n$ and $p = \frac{x - x_n}{h}$.
The Newton's backward interpolation formula is

$$P_n(x) = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \frac{p(p+1)(p+2)}{3!}\nabla^3 y_n + \frac{p(p+1)(p+2)(p+3)}{4!}\nabla^4 y_n + \frac{p(p+1)(p+2)(p+3)(p+4)}{5!}\nabla^5 y_n + \cdots$$

Differentiating this formula with respect to x successively, the formulae for derivatives of different order can be derived as

$$P_n'(x) = \frac{1}{h}\left[\nabla y_n + \frac{2p+1}{2!}\nabla^2 y_n + \frac{3p^2+6p+2}{3!}\nabla^3 y_n + \frac{4p^3+18p^2+22p+6}{4!}\nabla^4 y_n + \frac{5p^4+40p^3+105p^2+100p+24}{5!}\nabla^5 y_n + \cdots\right] \tag{1.7}$$

$$P_n''(x) = \frac{1}{h^2}\left[\nabla^2 y_n + \frac{6p+6}{3!}\nabla^3 y_n + \frac{12p^2+36p+22}{4!}\nabla^4 y_n + \frac{20p^3+120p^2+210p+100}{5!}\nabla^5 y_n + \cdots\right] \tag{1.8}$$

$$P_n'''(x) = \frac{1}{h^2}\left[\nabla^3 y_n + \frac{24p+36}{4!}\nabla^4 y_n + \frac{60p^2+240p+210}{5!}\nabla^5 y_n + \cdots\right] \tag{1.9}$$

and so on.

The above formulae give the approximate value of $\frac{dy}{dx}, \frac{d^2y}{dx^2}, \frac{d^3y}{dx^3}$, and so on, at any point value of x, where $\min\{x, x_0, \cdots, x_n\} < x < \max\{x, x_0, \cdots, x_n\}$.
When $x = x_n$ then $v = 0$. In this particular case, the above formulae reduced to the following form.

$$P_n'(x_n) = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \frac{1}{5}\nabla^5 y_n + \cdots\right] \tag{1.10a}$$

$$P_n''(x_n) = \frac{1}{h}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \cdots\right] \tag{1.10b}$$

$$P_n'''(x_n) = \frac{1}{h}\left[\nabla^3 y_n + \frac{3}{2}\nabla^4 y_n + \frac{7}{5}\nabla^5 y_n + \cdots\right] \tag{1.10c}$$

Error in Newton's backward differentiation formula

The error can be calculated by differentiating the error in Newton's backward interpolation formula. Such error is given by

$$E_n(x) = p(p+1)(p+2)\cdots(p+n)h^{n+1}\frac{f^{(n+1)}(\xi)}{(n+1)!}.$$

where $p = \frac{x - x_n}{h}$ and ξ lies between $\min\{x, x_0, \cdots, x_n\}$ and $\max\{x, x_0, \cdots, x_n\}$. Differentiating $E_n(x)$, we get

$$\begin{aligned} E_n'(x) &= h^n \frac{d}{dp}\left[p(p+1)(p+2)\cdots(p+n)\right]\frac{f^{(n+1)}(\xi)}{(n+1)!} \\ &\quad + h^{n+1}\frac{p(p+1)(p+2)\cdots(p+n)}{(n+1)!}f^{(n+2)}(\xi_1) \end{aligned} \tag{1.11}$$

where ξ and ξ_1 are two quantities depend on x and $\min\{x, x_0, \cdots, x_n\} < \xi, \xi_1 < \max\{x, x_0, \cdots, x_n\}$.
This expression gives the error in differentiation at any argument x. In particular, when $x = x_n$, i.e. when $p = 0$ then

$$\begin{aligned} E_n'(x_n) &= h^n \frac{f^{(n+1)}(\xi)}{(n+1)!}\frac{d}{dp}\left[p(p+1)\cdots(p+n)\right]_{p=0} + 0 \\ &= \frac{h^n n!}{(n+1)!}f^{(n+1)}(\xi) \qquad \left[\text{as } \frac{d}{dp}\left[p(p+1)\cdots(p+n)\right]_{p=0} = n!\right] \\ &= \frac{h^n f^{(n+1)}(\xi)}{n+1}, \end{aligned}$$

Example 1.2

A slider in a machine moves along a fixed straight rod. It's distance x (in cm) along the rod are given in the following table for various values of the time t (in second):

(sec) t	:	0	2	4	6	8
(cm) x	:	20	50	80	120	180

Find the velocity and acceleration of the slider at time $t = 8$.
Solution: *The backward difference table is*

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
0	20				
		30			
2	50		0		
		30		10	
4	80		10		**0**
		40		**10**	
6	120		**20**		
		60			
8	**180**				

Here $t = 8 = t_n$ and $h = 2$,the velocity at $t = 8$ is given by

$$\begin{aligned} v(8) = \frac{dx}{dt}|_{t=8} &\approx \frac{1}{h}\left[\nabla y_4 + \frac{1}{2}\nabla^2 y_4 + \frac{1}{3}\nabla^3 y_4 + \frac{1}{4}\nabla^4 + \frac{1}{5}\nabla^5 + \cdots\right] \\ &= \frac{1}{2}\left[60 + \frac{1}{2} \times 20 + \frac{1}{3} \times 10 + 0\right] \\ &= 0.5 \times \left[70 + \frac{10}{3}\right] \\ &= 36.66667 \end{aligned}$$

Thus, the velocity of the slider when $t = 8$ is $v = 36.6667$.
The acceleration at $t = 8$ is

$$\begin{aligned} a(8) = \frac{d^2x}{dt^2}|_{t=8} &\approx \frac{1}{h^2}\left[\nabla^2 y_4 + \nabla^3 y_4 + \frac{11}{12}\nabla^4 y_4 + \frac{5}{6}\nabla^5 y_4 + \cdots\right] \\ &= \frac{1}{2}[20 + 10 + 0] \\ &= \frac{2}{2^2} \times \left[70 + \frac{10}{3}\right] \\ &= 7.50 \end{aligned}$$

1.1.3 Finite Difference Formulas for Derivatives

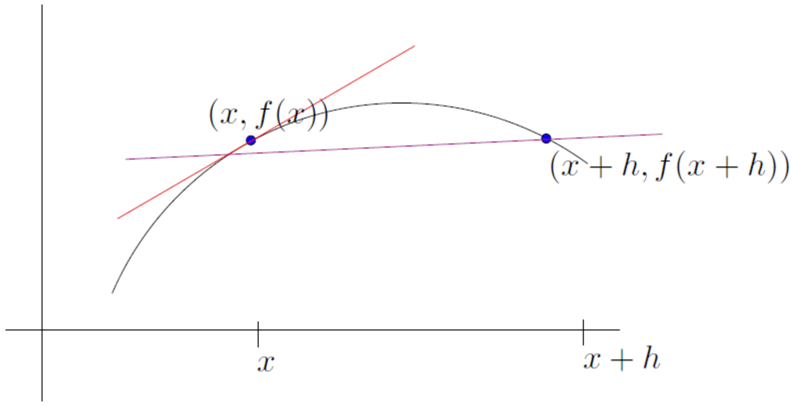
The derivative of a function $f(x)$ is defined as:

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

Thus, it is the slope of the tangent line at the point $(x, f(x))$. The difference quotient (DQ)

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

is the slope of the secant line passing through $(x, f(x))$ and $(x+h, f(x+h))$.



As $h$gets smaller and smaller, the difference quotient gets closer and closer to $f'(x)$. However, if h is too small, then the round-off error becomes large, yielding an inaccurate value of the derivative.

