Chapter 5

Numerical Differentiation and Integration

5.1 Introduction

As discussed in the previous chapter, a number of times we will have to estimate the function derivative or integral from a set of tabulated values of the function. For example, in our *Batman* problem, if Joker notes down the time as the wheel passes each floor, he may be asked to estimate the velocity of the wheel at these times. On the other hand, if he measures the velocity of the wheel, he may be asked to estimate the distance between the floors. In this chapter we discuss the methods which would enable him to do so. These methods are categorized as follows:

- *numerical differentiation* (estimating the function derivatives, e.g., to obtain the velocity or acceleration from distance measurements, finding the heat flux from temperature measurements), and
- *numerical integration* (estimating the integral of the function, e.g., to obtain distance from velocity measurements, finding the area of an object)

As before, we have two possibilities as to how the function values are given: the *continuous* case in which the function *f(x)* is known and the *discrete* case in which the function values are given corresponding to a few values of x. We mention again that the continuous case is a superset of the discrete case since the function values at selected points can be readily generated if the function is known. Also, since differentiation is a relatively straightforward operation, we would hardly ever need to perform *numerical* differentiation of a given function. Therefore, we first discuss numerical differentiation for the discrete case and then look at numerical integration for both the discrete and continuous cases.

5.2 Numerical Differentiation

Suppose we have a table of data listing the values of the dependent variable, f(x), corresponding to a few values of the independent variable, x, and we want to estimate the function derivative at one of these points[1]. Again, we denote the data points by the set of values$\{(x_k,f(x_k)), k=0,1,\ldots,n\}$[2]. As described in the previous chapter, we should be able to find the interpolating or regression polynomial and then, the derivative at any point. However, we have also seen that a higher order interpolating polynomial may show severe oscillations if the underlying function is not suitable for polynomial representation. Therefore, almost always, we will approximate the function by a *piecewise* polynomial[3] and then find its derivative using the relevant polynomial. The simplest continuous approximation would be a piecewise linear interpolation obtained by joining the function values at consecutive grid points, which will provide us with the *piecewise constant* first derivative. However, we will face two problems: (i) there would be two values of the first derivative at each node, one from either side, which may be significantly different from each other and (ii) the second and higher derivatives would be zero everywhere except at the grid points, where they would be undefined. Thus there is a need to look for alternative ways of performing the numerical differentiation. We discuss some of these techniques in the next sections. Since commonly the given data corresponds to evenly spaced grid points, we first describe the techniques for this case and then discuss the irregularly spaced data.

5.2.1 Evenly spaced grid points

In this section, we consider the case when $x_i - x_{i-1} = h$ for $i = 1,2,\ldots,n$. If we assume that the function is represented by a piecewise linear polynomial, the first derivative of the function at any point, x_i, may be obtained as

- the slope of the line in the previous segment (backward difference)[4]

$$f_i' = \frac{f(x_i) - f(x_{i-1})}{h} \tag{5.1}$$

- the slope of the line in the next segment (forward difference)

$$f_i' = \frac{f(x_{i+1}) - f(x_i)}{h} \tag{5.2}$$

- the average of these two slopes (or the slope of the line joining the previous point and the next point) (central difference)

$$f_i' = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \tag{5.3}$$

Clearly, the backward difference will not be valid at the first node, the forward difference will not work at the last node, and the central difference cannot be used at the first *and* last nodes. Now, if we want the second derivative at x_i, we may argue that the first derivative of the

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[1] Some times, though it is not very common, we may be asked to evaluate the derivative at a point which does not coincide with a grid point. A few techniques discussed here would be applicable in such cases. However, we would not address this issue further.

[2] As we did earlier for the interpolation problem, we assume that all x_k are distinct and there is no error in data. If the data is subjected to errors of measurement, we could first obtain the regression polynomial and then obtain the derivative at any point *analytically*. We also assume that the x_k are arranged in increasing order.

[3] We may go for nonpolynomial (e.g., rational, sinusoidal) interpolation but the procedure, and especially the error analysis, is more complicated.