In any case, if the DQ is taken as an approximate value of $f'(x)$, then it is called two-point forward difference formula (FDF) for $f'(x)$.

Thus, two-point backward difference and two-point central difference formulas, are similarly defined, respectively, in terms of the functional values $f(x-h)$ and $f(x)$, and $f(x-h)$ and $f(x+h)$.

Begin with the Taylor series as seen in Equation 1.12.

$$f(x+h) = f(x) + f^{'}(x)h + \frac{f^{(2)}(x)}{2!}h^2 + \frac{f^{(3)}(x)}{3!}h^3 + \cdots \tag{1.12}$$

Next by cutting off the Taylor series after the fourth term and evaluating it at h and $-h$ yields Equations (1.13) and (1.14).

$$f(x+h) = f(x) + f^{'}(x)h + \frac{f^{(2)}(x)}{2!}h^2 + \frac{f^{(3)}(c_1)}{3!}h^3 \tag{1.13}$$

$$f(x-h) = f(x) - f^{'}(x)h + \frac{f^{(2)}(x)}{2!}h^2 - \frac{f^{(3)}(c_2)}{3!}h^3 \tag{1.14}$$

Then by subtracting Equation (1.13) by Equation (1.14) yields.

$$f(x+h) - f(x-h) = 2f^{'}(x)h + \frac{f^{(3)}(c_1)}{3!}h^3 + \frac{f^{(3)}(c_2)}{3!}h^3 \tag{1.15}$$

Two-point Forward Difference Formula (FDF):

$$f^{'}(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

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

Two-point Backward Difference Formula (BDF):

$$f^{'}(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

Two-point Central Difference Formula (CDF):

$$f^{'}(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

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

Second Derivative

The second order derivatives can be obtained by adding equations (1.13) and (1.14) (if properly expanded to include the fourth-derivative-term):

$$f^{''}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$

Example 1.3

Given the following table, where the functional values correspond to $f(x) = x \ln x$:

x	f(x)
1	0
2	1.3863
3	3.2958

Approximate $f'(2)$ by using two-point (i) FDF, (ii) BDF, and (iii) CDF. (Note that $f'(x) = 1 + \ln x$, $f'(2) = 1 + ln2 = 1.6931$.) Input Data: $x = 2, h = 1, x + h = 3$.
Solution:

1. ***Two-point FDF:***

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} = \frac{f(3) - f(2)}{1} = 1.9095.$$

Absolute Error: $|(1 + \ln 2) - 1.9095| = |1.6931 - 1.9095| = 0.2164.$

2. ***Two-point BDF:***

$$f'(x) \approx \frac{f(x) - f(x-h)}{h} = \frac{f(2) - f(2)}{h} = 1.3863.$$

Absolute Error: $|1.6931 - 1.3863| = 0.3068.$

3. ***Two-point CDF:***

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} = \frac{f(3) - f(1)}{2} = \frac{3.2958}{2} = 1.6479.$$

Absolute Error: $|1.6931 - 1.6479| = 0.0452.$

Remarks: The above example shows that two-point CDF is more accurate than two-point FDF and BDF. The reason will be clear from our discussion on truncation errors in the next section.

Derivations of the Two-Point Finite Difference Formulas: Taylor base

In this section, we will show how to derive the two-point difference formulas and the truncation errors associated with them using the Taylor series and state without proofs, the three-point FDF and BDF. The derivatives of these and other higher-order formulas and their errors will be given in the next Section, using Lagrange interpolation techniques. Consider the two-term Taylor series expansion of $f(x)$ about the points $x+h$ and $x-h$, respectively:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\xi_0) \quad \text{where} \quad x < \xi_0 < x+h \tag{1.16}$$

and

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(\xi_1) \quad \text{where} \quad x < \xi_1 < x+h \tag{1.17}$$

Solving for $f'(x)$ from (1.16), we get

$$f'(x) = \left[\frac{f(x+h) - f(x)}{h}\right] - \frac{h^2}{2}f''(\xi_0) \tag{1.18}$$

The term within brackets on the right-hand side of (1.18) is the two-point FDF. The second term (remainder) on the right-hand side of (1.18) is the truncation error for two-point FDF. Similarly, solving for $f'(x)$ from (1.17), we get

$$f'(x) = \left[\frac{f(x) - f(x-h)}{h}\right] + \frac{h^2}{2}f''(\xi_1) \tag{1.19}$$

The first term within brackets on the right-hand side of (1.19) is the two-point BDF. The second term (remainder) on the right-hand side of (1.19) is the truncation error for two-point BDF.

Assume that $f''(x)$ is continuous. Consider this time a three-term Taylor series expansion of $f(x)$ about the points $(x+h)$ and $(x-h)$:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{3!}f'''(\xi_2) \tag{1.20}$$

where $x < \xi_2 < x+h$ and

$$f(x+h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{3!}f'''(\xi_3) \tag{1.21}$$

where $x-h < \xi_3 < x$ and Subtracting (1.21) from (1.20), we obtain

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3!}[f'''(\xi_2) + f'''(\xi_3)] \tag{1.22}$$

Solving (1.22) for $f'(x)$, we get

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{12}[f'''(\xi_2) - f'''(\xi_3)] \tag{1.23}$$

Thus, by IVT, there exists a number ξ in $[x-h, x+h]$ such that

$$f'''(xi_2) + f'''(xi_3) = f'''(\xi)$$

Thus, (1.23) becomes

$$f'(x) = \left[\frac{f(x+h) - f(x-h)}{2h}\right] - \frac{h^2}{6}f'''(\xi) \tag{1.24}$$

The term within brackets on the right-hand side of (1.24) is the two-point CDF, and the term $-\frac{h^2}{6}f''(\xi)$ is the **truncation error for two-point CDF**.

Three-point and Higher Order Formulas for $f'(x)$: Lagrange Approach

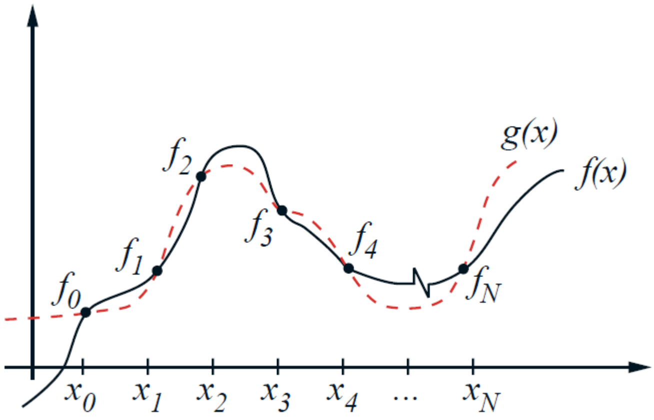
Three-point and higher-order derivative formulas and their truncation errors can be derived in the similar way as in the last section. Three-point FDF and BDF approximate $f'(x)$ in terms of the functional values at three points: $x, x+h,$ and $x+2h$ for FDF and $x, x-h, x-2h$ for BDF, respectively.

- **Three-point FDF for $f'(x)$:** $f'(x) \approx \dfrac{-3f(x)+4f(x+h)-f(x+2h)}{2h}$
- **Three-point BDF for $f'(x)$:** $f'(x) \approx \dfrac{3f(x)-4f(x-h)+f(x-2h)}{2h}$

1.1.4 General 1^{st} derivative approximation

The interpolation nodes are given as: $(x_1, f_1), (x_2, f_2), \cdots, (x_N, f_N)$.Then recall the Lagrange interpolating polynomial $P_n(x)$ of degree at most, n is given by:

$$f(x) = \sum_{k=0}^{n} f(x_k)L_{N,k}(x) + \frac{(x-x_0)\cdots(x-x_N)}{(N+1)!} f^{N+1}(\xi(x)) \tag{1.25}$$



Take 1^{st} derivative for Eq. (1.25):

$$f'(x) = \sum_{k=0}^{n} f(x_k)L'_{N,k}(x) + \frac{(x-x_0)\cdots(x-x_N)}{(N+1)!}\left(\frac{d\left(f^{N+1}(\xi(x))\right)}{dx}\right) + \frac{1}{(N+1)!}\left(\frac{d((x-x_0)\cdots(x-x_N))}{dx}\right) f^{N+1}(\xi(x))$$

Set $x = x_j$, with x_j being x-coordinate of one of interpolation nodes $j = 1, 2, \cdots, N$

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L'_{N,k}(x_j) + \frac{f^{N+1}(\xi(x_j))}{(N+1)!} \prod_{k=0 k\neq j}^{n} (x_j - x_k) \tag{1.26}$$

which is called an $(n+1)$-point formula to approximate $f'(x_j)$. The most common formulas are those involving three and five evaluation points. We first derive some useful three-point formulas and consider aspects of their errors. Because

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \text{ we have } L'_0(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

Similarly

$$L_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \text{ and } L_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_1)(x_2 - x_0)}$$

Hence, from Eq. (1.26)

$$f'(x_j) = f(x_0)\left[\frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] + f(x_1)\left[\frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right] + f(x_2)\left[\frac{2x - x_0 - x_1}{(x_2 - x_1)(x_2 - x_0)}\right] + \frac{f^{(3)}(\xi_j)}{6}\prod_{k=0,k\neq j}^{2}(x_j - x_k) \tag{1.27}$$

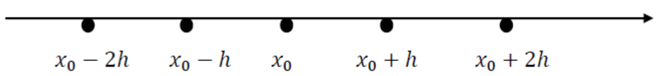
Three-Point Formulas

The formulas from Eq. (1.27) become especially useful if the nodes are equally spaced, that is, when $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, for some $h \neq 0$. We will assume equally spaced nodes throughout the remainder of this section. Using Eq. (1.27) with $x_j = x_0, x_1 = x_0 + h$, and $x_2 = x_0 + 2h$ gives

1. $f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_1) - f(x_2)] + \frac{h^2}{3}f^{(3)}(\xi(x_0))$ (three-point endpoint formula)
2. $f'(x_1) = \frac{1}{2h}[-f(x_0) + f(x_2)] + \frac{h^2}{6}f^{(3)}(\xi(x_1))$ (three-point midpoint formula)
3. $f'(x_1) = \frac{1}{2h}[f(x_0) - 4f(x_1) + 3f(x_2)] + \frac{h^2}{3}f^{(3)}(\xi(x_2))$ (three-point endpoint formula)

Mostly used five-point formula

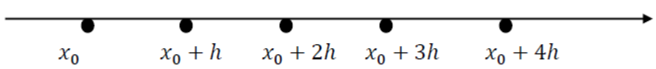
1. Five-point midpoint formula



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

where $\xi \in [x_0 - 2h, x_0 + 2h]$

2. Five point end point



$$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5}f^5(\xi) \tag{1.28}$$

where $\xi \in [x_0, x_0 + 4h]$.

Second Derivative Midpoint Formula

Expand a function f in a third Taylor polynomial about a point x_0 and evaluate at $x_0 + h$ and $x_0 - h$. Then

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

Example 1.4

Given the following data

x	1.1	1.2	1.3	1.4	1.5
f(x)	0.6133	0.7822	0.9716	1.1814	1.4117

find the first derivative $f'(x)$ *at the point* $x = 1.3$.

(a) *Use the three-point forward difference formula.*

(b) *Use the three-point backward difference formula.*

(c) *Use the two-point central difference formula.*

Example 1.5

Let $f(x) = \sin x$. *Use formulas forward and central difference formula with* $h = 0.1$ *to approximate* $f'(0.5)$ *and* $f''(0.5)$. *Compare with the true values,* $f'(0.5) = 0.87758256$ *and* $f''(0.5) = -0.47942554$.
Solution: *Using forward formula we get*

$$\begin{aligned} f'(0.5) &\approx \frac{f(0.6) - f(0.5)}{0.1} \\ &\approx \frac{0.56464247 - 0.47942554}{0.1} \approx 0.8521693 \\ \textit{Error} &= 0.02541326. \end{aligned}$$

Similarly, using central formula, we get

$$\begin{aligned} f''(0.5) &\approx \frac{f(0.6) - 2f(0.5) + f(0.4)}{(0.1)^2} \\ &\approx \frac{0.56464247 - 0.95885108 + 0.38941834}{(0.1)^2} \approx -0.479027 \\ \textit{Error} &= 0.000399. \end{aligned}$$

1.1.5 Richardson Extrapolation

under construction

1.2 Numerical Integration

This section deals with the problem of estimating the definite integral

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

with $[a, b]$ finite.
In most cases, the evaluation of definite integrals is either impossible, or else very difficult, to evaluate analytically. It is known from calculus that the integral I represents the area of the region between the curve $y = f(x)$ and the lines $x = a$ and $x = b$. So the basic idea of approximating I is to replace $f(x)$ by an interpolating polynomial $p(x)$ and then integrate the polynomial by finding the area of the region bounded by $p(x)$, the lines $x = a$ and $x = b$, and the x-axis. This process is called **numerical quadrature**. The integration rules that we will be developing correspond to the varying degree of the interpolating polynomials.

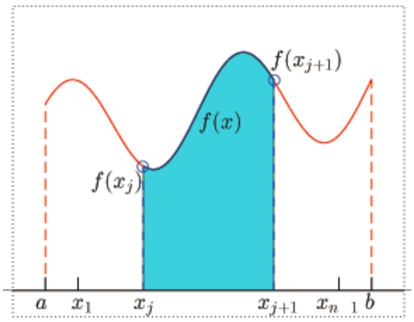
There are two primary means of improving Numerical integration

1. If $a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b$, then properties of the integral give

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

   We create **composite integrals** and choose appropriate $x_i's$, which subdivide our function $f(x)$ into n sub-intervals with each sub-interval providing a smaller domain and better approximation of f on that subinterval.

2. Take a particular subinterval, then partition that subinterval further to obtain a reasonable approximation of $f(x)$ on the subinterval by an interpreting polynomial, which is precisely integrable and has a known error bound.



Our aim is to obtain the greatest accuracy approximating the integral with the minimum amount of computation. We can vary the spacing x_j , not necessarily uniform We can alter how $f(x)$ is approximated using polynomials, which are exactly integrable.

1.2.1 Numerical Quadrature - Basics

We begin our analysis with the second point above (avoiding the composite integral for now). We focus on a single interval and consider interpolating polynomials approximating $f(x)$ on the single interval. The basic idea is to replace integration by a clever summation:

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

where $a \leq x_0 < x_1 < \cdots < x_n \leq b,\ f_i = f(x_i)$.

The coefficients a_i and the nodes x_i are to be selected.