[4] We will denote the estimated derivatives of the function at x_i by f_i' and the *exact* value by $f'(x_i)$.

function at the midpoint[1] of the previous segment is given by Eq. (5.1) and that at the midpoint of the next segment is given by Eq. (5.2). Therefore, the second derivative may be approximated as

$$f_i'' = \frac{\dfrac{f(x_{i+1}) - f(x_i)}{h} - \dfrac{f(x_i) - f(x_{i-1})}{h}}{h} = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} \tag{5.4}$$

Another alternative may be to fit a second degree polynomial through the three points (x_{i-1}, x_i, x_{i+1}) and find its second derivative (which would be a constant over the interval), which results in the same expression. Of course, the same argument could be extended to arrive at expressions of the higher derivatives, which would generally involve an increasing number of grid points around (or on one side of) the point at which we want the derivative value. However, there is a more convenient way, based on the Taylor's series, of deriving these expressions, which also provides an estimate of the error in the approximation. For convenience, we first analyze the first derivative of the function and then briefly describe the higher derivatives.

Using the Taylor's series expansion (you may want to review section 4.2 at this stage) about the point x_i, we may write

$$\begin{aligned} f(x_{i-1}) &= f(x_i) - hf'(x_i) + \frac{h^2}{2!} f''(x_i) - \frac{h^3}{3!} f'''(x_i) + \dots \\ f(x_{i+1}) &= f(x_i) + hf'(x_i) + \frac{h^2}{2!} f''(x_i) + \frac{h^3}{3!} f'''(x_i) + \dots \end{aligned} \tag{5.5}$$

from which the following can be easily obtained

$$\begin{aligned} f'(x_i) &= \frac{f(x_i) - f(x_{i-1})}{h} + h\frac{f''(x_i)}{2!} - h^2\frac{f'''(x_i)}{3!} - \dots = \frac{f(x_i) - f(x_{i-1})}{h} + h\frac{f''(x_b)}{2!} \\ f'(x_i) &= \frac{f(x_{i+1}) - f(x_i)}{h} - h\frac{f''(x_i)}{2!} - h^2\frac{f'''(x_i)}{3!} - \dots = \frac{f(x_{i+1}) - f(x_i)}{h} - h\frac{f''(x_f)}{2!} \\ f'(x_i) &= \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - h^2\frac{f'''(x_i)}{3!} - h^4\frac{f^{v}(x_i)}{5!} - \dots = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - h^2\frac{f'''(x_c)}{3!} \end{aligned} \tag{5.6}$$

in which ξ represents a point in the appropriate interval for the **b**ackward, **f**orward, and **c**entral difference schemes, i.e., $x_b \in (x_{i-1}, x_i); x_f \in (x_i, x_{i+1});$ and $x_c \in (x_{i-1}, x_{i+1})$. From these relationships, the following may be noted:

- The forward and backward difference schemes for the first derivative have error[2] of order h while the central difference scheme has O(h^2) error. This implies that if the

[1] Since the slope is constant throughout a segment, any other point could also be taken. However, as we will see a little latter, the central difference gives a better accuracy.

[2] The error, defined as *true value – approximate value*, refers here to only the truncation error arising out of the chopping off of Taylor's series after finite number of terms. For small step size, h, the function values at two neighbouring points would be very close and there may be significant round-off errors in computation of the derivatives. There is, therefore, a trade-off between the truncation and round-off errors and there would be an optimum step size which would result in the minimum *total* error. However, in this chapter, we will concentrate

step size, h, is halved, the error will also be *roughly*[1] half in the forward and backward schemes and one-fourth in the central difference scheme.

- If the actual function is a straight line, i.e., the second derivative is zero, both the forward and backward schemes will be exact. Similarly, if the function is a 2nd degree polynomial, the central difference scheme will provide the exact first derivative.
- The point ξ is not known and therefore an error estimate cannot be obtained for a general case. However, for known functions, upper and lower bounds for the second or third derivatives may be obtained and utilized to obtain the error bounds. As already discussed, though, the function is typically not known.
- Generally, but not always (see Exercise 5.2.1) the error reduces as the step size, *h*, becomes small. For an acceptable accuracy, therefore, the step size should be "small." Of course, the acceptable step size depends on how fast the function is varying (see Exercise 5.2.2). Choosing a proper step size for sampling the function is more a matter of the *design of experiment* and will not be considered here. The issue which we address is: once the step size is chosen and function values are available at a few (evenly spaced) points, how to estimate the derivatives accurately.

Example 5.1: The location of an object at various times was measured as follows:

Time (s)	0	1	2	3	4	5	6	7	8	9
Distance (cm)	0	3	14	39	84	155	258	399	584	819

Estimate the speed of the object at 5 seconds using (a) Backward difference, O(h); (b) Forward difference, O(h); and (c) Central difference, O(h^2). First use a step size, h=1 s, and then double this size (h = 2 s).

Solution: With a step size of 1 min, using Eqs. (5.6), the speed (i.e., the first derivative of the distance) is estimated as

$$\text{Backward difference,}\quad f_5' = \frac{f(5) - f(4)}{1} = 71 \text{ cm/s}$$

$$\text{Forward difference,}\quad f_5' = \frac{f(6) - f(5)}{1} = 103 \text{ cm/s}$$

$$\text{Central difference,}\quad f_5' = \frac{f(6) - f(4)}{2} = 87 \text{ cm/s}$$

for double the step size, these estimates are

$$\text{Backward difference,}\quad f_5' = \frac{f(5) - f(3)}{2} = 58 \text{ cm/s}$$

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on the truncation error assuming that use of higher precision computation will make the round-off error negligible in comparison, even for very small step sizes.

[1] If the second derivative of the function is constant, the error in forward and backward difference approximation of the first derivative would be *exactly* halved by halving the step size. Similarly, if the third derivative is constant, the error in central difference will be exactly one-fourth. For a general case, the error will vary linearly (or quadratically) with *h* only for small *h*.

$$\text{Forward difference,}\quad f_5' = \frac{f(7) - f(5)}{2} = 122 \text{ cm/s}$$

$$\text{Central difference,}\quad f_5' = \frac{f(7) - f(3)}{4} = 90 \text{ cm/s}$$

We expect the central difference estimate with the smaller step size of 1 second to be the most accurate estimate out of those obtained here. It is apparent that the forward and backward difference estimates have larger errors and the increase in error with increase in step length is also evident.

Improving the accuracy

As seen in the previous section, a simple forward or backward difference scheme estimates the first derivative with an O(h) error. One way to reduce the error is to reduce the step size. However, since we do not have function measurements at closer intervals, it would generally not be feasible to do so. Using the central difference formula is likely to improve the accuracy since the error is $O(h^2)$. However, if we are at either end of the data grid, the central difference scheme is not directly applicable. This provides the motivation to devise schemes which achieve higher order of accuracy (by utilizing additional function values). Although the basic philosophy is the same, i.e., using a higher order interpolation, there are several ways of arriving at the required formula. We discuss below some of these methods taking example of a forward difference formula which has $O(h^2)$ error:

a. Interpolation followed by differentiation: If, instead of the linear interpolation used in Eq. (5.2), we use the point x_{i+2} to fit a parabola through the three points and then differentiate it, we obtain a more accurate approximation. Since the derivative is invariant under translation, we may, without any loss of generality, take x_i=0, x_{i+1}=h, and x_{i+2}=2h. The interpolating polynomial is then given by

$$f_2(x) = f(x_i) + \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}x + \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}x^2 \qquad (5.7)$$

and, its slope at x=0 as

$$f_i' = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} \qquad (5.8)$$

b. Using Taylor's series: Writing the Taylor's series expansion

$$f(x_{i+2}) = f(x_i) + 2hf'(x_i) + \frac{4h^2}{2!}f''(x_i) + \frac{8h^3}{3!}f'''(x_i) + \ldots \quad (5.9)$$

and using Eq. (5.5) for the expansion of $f(x_{i+1})$ to eliminate the term involving the second derivative, it can be shown that

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + \frac{h^2}{3}f'''(x_i) + \ldots \qquad (5.10)$$

c. Method of undetermined coefficients: Assuming an expression of the form

$$f_i' = c_i f(x_i) + c_{i+1} f(x_{i+1}) + c_{i+2} f(x_{i+2}) \qquad (5.11)$$

in which the $c^{'s}$ are undetermined coefficients, we require that the first derivative be exact for all polynomials of 2nd degree. Taking the function as f(x)=1, x, and x^2, respectively, we obtain three linear equations (recall that we have taken the three points as x=0, h, and 2h) which can be solved to obtain the coefficients:

$$
\begin{aligned}
&c_i + c_{i+1} + c_{i+2} = 0 \\
&0.c_i + h.c_{i+1} + 2h.c_{i+2} = 1 \\
&0.c_i + h^2.c_{i+1} + 4h^2.c_{i+2} = 0
\end{aligned}
\tag{5.12}
$$

which results in $c_i = -\frac{3}{2h}; c_{i+1} = \frac{2}{h}; c_{i+2} = -\frac{1}{2h}$.