Various means of selecting a_i and x_i alter the efficiency and accuracy of our algorithm

Building Integration Schemes with Lagrange Polynomials

Given the nodes $\{x_0, x_1, \cdots, x_n\}$ we can use the **Lagrange interpolating polynomial**

$$P_n(x) = \sum_{i=0}^{n} f_i L_{n,i}(x), \text{ with error } E_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n}(x - x_i)$$

to obtain

$$\int_a^b f(x)dx = \underbrace{\int_a^b P_n(x)dx}_{\text{The approximation}} + \underbrace{\int_a^b E_n(x)dx}_{\text{The Error Estimate}}$$

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

Where $\xi(x))in[a, b]$

Identifying the Coefficients

The Lagrange interpolating polynomials are readily integrated to give the weighting coefficients a_i

$$\int_a^b P_n(x)dx = \int_a^b \sum_{i=0}^{n} f_i L_{n,i}(x) = \sum_{i=0}^{n} f_i \underbrace{\int_a^b L_{n,i}(x)dx}_{a_i} = \sum_{i=0}^{n} f_i a_i$$

Hence we write

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

with error given by

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

Before discussing the general situation of quadrature formulas, let us consider formulas produced by using first and second Lagrange polynomials with equally spaced nodes. This gives the Trapezoidal rule and Simpson's rule, which are commonly introduced in calculus courses.

1.2.2 Rectangular Rule

In the rectangular rule, the definite integral $\int_a^b f(x)dx$ is approximated by the area of a rectangle. This rectangle may be built using the left endpoint, the right endpoint, or the midpoint of the interval $[a, b]$ (Figure 1.1). The one that uses the midpoint is sometimes called the midpoint method and is only applicable when the integrand is an analytical expression

1.2.3 Composite Rectangular Rule

In applying the composite rectangular rule, the interval $[a, b]$ is divided into n subintervals defined by $n + 1$ points labeled $a = x_1, x_2 \cdots, x_n, x_{n+1} = b$. The subintervals can generally have different widths so that longer intervals may be chosen for regions where the integrand exhibits slow variations and shorter intervals where the integrand experiences rapid changes. Over each subinterval $[x_i, x_{i+1}]$, the integral is approximated by the area of a rectangle. These rectangles are constructed using the left endpoint, the right endpoint, or the midpoint as described earlier (Figure 1.2). Adding the areas of rectangles yields the approximate value of the definite integral $\int_a^b f(x)dx$.

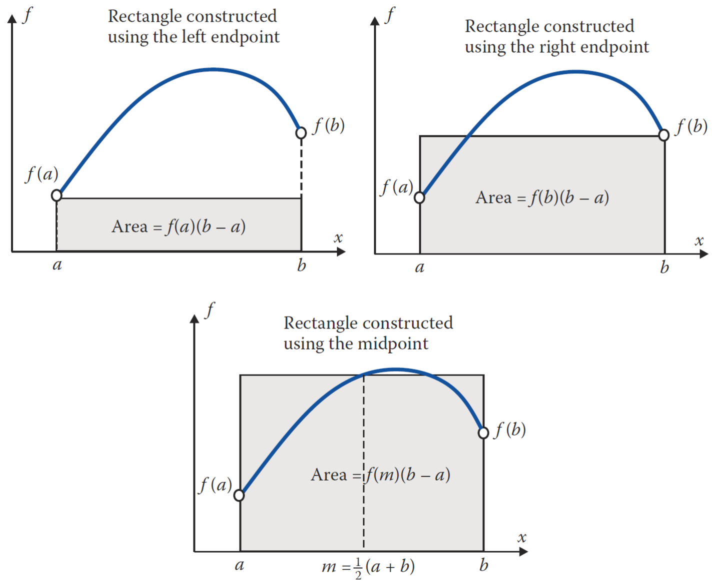


Figure 1.1: Rectangular rule.

1. Composite Rectangular Rule (Using Left Endpoint)

$$\int_a^b f(x)dx = \sum_{i=1}^{n} \{f(x_i)\,(x_{i+1} - x_i)\} + O(h) = h\sum_{i=1}^{n} f(x_i) + O(h) \quad \text{for equal space}$$

2. Composite Rectangular Rule (Using Right Endpoint)

$$\int_a^b f(x)dx = \sum_{i=2}^{n+1} \{f(x_i)\,(x_i - x_{i-1})\} + O(h) = h\sum_{i=2}^{n+1} f(x_i) + O(h) \quad \text{for equal space}$$

3. Composite Rectangular Rule (Using Midpoint)

$$\begin{aligned}\int_a^b f(x)dx &= \sum_{i=1}^{n} \{f(m_i)\,(x_{i+1} - x_i)\} + O(h^2) \\ &= h\sum_{i=1}^{n} f(m_i) + O(h^2) \quad \text{for equal space} \quad m_i = \frac{1}{2}\,(x_{i+1} - x_i)\end{aligned}$$

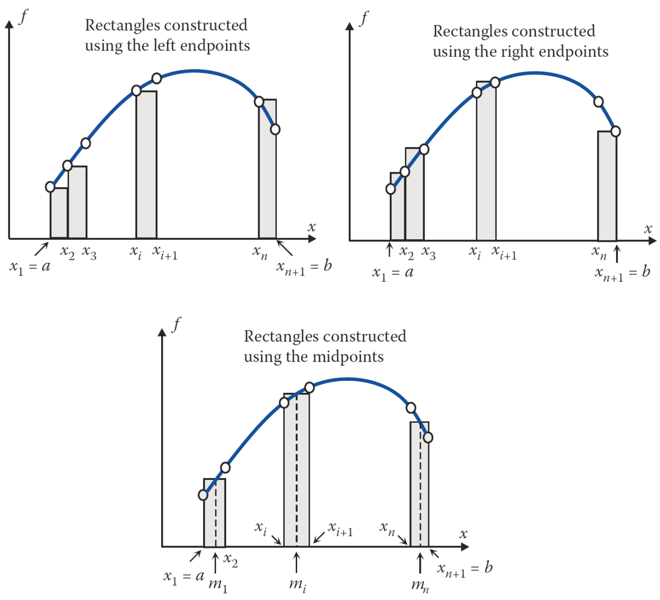


Figure 1.2: Composite rectangular rules.

Example 1.6

Evaluate the following definite integral using all three composite rectangular rule strategies with $n = 8$

$$\int_{-1}^{1} \frac{1}{x+1}$$

Solution

With the limits of integration at $b = 1, a = -1$, *we ind the spacing size as* $h = (b-a)/n = 2/8 = 0.25$. *The nine nodes are thus defined as* $x_1 = -1, -0.75, -0.5, \cdots, 0.75, 1 = x_9$. *Letting* $f(x) = 1/(x+2)$, *the three integral estimates are found as follows:*

1. *Using left endpoint*

$$\int_{-1}^{1} f(x)dx = h\sum_{i=1}^{8} f(x_i) = 0.25\left[f(-1) + f(-0.75) + \cdots + f(0.75)\right] = 1.1865$$

2. *Using Right Endpoint*

$$\int_{-1}^{1} f(x)dx == h\sum_{i=2}^{9} f(x_i) = 0.25\left[f(-0.75) + \cdots + f(0.75) + f(1)\right] = 1.0199$$

3. *Using Midpoint*

$$\int_{-1}^{1} f(x)dx = h\sum_{i=1}^{n} f(m_i) = 0.25\left[f(-0.875) + f(-0.625)\cdots + f(0.875)\right] = 1.0963$$

$$m_i = \frac{1}{2}(x_{i+1} - x_i)$$

Noting that the actual value of the integral is $\ln 3 = 1.0986$, *the above estimates come with relative errors of* $8\%, 7.17\%$, *and* 0.21%, *respectively.The midpoint method yields the best accuracy.*