d. Richardson's extrapolation: From Eq. 5.6, the leading error term in the two point forward difference formula is equal to $-\frac{hf''(x_i)}{2}$. If we use a step size of *2h,*[1] the leading error term should be roughly twice that for the step size of *h*. Denoting the estimate of the first derivative with step size h as $f_i'(h)$, we have

$$
\begin{aligned}
f'(x_i) &= f_i'(h) + E + O(h^2) \\
f'(x_i) &= f_i'(2h) + 2E + O(h^2)
\end{aligned}
\tag{5.13}
$$

E being the O(h) error. A new, and hopefully more accurate, estimate of $f'(x_i)$ is obtained from the above as

$$
\begin{aligned}
f'(x_i) &= 2 f_i'(h) - f_i'(2h) + O\left(h^2\right) \\
&= 2\frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - f(x_i)}{2h} + O\left(h^2\right) \\
&= \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O\left(h^2\right)
\end{aligned}
\tag{5.14}
$$

In fact, we may carry out another step of extrapolation by using two $O(h^2)$ estimates to obtain an $O(h^3)$[2] estimate as[3]

$$
\begin{aligned}
f'(x_i) &= \frac{4 f_i'(h) - f_i'(2h)}{3} + O\left(h^3\right) \\
&= \frac{4}{3}\frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} - \frac{1}{3}\frac{-f(x_{i+4}) + 4f(x_{i+2}) - 3f(x_i)}{4h} + O\left(h^3\right) \\
&= \frac{f(x_{i+4}) - 12f(x_{i+2}) + 32f(x_{i+1}) - 21f(x_i)}{12h} + O(h^3)
\end{aligned}
\tag{5.15}
$$

Thus, all the methods result in the same expression for the O(h^2) estimate of the first derivative using the forward difference. Method (a) of direct interpolation is quite cumbersome. Moreover, it does not provide an estimate of the error and is not recommended for use[4]. Method (b) is the most commonly used technique for performing the numerical differentiation and is discussed in detail in the next section. Note that it provides an estimate of the error in approximating the derivative. Method (c) is quite straightforward but does not

[1] In other words, we use every alternate data point.
[2] We assume that the next term in the error is $O(h^3)$. When using the central difference, the next higher order term would be $O(h^4)$.
[3] In practice, we will be writing out the expression for the "more accurate" derivative in terms of "less accurate" derivatives and not in terms of the function values. Thus, we typically stop at the first line in Eqs. (5.14) and (5.15) and do not need to obtain the third line.
[4] An advantage of this method is that the second derivative is also easily obtained from Eq. (5.7).

provide an error estimate[1]. Method (d) is a powerful technique and may be used repeatedly to obtain more and more accurate estimates. However, the same could be accomplished by a direct use of the Taylor's series and would provide an estimate of the error also. Moreover, the higher order estimates typically *skip* some points [e.g., x_{i+3} in Eq. (5.15)] which is not desirable. Therefore, the method of undetermined coefficients and the Richardson's extrapolation method would not be discussed for the numerical differentiation. As we will see latter in this chapter, both of these techniques are quite useful in numerical integration.

Example 5.2: For the problem discussed in Example 5.1, estimate the speed using (a) forward difference, $O(h^2)$, using step sizes of 1 min and 2 min; and (b) Richardson extrapolation, $O(h^3)$.

Solution: With a step size of 1 s, using Eqs. (5.10), the speed is estimated as

$$f_5'(h) = \frac{-f(7)+4f(6)-3f(5)}{2} = 84 \text{ cm/s}$$

for double the step size, the estimate is

$$f_5'(2h) = \frac{-f(9)+4f(7)-3f(5)}{4} = 78 \text{ cm/s}$$

Using Eq. (5.15), first line, we obtain the $O(h^3)$ estimate with Richardson extrapolation as

$$f_5' = \frac{4f_5'(h) - f_5'(2h)}{3} = 86 \text{ cm/s}$$

As it turns out, this value is equal to the true value for this problem since the fourth derivative of the function is zero (we did not mention it earlier, and it was not really needed, but the distance was assumed to vary with time as $t+t^2+t^3$ resulting in a speed equal to $1+2t+3t^2$). It should also be noted that the error in the estimate with h=2 s (which is 86-78=8 cm/s) is exactly 4 times that with h=1 s (which is 2 cm/s). It is expected since the error is $O(h^2)$ and the third derivative of the function is constant (see Eq. 5.10 for the error term). Moreover, the error is positive (note that the third derivative is positive) and the forward difference formulas underpredict the speed of the object.

General formulation using Taylor's series

We write the finite difference approximation of the n^{th} derivative at x_i, as

$$f_i^n = \frac{1}{h^n} \sum_{j=-n_b}^{n_f} c_{i+j} f\left(x_{i+j}\right) \tag{5.16}$$

Where n_b and n_f denote the number of backward and forward grid points used in the expression. Thus, n_b=0 for forward difference schemes, n_f =0 for backward difference schemes, and n_b=n_f for central difference schemes[2]. The coefficients[1], c, are obtained by

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[1] However, an *approximate* estimate of the error may be obtained if we assume that the error is proportional to $h^2 f'''(x_f)$. Then, using the function $f(x)=x^3$, it can be shown from an extension of Eq. (5.15) that the error is equal to $\frac{h^2 f'''(x_f)}{3}$.

[2] We may, of course, use different number of points before and after x_i. However, the nonsymmetrical distribution of the grid points will imply that we lose the advantage of the cancellation of errors. Even then,

expanding $f\left(x_{i+j}\right)$ in a Taylor's series about the point x_i and equating the coefficients of like terms[2] on both sides. For example, the forward difference approximation for the first derivative using three points (n_b=0, n_f =2) is written as

$$\begin{aligned} f_i' &= \frac{c_i f\left(x_i\right)+c_{i+1} f\left(x_{i+1}\right)+c_{i+2} f\left(x_{i+2}\right)}{h} \\ &= \frac{c_i+c_{i+1}+c_{i+2}}{h} f\left(x_i\right)+\left(c_{i+1}+2c_{i+2}\right) f'\left(x_i\right)+\frac{h}{2}\left(c_{i+1}+4c_{i+2}\right) f''\left(x_i\right)+\frac{h^2}{6}\left(c_{i+1}+8c_{i+2}\right) f'''\left(x_i\right)+\ldots \end{aligned}$$

(5.17)

Equating the coefficients of f, f', and f'' we get equations similar to Eq. (5.12), resulting in $c_i=-\frac{3}{2}; c_{i+1}=2; c_{i+2}=-\frac{1}{2}$. The error[3] is obtained from the last term in Eq. (5.17) as $\frac{h^2 f'''\left(x_f\right)}{3}$, with $x_f \in \left(x_i, x_{i+2}\right)$. Similarly, if we want the second derivative using the same three points, we get $c_i=1; c_{i+1}=-2; c_{i+2}=1$ and the error as $-hf'''\left(x_f\right)$. For the central difference scheme using three points (n_b=n_f =1), the first derivative is written as

$$\begin{aligned} f_i' &= \frac{c_{i-1} f\left(x_{i-1}\right)+c_i f\left(x_i\right)+c_{i+1} f\left(x_{i+1}\right)}{h} \\ &= \frac{c_{i-1}+c_i+c_{i+1}}{h} f\left(x_i\right)+\left(-c_{i-1}+c_{i+1}\right) f'\left(x_i\right)+\frac{h}{2}\left(c_{i-1}+c_{i+1}\right) f''\left(x_i\right)+\frac{h^2}{6}\left(-c_{i-1}+c_{i+1}\right) f'''\left(x_i\right)+\ldots \end{aligned} \qquad (5.18)$$

from which, we get $c_{i-1}=-\frac{1}{2}; c_i=0; c_{i+1}=\frac{1}{2}$ and the error as $-\frac{h^2}{6} f'''\left(x_c\right)$ with $x_c \in \left(x_{i-1}, x_{i+1}\right)$.

For, the second derivative, we get the three equations as

$$\begin{aligned} c_{i-1}+c_i+c_{i+1}&=0 \\ -c_{i-1}+c_{i+1}&=0 \\ c_{i-1}+c_{i+1}&=2 \end{aligned}$$

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sometimes it may be preferable to use nonsymmetric central difference (e.g., at the second point of the data grid, it may be better to use a 5-point central difference scheme with n_b=1 and n_f=3 rather than a 5-point forward difference scheme with n_f=4).

[1] Comparing the Lagrange interpolating polynomial [Eq. (4.19) with the basis functions given by Eq. (4.21)] and Eq. (5.16), it is apparent that the coefficients may be obtained by taking the n^{th} derivative of the Lagrange polynomial. However, it is generally easier to use Taylor's series expansion.

[2] Since there are n_b+n_f+1 unknown coefficients to be obtained, we would need to equate the coefficients of the function, *f(xi)*, and its derivatives up to the order n_b+n_f .