1.2.4 Trapezoidal Rule

One of the simplest methods of finding the area under a curve, known as the trapezoidal rule, is based on approximating $f(x)$ by a piecewise linear polynomial that interpolates $f(x)$ at the nodes $x_0, x_1, \cdots, x_n$. Let $a = x_0 < x_1 = b$, and use the linear Lagrange polynomial

$$p_1(x) = f_0\left[\frac{x-x_1}{x_0-x_1}\right] + f_1\left[\frac{x-x_0}{x_1-x_0}\right].$$

Then

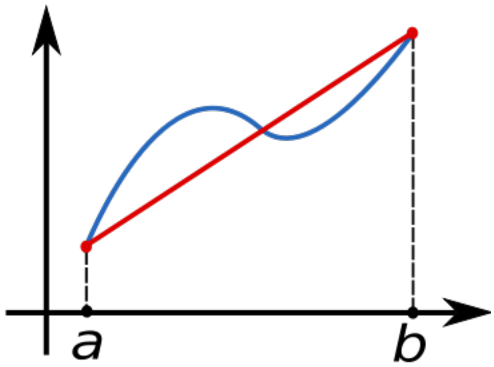


Figure 1.3: Trapezoidal rule illustration

$$\int_a^b f(x)dx = \int_{x_0}^{x_1}\left[f_0\left[\frac{x-x_1}{x_0-x_1}\right] + f_1\left[\frac{x-x_0}{x_1-x_0}\right]\right]dx + \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)dx.$$

Hence,

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

Truncation Error= $\frac{h^3}{12}f''(\xi)$
If $|f''(x)| \leq$M for all x in the interval $[a,b]$, then

$$|E_i| \leq \frac{h^3}{12}M$$

Applying above over the entire interval, we obtain the total error E_T

$$|E_T| \leq n\frac{h^3}{12}M = (b-a)\frac{h^2}{12}$$

Hence, as we expected, the error term for the composite trapezoidal rule is zero if $f(x)$ is linear; that is, for a first-degree polynomial, the trapezoidal rule gives the exact result.

1.2.5 Composite Trapezoidal Rule

We define $h = \frac{b-a}{n} = x_j - x_{j-1}$

$$\begin{aligned}\int_{a=x_0}^{b=x_n} f(x)dx &= \sum_{j=1}^{n}\int_{x_{j-1}}^{x_j} f(x)dx = \sum_{j=1}^{n}\left(\frac{h}{2}[f(x_{j-1}+f(x_j)] - \frac{h^3}{12}f''(\xi_j)\right)\\ &= \sum_{j=1}^{n}\frac{h}{2}[f(x_{j-1}+f(x_j)] - \frac{h^3}{12}\sum_{j=1}^{n}f''(\xi_j)\\ &= \sum_{j=1}^{n}\frac{h}{2}[f(x_{j-1}+f(x_j)] - \frac{h^2}{12}(b-a)f''(\xi) \quad (\text{since } nh = b-a)\end{aligned}$$

Thus, the Composite Trapezoidal rule is

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

Example 1.7

Evaluate the following definite integral using composite trapezoidal rule strategies with $n = 8$

$$\int_{-1}^{1} \frac{1}{x+1}$$

Solution:

$$\int_{-1}^{1} f(x)dx = \frac{0.25}{2}\left[f(-1) + 2f(-0.75) + 2f(-0.5) + \cdots + 2f(0.75) + f(1)\right] = 1.1032$$

Recalling the actual value 1.0986, the relative error is calculated as 0.42%. As expected, and stated earlier, the accuracy of composite trapezoidal rule is compatible with the midpoint rectangular method and better than the composite rectangular rule using either endpoint.

Example 1.8

Use the composite trapezoidal rule with $n = 1$ to compute the integral

$$\int_1^3 2x + 1dx$$

Solution:
We have

$$\int_1^3 2x + 1dx = \frac{2}{2}[f(1) + f(3)] = 3 + 7 = 10.$$

As expected, the trapezoidal rule gives the exact value of the integral because $f(x)$ is linear.

Example 1.9

Determine the number of subintervals n required to approximate

$$\int_0^2 \frac{1}{x+4}$$

with an error E_T less than 10^{-4} using the composite trapezoidal rule.
Solution: *We have*

$$|E_T| \leq (b-a)\frac{h^2}{12} \leq 10^{-4}$$

In this example, the integrand is $f(x) = 1/(x+4)$, and $f''(x) = 2(x+4)^{-3}$. The maximum value of $|f''(x)|$ on the interval $[0, 2] is 1/32$, and thus, $M = 1/32$. This is used with the above formula to obtain

$$\frac{1}{192}h^2 \leq 10^{-4} \quad \text{or} \quad h = 0.13856$$

Since $h = 2/n$, the number of subintervals n required is $n \geq 15$.

1.2.6 Simpson Rules

The trapezoidal rule estimates the value of a definite integral by approximating the integrand with a first-degree polynomial, the line connecting the points $(a, f(a))$ and $(b, f(b))$. Any method that uses a higher-degree polynomial to connect these points will provide a more accurate estimate. Simpson's 1/3 and 3/8 rules, respectively, use second and third degree polynomials to approximate the integrand.

Simpson's 1/3 rule

In evaluating $\int_a^b f(x)dx$, the Simpson's 1/3 rule uses a second-degree polynomial to approximate the integrand $f(x)$. The three points that are needed to determine this polynomial are picked as $x_0 = a, x_1 = (a+b)/2$, and $x_2 = b$ with $h = \frac{b-a}{2}$, the second degree Lagrange interpolating polynomial is constructed as

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

$$\boxed{\int_a^b \mathbf{f(x)dx = h\left[\frac{f(x_0)+4f(x_1)+f(x_2)}{6}\right] + O(h^5)f^{(4)}}(\xi)}$$

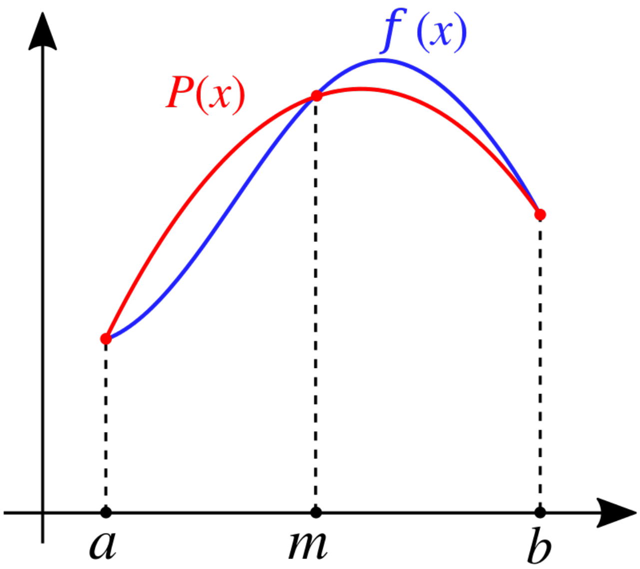


Figure 1.4: Simpsons method illustration

Composite Simpson's 1/3 rule

In the composite Simpson's 1/3 rule, the interval $[a, b]$ is divided into n subintervals defined by $n + 1$ points labeled $a = x_0, x_2, \cdots, x_n = b$. Although the subintervals can have different widths, the results that follow are based on the assumption that the points are equally spaced with spacing size $h = (b-a)/n$. Since three points are needed to construct a second degree interpolating polynomial, the Simpson's 1/3 rule must be applied to two adjacent subintervals at a time. Therefore, $[a, b]$ must be divided into an even number of subintervals for the composite 1/3 rule to be implemented. As a result,

$$\int_a^b f(x)dx \approx \sum_{j=1}^{n} \frac{x_{j-1} - x_j}{6} \left[f(x_{j-1}) + 4f\left(\frac{x_{j-1} + x_j}{2}\right) + f(x_j) \right]$$

Example 1.10

Evaluate the definite integral of the above example using the composite Simpson's 1/3 rule with $n = 8$:

$$\int_{-1}^{1} \frac{1}{x+2} dx$$

Solution:

The spacing size is $h = (b-a)/n = 0.25$ and the nine nodes are defined as

$$x_0 = -1, -0.75, -0.5, \cdots, 0.75, 1 = x_8.$$

$$\int_{-1}^{1} \frac{1}{x+2} dx = \frac{0.25}{3} \begin{bmatrix} f(-1) + 4f(-0.75) + 2f(-0.5) + 4f(-0.25) \\ + 2f(0) + 4f(0.25) + 2f(0.5) + 4f(0.75) + f(1) \end{bmatrix} = 1.0987$$

Knowing the actual value is 1.0986, the relative error is calculated as 0.01%. As expected, the accuracy of the composite Simpson's 1/3 rule is superior to the composite trapezoidal rule.