[3] Recall that the error is given by *true value – approximate value*.

and the error as $-\frac{h}{6}\left(-c_{i-1}+c_{i+1}\right) f'''\left(x_i\right)-\frac{h^2}{24}\left(c_{i-1}+c_{i+1}\right) f^{iv}\left(x_c\right)$ [1]. This results in $c_{i-1}=1; c_i=-2; c_{i+1}=1$ and the error is obtained as $-\frac{h^2 f^{iv}\left(x_c\right)}{12}$.

It is readily seen that the leading error term in the generalized form of the finite difference approximation for the nth derivative is proportional to[2] $h^{-n} h^{n_b+n_f+1} f^{n_b+n_f+1}\left(x_i\right)$. For forward/backward difference, therefore, if we want an expression for the nth derivative of $O(h^a)$ accuracy, we would need to use $a+n-1$ additional points after/before x_i. For central difference, however, as we just saw, the coefficient of the leading error term may become zero[3]. So, in the central difference scheme for the nth derivative using n_c points before and same number of points after x_i, the accuracy would be $O(h^a)$ with $a=2n_c+1-n$ for odd n and $a=2n_c+2-n$ for even n, implying that a is always even.

It is not desirable to skip points close to x_i and include points farther away. For example, when using Richardson's extrapolation to obtain $O(h^3)$ estimate of the first derivative using the forward difference approximation, we effectively skip x_{i+3} but include x_{i+4}. It may be better to use the generalized form and obtain $c_i=-\frac{11}{6}; c_{i+1}=3; c_{i+2}=-\frac{3}{2}; c_{i+3}=\frac{1}{3}$ and the error as $-\frac{h^3 f^{iv}\left(x_f\right)}{4}$. On the other hand, if we include the point x_{i+4}, and assume that $c_{i+3}=0$, we get $c_i=\frac{7}{4}; c_{i+1}=\frac{8}{3}; c_{i+2}=-1; c_{i+4}=\frac{1}{12}$ and the error as $-\frac{h^3 f^{iv}\left(x_f\right)}{3}$. Thus we get the same expression as was obtained using Richardson's extrapolation [Eq. (5.15)] and see that the error is larger than that obtained using 4 *consecutive* points[4].

A listing of some expressions is given in a convenient tabular form in Tables 5.1, 5.2, and 5.3 for the forward, backward, and central difference schemes (note that the backward difference scheme is similar to the forward difference scheme with using –h in place of h and i−j in place of i+j). An extensive table is available in a number of references (e.g., Abramowitz and Stegun).

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[1] Although the leading term in the error is *O(h)*, its coefficient becomes zero. Therefore, we use an additional term in the error.

[2] A dimensional analysis will show that the error in nth derivative will contain terms of the form $h^{a-n} f^{a}(x)$.

[3] It can be shown that for symmetrically placed points, all *even* derivatives would have symmetric coefficients and the coefficient of the leading error term will be zero. Similarly, all *odd* derivatives would have antisymmetric coefficients with $c_i = 0$.

[4] The expression for the first derivative of $O(h^2)$ accuracy using central difference approximation contains points x_{i-1} and x_{i+1} but not x_i. However, this does not mean that we have skipped the point x_i. A quick look at the derivation indicates that we did consider the coefficient c_i, it just *turned out* to be zero. In contrast, for the Richardson's extrapolation, we *forced* c_{i+3} to be zero.

Table 5.1 Forward difference formulae $f_i^n = \frac{1}{h^n}\sum_{j=0}^{n_f} c_{i+j} f\left(x_{i+j}\right)$

Accuracy	Derivative	c_i	c_{i+1}	c_{i+2}	c_{i+3}	c_{i+4}	Error[1]
O(h)	f_i'	-1	1				$-\frac{hf''}{2}$
	f_i''	1	-2	1			$-hf'''$
	f_i'''	-1	3	-3	1		$-\frac{3hf^{iv}}{2}$
	f_i^{iv}	1	-4	6	-4	1	$-2hf^{v}$
O(h^2)	f_i'	$-3/2$	2	$-1/2$			$\frac{h^2 f'''}{3}$
	f_i''	2	-5	4	-1		$\frac{11h^2 f^{iv}}{12}$
	f_i'''	$-5/2$	9	-12	7	$-3/2$	$\frac{7h^2 f^{v}}{4}$
O(h^3)	f_i'	$-11/6$	3	$-3/2$	1/3		$-\frac{h^3 f^{iv}}{4}$
	f_i''	35/12	$-26/3$	19/2	$-14/3$	11/12	$-\frac{5h^3 f^{v}}{6}$

Table 5.2 Backward difference formulae $f_i^n = \frac{1}{h^n}\sum_{j=-n_b}^{0} c_{i+j} f\left(x_{i+j}\right)$

Accuracy	Derivative	c_{i-4}	c_{i-3}	c_{i-2}	c_{i-1}	c_i	Error
O(h)	f_i'				-1	1	$\frac{hf''}{2}$
	f_i''			1	-2	1	hf'''
	f_i'''		-1	3	-3	1	$\frac{3hf^{iv}}{2}$
	f_i^{iv}	1	-4	6	-4	1	$2hf^{v}$
O(h^2)	f_i'			1/2	-2	3/2	$\frac{h^2 f'''}{3}$
	f_i''		-1	4	-5	2	$\frac{11h^2 f^{iv}}{12}$

[1] The derivatives in the error expressions are evaluated at some point in the appropriate interval.

	f_i'''	3/2	-7	12	-9	5/2	$\frac{7h^2 f^{v}}{4}$
$O(h^3)$	f_i'		$-1/3$	3/2	-3	11/6	$\frac{h^3 f^{iv}}{4}$
	f_i''	11/12	$-14/3$	19/2	$-26/3$	35/12	$\frac{5h^3 f^{v}}{6}$

Table 5.3 Central difference formulae $f_i^n = \frac{1}{h^n} \sum_{j=-n_c}^{n_c} c_{i+j} f\left(x_{i+j}\right)$

Accuracy	Derivative	c_{i-2}	c_{i-1}	c_i	c_{i+1}	c_{i+2}	Error
$O(h^2)$	f_i'		$-1/2$	0	1/2		$-\frac{h^2 f'''}{6}$
	f_i''		1	-2	1		$-\frac{h^2 f^{iv}}{12}$
	f_i'''	$-1/2$	1	0	-1	1/2	$-\frac{h^2 f^{v}}{4}$
	f_i^{iv}	1	-4	6	-4	1	$-\frac{h^2 f^{vi}}{6}$
$O(h^4)$	f_i'	1/12	$-2/3$	0	2/3	$-1/12$	$\frac{h^4 f^{v}}{30}$
	f_i''	$-1/12$	4/3	$-5/2$	4/3	$-1/12$	$\frac{h^4 f^{vi}}{90}$

Example 5.3: For the problem described in Example 5.1, estimate the speed using (a) backward difference, $O(h^2)$, using step sizes of 1 s and 2 s; (b) Richardson extrapolation, $O(h^3)$, using the two estimates obtained in (a); and (c) central difference, $O(h^4)$. Also estimate the acceleration using (a) the forward difference, $O(h)$, $O(h^2)$ and $O(h^3)$; and (b) central difference $O(h^2)$.

Solution: Using tables 5.2 and 5.3, the speed is estimated as

$$\text{Backward difference, } O(h^2),\ h=1 \text{ s:}\quad f_5' = \frac{\frac{1}{2} f(3) - 2f(4) + \frac{3}{2} f(5)}{1} = 84 \text{ cm/s}$$

$$\text{Backward difference, } O(h^2),\ h=2 \text{ s:}\quad f_5' = \frac{\frac{1}{2} f(1) - 2f(3) + \frac{3}{2} f(5)}{2} = 78 \text{ cm/s}$$

$$\text{Ricardson Extrapolation:}\quad f_5' = \frac{4 f_5'(h=1) - f_5'(h=2)}{3} = 86 \text{ cm/s}$$

Central difference, $O(h^4)$: $f_5' = \dfrac{\frac{1}{12} f(3) - \frac{2}{3} f(4) + \frac{2}{3} f(6) - \frac{1}{12} f(7)}{1} = 86$ cm/s

The acceleration estimates (using tables 5.1 and 5.3) are:

$$\text{Forward difference, } O(h)\text{: } f_5' = \frac{f(5) - 2f(6) + f(7)}{1^2} = 38 \text{ cm/s}$$

$$\text{Forward difference, } O(h^2)\text{: } f_5' = \frac{2f(5) - 5f(6) + 4f(7) - f(8)}{1^2} = 32 \text{ cm/s}$$

$$\text{Forward difference, } O(h^3)\text{: } f_5' = \frac{\frac{35}{12} f(5) - \frac{26}{3} f(6) + \frac{19}{2} f(7) - \frac{14}{3} f(8) + \frac{11}{12} f(9)}{1^2} = 32 \text{ cm/s}$$

$$\text{Central difference, } O(h^4)\text{: } f_5' = \frac{f(4) - 2f(5) + f(6)}{1^2} = 32 \text{ cm/s}$$

Knowing the function, it is easy to draw conclusions about the error along similar lines as described in Example 5.2.