Simpson Rules 3/8 rule

The Simpson's 3/8 rule uses a third-degree polynomial to approximate the integrand $f(x)$. The four points that are needed to form this polynomial are picked as the four equally spaced points $x_0 = a, x_1 = (2a + b)/3, x_2 = (a + 2b)/3$, and $x_3 = b$ with spacing size $h = (b - a)/3$

Simpson's 3/8 is defined by the formula

$$\int_a^b f(x)dx = \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_4)] - \frac{3h^5}{80} f^4\xi$$

Definition 1.1

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 all $k = 0, 1, \cdots, n$.

With this definition:

Scheme	Degree of Accuracy
Trapezoidal	1
Simpson's	3

Trapezoidal and Simpson's are examples of a class of methods known as **Newton-Cotes formulas**.

Example 1.11

Evaluate the definite integral of the above example using the composite Simpson's 3/3 *rule with* $n = 8$:

$$\int_{-1}^{1} \frac{1}{x+2} dx$$

Solution:

The spacing size is $h = (b-a)/n = 0.25$ *and the nine nodes are defined as*

$$x_0 = -1, -0.75, -0.5, \cdots, 0.75, 1 = x_8.$$

$$\int_{-1}^{1} \frac{1}{x+2} dx = \frac{0.75}{8} \begin{bmatrix} f(-1) + 3f(-0.75) + 3f(-0.5) + f(-0.25) \\ + f(0) + 3f(0.25) + 3f(0.5) + f(0.75) \\ + f(1) \end{bmatrix} = 1.0986$$

Knowing the actual value is 1.0986, *the relative error is calculated as* 0.0%.

1.2.7 Newton-Cotes formulas

Newton-Cotes formulae can be useful if the value of the integrand at equally spaced points is given. It is assumed that the value of a function f defined on $[a, b]$ is known at equally spaced points x_i, for $i = 0, \cdots, n$, where $x_0 = a$ and $x_n = b$. There are two types of Newton-Cotes formulae, the "closed" type which uses the function value at all points, and the "open" type which does not use the function values at the endpoints. The closed Newton-Cotes formula of degree n is stated as

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

where $x_i = h_i + x_0$, with h (called the step size) equal to $\frac{x_n - x_0}{n} = \frac{b-a}{n}$. The w_i are called weights.

As can be seen in the following derivation the weights are derived from the Lagrange basis polynomials. They depend only on the x_i and not on the function f. Let $L(x)$ be the interpolation polynomial in the Lagrange form for the given data points $(x_0, f(x_0)), \cdots, (x_n.f(x_n))$, then

$$\int_a^b f(x)\, dx \approx \int_a^b L(x)\, dx = \int_a^b \Big(\sum_{i=0}^{n} f(x_i)\, l_i(x)\Big)\, dx = \sum_{i=0}^{n} f(x_i) \underbrace{\int_a^b l_i(x)\, dx}_{w_i}.$$

The open Newton-Cotes formula of degree n is stated as

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

The weights are found in a manner similar to the closed formula.

Newton's cotes Quadrature formula

Let $f(x)$ be an unknown function whose numerical values are given at $(n+1)$ equidistant points x_i in the interval $[a, b]$, where $x_i = x_0 + ih$, $i = 0, 1, \cdots, n$ such that $a = x_0$ and $b = x_n$, i.e.,

$b-a=nh$. Then

$$\begin{aligned}\int_a^b f(x)dx &\approx \int_{x_0}^{x_n} P_n(x)dx \\ &= h\int_0^n P_n(p)dp, \qquad \text{where} \quad x=x_0+ph, \text{ and } dx=hdp.\end{aligned}$$

Expressing $P_n(p)$ by Newton's forward difference formula (1.29) , we get

$$\begin{aligned}\int_a^b f(x)dx &\approx h\int_0^n \left[f_0+p\Delta f_0+\frac{p(p-1)}{2!}\Delta^2 f_0+\cdots\frac{p(p-1)\cdots(p-n+1)}{n!}\Delta^n f_0\right]dk \\ &= h\left[pf_0+\frac{p^2}{2}\Delta f_0+\frac{1}{2!}\left(\frac{p^3}{3}-\frac{p^2}{2}\right)\Delta^2 f_0+\cdots+\text{last term}\right]_0^n\end{aligned}$$

Thus, the Newton's Cotes quadrature formula is given by:

$$\int_a^b f(x)dx \approx h\left[nf_0+\frac{n^2}{2}\Delta f_0+\frac{1}{2!}\left(\frac{n^3}{3}-\frac{n^2}{2}\right)\Delta^2 f_0+\cdots+\text{last term}\right] \qquad (1.29)$$

From this formula one can derive many simple formulae for different values of $n=1,2,3,\cdots$. Some particular cases are discussed below.

1.2.8 Trapeziodal Rule

One of the simple quadrature formula is trapezoidal formula. To obtain this formula, we substitute $n=1$ to the Equation (1.29). Obviously, we can fit a straight line through these two points or we can say, one can obtain only first order differences from two points then neglecting second and high order differences in Equation (1.29) we get,

$$\begin{aligned}\int_a^b f(x)dx &\approx h\left[f_0+\frac{1}{2}\Delta f_0\right] \ = h\left[f_0+\frac{1}{2}(f_1-f_0)\right] \\ &= \frac{h}{2}(f_0+f_1)\end{aligned}$$

Hence

$$\int_a^b f(x)dx \approx \frac{h}{2}(f_0+f_1) \qquad (1.30)$$

This is known as **Trapezoidal quadrature formula** or the **Trapezoidal rule.**

Note that the formula is very simple and it gives a very rough approximation of the integral. So, if the interval $[a,b]$ is divided into some subintervals and the formula is applied to each of these subintervals, then much better approximate result may be obtained. This formula is known as **composite trapezoidal formula**, described below.

Composite Trapezoidal formula

Suppose the interval $[a,b]$ be divided into n equal subintervals as $a=x_0,x_1,x_2,\cdots,x_n=b$. That is, $x_i=x_0+ih, i=1,2,\cdots,n$, where h is the length of the intervals.

Now, the trapezoidal formula is applied to each of the subintervals, and we obtained the composite formula as follows:

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx \\ &\approx \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \cdots + \frac{h}{2}(f_{n-1} + f_n) \\ &= \frac{h}{2}\left[f_0 + 2(f_1 + f_2 + \cdots + f_{n-1}) + f_n\right].\end{aligned}$$

Therefore, the Composite trapezoidal rule is given by

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f_0 + 2\sum_{j=1}^{n-1} f_j + f_n\right]. \qquad (1.31)$$

Example 1.12

The following points were found empirically.

x	2.1	2.4	2.7	3.0	3.3	3.6
y	3.2	2.7	2.9	3.5	4.1	5.2

Use the trapezoidal rule to estimate

$$dsplaystyle \int_{2.1}^{3.6} ydx$$

Solution: *Here we have* $h = 0.3$, *therefore we have*

$$\begin{aligned}\int_{2.1}^{3.6} ydx &= \frac{0.3}{2}\left[3.2 + 2 \times (2.7 + 2.9 + 3.5 + 4.1) + 5.2\right] \\ &= 5.22\end{aligned}$$

Error in Trapezoidal Rule

Since Trapezoidal rule is a numerical formula, it must have an error. The error in trapezoidal formula is calculated below.

Error of Trapezoidal in one step, i.e., Local error is

$$\begin{aligned}E_{L_0} &= \int_{x_0}^{x_1} \frac{p(p-1)}{2!} h^2 f''(\xi_1) dp \\ &= \frac{h^3}{2} f''(\xi_1) \int_0^1 \left(p^2 - p\right) dp = \quad = -\frac{h^3}{12} f''(\xi_1) \to \mathcal{O}(h^3),\end{aligned}$$

i.e., the local error of Trapezoidal rule is $\mathcal{O}(h^3)$. Now, Global error in Trapezoidal rule means the sum of all n local errors, which is

$$\sum_{i=0}^{n-1} E_{L_i} = -\frac{h^3}{12}\left[f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_n)\right], x_i \le \xi_i \le x_{i+1}, i = 0, 1, 2 \cdots, n-1.$$

If we assume that $f''(x)$ is continuous on (a,b) then there exists some value of x in (a,b), say ξ such that $\sum_{i=1}^{n} f''(\xi_i) = nf''(\xi)$.

Therefore, the global error of Trapezoidal rule is given by

$$E_T = -\frac{h^3}{12}nf''(\xi) = -\frac{b-a}{12}h^2 f''(\xi) \to \mathcal{O}(h^2) \qquad \text{since } nh = b-a, \quad (1.32)$$

which is one less to the order of local error.

Note: The error term in trapezoidal formula indicates that if the second and higher order derivatives of the function $f(x)$ vanish, then the trapezoidal formula gives exact result. That is, the trapezoidal formula gives exact result when the integrand is linear.

Geometrical interpretation of trapezoidal formula

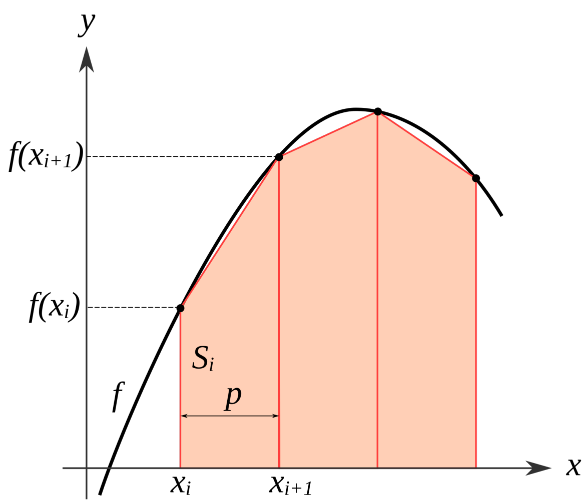


Figure 1.5: Geometrical interpretation of trapezoidal formula

In trapezoidal formula, the integrand $y = f(x)$ is replaced by the straight line, let AB joining the points (x_i, y_i) and (x_1, y_1) (see Figure 1.5). Then the area bounded by the curve $y = f(x)$, the ordinates $x = x_i$, $x = x_{i+1}$ and the x-axis is approximated by the area of the trapezium bounded by the straight line AB, the straight lines $x = xx_i$, $x = x_{i+1}$ and x-axis. That is, the value of the integration $\int_{x_i}^{x_{i+1}} f(x)dx$ obtained by the a trapezoidal formula is nothing but the area of the trapezium.

1.2.9 Simpson's Rule

When substituting $n = 2$ in the formula (1.29) and similar to $n = 1$, neglecting third and higher order differences in (1.29), we get

$$\begin{aligned}\int_a^b f(x)dx &\approx h\left[2f_0 + \frac{2^2}{2}\Delta f_0 + \frac{1}{2!}\left(\frac{2^3}{3} - \frac{2^2}{2}\right)\Delta^2 f_0\right] \\ &= h\left[2f_0 + 2(f_1 - f_0) + \frac{1}{3}(f_2 - 2f_1 + f_0)\right] \\ &= \frac{h}{3}[f_0 + 4f_1 + f_2]\end{aligned}$$

Hence, the Simpson's 1/3 formula is given by

$$\int_a^b f(x)dx \approx \frac{h}{3}[f_0 + 4f_1 + f_2] \qquad (1.33)$$

Composite Simpson???s 1/3 Rule

In the above formula, the interval of integration $[a, b]$ is divided into two subdivisions. Now, we divide the interval $[a, b]$ into n (even number) equal subintervals by the arguments $x_0, x_1, x_2, \cdots, x_n$, where $x_i = x_0 + ih,\ i = 1, 2, \cdots, n$.

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx \\ &\approx \frac{h}{3}(f_0 + 4f_1 + f_2) + \frac{h}{3}(f_2 + 4f_3 + f_4) + \cdots + \frac{h}{3}(f_{n-2} + 4f_{n-1} + f_n) \\ &= \frac{h}{3}[f_0 + 4(f_1 + f_3 + \cdots + f_{n-1}) + 2(f_2 + f_4 + \cdots + f_{n-2}) + f_n]. \\ &= \frac{h}{3}[f_0 + 4(\text{sum of } f_i \text{ with odd subscripts}) + 2(\text{sum of } f_i \text{ with even subscripts}) + f_n].\end{aligned} \qquad (1.34)$$

Thus, the **Simpson's 1/3 composite quadrature formula** is given by

$$\int_a^b f(x)dx \approx \frac{h}{3}\left[f_0 + 4\sum_{j=1}^{\frac{n}{2}} f_{2j-1} + 2\sum_{j=1}^{\frac{n}{2}-1} f_{2j} + f_n\right]. \qquad (1.35)$$

Note: Simpson's 1/3 -rule requires the division of the whole range into an even number of subintervals of width h.

Error in Simpson's 1/3 quadrature formula

The Local error expression in Simpson's 1/3 rule on the interval $[x_0, x_2]$ is given by

$$E_L \approx -\frac{h^5}{90} f^{(iv)}(\xi)$$

where $x_0 < \xi < x_2$ and the Global error in the composite Simpson's 1/3 rule is given by

$$E_T = -\frac{b-a}{180}h^4 f^{(iv)}(\xi), \quad \text{where} \quad f^{(iv)(\xi)} = \max\{f^{(iv)}(x_0), f^{(iv)}(x_1), \cdots, f^{(iv)}(x_n)\} \tag{1.36}$$

Example 1.13

Approximate the value of the integral

$$\int_0^1 e^{-x} dx$$

using the composite Simpson???s rule with $n = 4$ subintervals. Determine an upper bound for the absolute error using the error term. Verify that the absolute error is within this bound.

Solution: *Here $n = 4$ and hence $h = \frac{1-0}{4} = \frac{1}{4}$. Using the Simpson's composite rule we get*

$$\int_0^1 e^{-x} dx \approx \frac{1}{3\times 4}\left(e^0 + 4e^{-0.25} + 2e^{-0.5} + 4e^{-0.75} + e^{-1}\right)$$
$$\approx 0.6321342$$

Next, we need to find an upper bound for the absolute error using the general error term for the composite Simpson's rule given by

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

where $a < \xi < b$. Taking absolute values, and inserting $a = 0, b = 1$ and $h = 1/4$, the absolute error E is

$$E = -\frac{1}{180\times 4^4}|f^{(4)}(\xi)|.$$

Since $|f^{(4)}(\xi) = e^{-x}|$ is a decreasing positive function, we have the bound $|f^{(4)}(\xi)| < e^{-0} = 1$. Therefore the error bound is given by

$$E \leq \frac{1}{46080} \approx 2.2\times 10^{-5}.$$

To verify that the bound holds here, we easily compute the exact value of the integral

$$\int_0^1 e^{-x} dx = \left[-e^{-x}\right]_0^1 = e^{-1} - e^0 = 1 - e^{-1} = 0.6321206$$

Thus the actual absolute error is (correct to the digits used)

$$|0.6321206 - 0.6321342 \approx 1.4\times 10^{-5}$$

so the absolute error is within our bound. The bound quite closely bounds the actual absolute error in this case.

Exercise 1.1

Evaluate $\int_1^3 (x+1)e^{x^2}dx$ *taking 10 intervals, by* (i) *Trapezoidal, and* (ii) *Simpson's 1/3 rule.* **Ans.** (i) *6149.2217* (ii) *5557.9445*

Simpson's 3/8 Rule:

We put $n = 3$ in Equation (1.29), and we will have the four points $(x_0, y_0), (x_1, y_1), (x_2, y_2), (x_3, y_3)$ so that all forward differences higher than third order in Equation (1.29) will be zero. Hence we obtain:

$$\begin{aligned}\int_a^b f(x)dx &\approx h\left[3f_0 + \frac{3^2}{2}\Delta f_0 + \frac{1}{2!}\left(\frac{3^3}{3} - \frac{3^2}{2}\right)\Delta^2 f_0 + \frac{1}{3!}\left(\frac{3^4}{4} - 3^3 + 3^2\right)\Delta^3 f_0\right]\\ &= h\left[3f_0 + \frac{9}{2}\Delta f_0 + \frac{9}{4}\Delta^2 f_0 + \frac{9}{24}\Delta^3 f_0\right]\\ &= \frac{3}{8}h\left[8f_0 + 12\Delta f_0 + 6\Delta^2 f_0 + \Delta^3 f_0\right]\\ &= \frac{3}{8}h\left[8f_0 + 12(f_1 - f_0) + 6(f_2 - 2f_1 + f_0) + (f_3 - 3f_2 + 3f_1 - f_0)\right]\\ &= \frac{3}{8}h\left[f_0 + 3f_1 + 3f_2 + f_3\right]\end{aligned}$$

Therefore, the **Simpson's 3/8 Rule** is given by

$$\int_a^b f(x)dx \approx \frac{3}{8}h\left[f_0 + 3f_1 + 3f_2 + f_3\right] \qquad (1.37)$$

Composite Simpson's 3/8 Rule

In the above formula, the interval of integration $[a, b]$ is divided into three subdivisions. Now, we divide the interval $[a, b]$ into n (a multiple of three) equal subintervals by the arguments $x_0, x_1, x_2, \cdots, x_n$, where $x_i = x_0 + ih,\ i = 1, 2, \cdots, n$.

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_3} f(x)dx + \int_{x_3}^{x_6} f(x)dx + \cdots + \int_{x_{n-3}}^{x_n} f(x)dx\\ &\approx \frac{3}{8}h\left(f_0 + 3f_1 + 3f_2 + f_3\right) + \frac{3}{8}h\left(f_3 + 3f_4 + 3f_5 + f_6\right) + \cdots\\ &\quad + \frac{3}{8}h\left(f_{n-3} + 3f_{n-2} + 3f_{n-1} + f_n\right)\\ &= \frac{3}{8}h\left[f_0 + 3\left(f_1 + f_2 + f_4 + f_5 + \cdots f_{n-1}\right) + 2\left(f_3 + f_6 + f_9 + \cdots + f_{n-3}\right) + f_n\right]\end{aligned}$$

Thus, the **composite Simpson's 3/8 quadrature formula** is given by

$$\int_a^b f(x)dx \approx \frac{3}{8}h\left[f_0 + 3\left(f_1 + f_2 + f_4 + f_5 + \cdots f_{n-1}\right) + 2\left(f_3 + f_6 + \cdots + f_{n-3}\right) + f_n\right] \qquad (1.38)$$

In using Equation (1.38) the number of subintervals should be taken as a multiple of 3.

Example 1.14

Approximate the value of the integral

$$dsplaystyle \int_0^6 \frac{1}{1+x^2}dx$$

by dividing the interval[0,6] in to six equal subintervals using:

i. *Trapezoidal rule*

ii. *Simpson's 1/3 rule*

iii. *Simpson's 3/8 rule*

Solution: *Since we have six subintervals, i.e.* $n = 6$, *we can obtain the the step size* h *as*

$$h = \frac{6-0}{6} = 1.$$

As a result we obtain the values of the function $f(x) = \frac{1}{1+x^2}$ *at the nodal points*

x_i	0	1	2	3	4	5	6
$f(x_i)$	1	0.5	0.2	0.1	0.0588	0.0385	0.027

i. ***Trapezoidal rule:***

$$\begin{aligned}\int_0^6 \frac{1}{1+x^2}dx &\approx \frac{1}{2}\left[f_0 + 2\left(f_1 + f_2 + f_3 + f_4 + f_5\right) + f_6\right]\\ &\approx \frac{1}{2}\left[1 + 2\left(0.5 + 0.2 + 0.1 + 0.0588 + 0.0385\right) + 0.027\right]\\ &\approx 1.4108\end{aligned}$$

ii. ***Simpson's*** $1/3$ ***rule:***

$$\begin{aligned}\int_0^6 \frac{1}{1+x^2}dx &\approx \frac{1}{3}\left[f_0 + 4\left(f_1 + f_3 + f_5\right) + 2\left(f_2 + f_4\right) + f_6\right]\\ &\approx \frac{1}{3}\left[1 + 2\left(0.5 + 0.1 + 0.0385\right) + \left(0.2 + 0.0588\right) + 0.027\right]\\ &\approx 1.3662\end{aligned}$$

iii. ***Simpson's*** $3/8$ ***rule:***

$$\begin{aligned}\int_0^6 \frac{1}{1+x^2}dx &\approx \frac{3}{8}\left[f_0 + 3\left(f_1 + f_2 + f_4 + f_5\right) + 2\left(f_3\right) + f_6\right]\\ &\approx \frac{3}{8}\left[1 + 2\left(0.5 + 0.2 + 0.0588 + 0.0385\right) + 2\left(0.1+\right) + 0.027\right]\\ &\approx 1.3571\end{aligned}$$

A more illuminating explanation of why Simpson's rule is "more accurate than it ought to be" can be had by looking at the extent to which it integrates polynomials exactly. This leads us to the notion of **degree of precision** for a quadrature rule.

Definition 1.2: Degree of Precision

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

Example 1.15

Determine the degree of precision of Simpson's rule.
Solution: *It will suffice to apply the rule over the interval $[0, 2]$.*

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

but,

$$\int_0^2 x^4 dx = \frac{32}{5} \neq \frac{1}{3}(0+4+16) = \frac{20}{3},$$

Therefore, the degree of precision is 3.