5.2.2 Unevenly spaced grid points

Let us now consider the case when $x_i - x_{i-1} = h_i$ for $i = 1, 2, ..., n$ such that not all h_i are equal. If we assume that the function is represented by a piecewise linear polynomial, the first derivative of the function at any point, x_i, may be obtained in a similar fashion as was done for equally spaced grid points. For example, we may use the backward difference: $f_i' = \dfrac{f(x_i) - f(x_{i-1})}{h_i}$, and the forward difference: $f_i' = \dfrac{f(x_{i+1}) - f(x_i)}{h_{i+1}}$. However, when we come to central difference, we may not be able to use the average of these two slopes or the slope of the line joining the function values at x_{i-1} and x_{i+1} because the segments may not be of equal length. The Taylor's series can again be utilized but the formulation must account for the unequal step sizes. For example, we may write

$$\begin{aligned} f(x_{i-1}) &= f(x_i) - h_i f'(x_i) + \frac{h_i^2}{2!} f''(x_i) - \frac{h_i^3}{3!} f'''(x_i) + ... \\ f(x_{i+1}) &= f(x_i) + h_{i+1} f'(x_i) + \frac{h_{i+1}^2}{2!} f''(x_i) + \frac{h_{i+1}^3}{3!} f'''(x_i) + ... \end{aligned} \quad (5.19)$$

and eliminate the term involving the second derivative to obtain

$$f_i' = -\frac{h_{i+1}}{h_i(h_i + h_{i+1})} f(x_{i-1}) + \frac{h_{i+1} - h_i}{h_{i+1} h_i} f(x_i) + \frac{h_i}{h_{i+1}(h_i + h_{i+1})} f(x_{i+1}) \quad (5.20)$$

with the leading error term being $-\dfrac{h_i h_{i+1} f'''}{6}$. (Note that for equal segments we do get the same expressions as obtained earlier.) Another alternative would be to use Lagrange interpolating polynomials and then perform analytical integration on them. Yet another option could be the use of cubic splines, which would directly give us the first/second derivatives at the nodes (see section 4.5). However, the general formulation discussed in the previous section can be readily applied to this case also and is described briefly here.

Similar to Eq. (5.11), writing[1]

$$f_i^n = \sum_{j=-n_b}^{n_f} c_{i+j} f\left(x_{i+j}\right) \quad (5.21)$$

the forward difference approximation for the first derivative using three points gives rise to

$$c_i + c_{i+1} + c_{i+2} = 0$$
$$0.c_i + h_{i+1}.c_{i+1} + \left(h_{i+1} + h_{i+2}\right).c_{i+2} = 1$$
$$0.c_i + h_{i+1}^2.c_{i+1} + \left(h_{i+1} + h_{i+2}\right)^2.c_{i+2} = 0$$

which results in

$$c_i = -\frac{2h_{i+1} + h_{i+2}}{h_{i+1}\left(h_{i+1} + h_{i+2}\right)}; c_{i+1} = \frac{h_{i+1} + h_{i+2}}{h_{i+1}h_{i+2}}; c_{i+2} = -\frac{h_{i+1}}{h_{i+2}\left(h_{i+1} + h_{i+2}\right)} \qquad (5.22)$$

and a leading error term of $\frac{h_{i+1}\left(h_{i+1} + h_{i+2}\right)}{6} f'''\left(x_f\right)$. Since the methodology is almost identical to that discussed for the evenly spaced points, we will not discuss this topic further.

Example 5.4: For the problem described in Example 5.1, assume that the measurement at t=7 s is missing. Estimate the speed at 5 s using the forward difference with the three measurements at 5, 6, and 8 s.

Solution: For i=5, using Eq. (5.22), with $h_{i+1} = 6 - 5 = 1$ and $h_{i+2} = 8 - 6 = 2$, we obtain the coefficients as $c_i = -\frac{4}{3}; c_{i+1} = \frac{3}{2}; c_{i+2} = -\frac{1}{6}$ and the speed is estimated from Eq. (5.21) as $f_5' = \sum_{j=0}^{2} c_{5+j} f\left(x_{5+j}\right) = -\frac{4}{3} f\left(5\right) + \frac{3}{2} f\left(6\right) - \frac{1}{6} f\left(8\right) = 83$ cm/s. The error is 3 cm/s, which matches with the expression of error listed after Eq. (5.22) (the third derivative is equal to 6).

5.2.3 Amplitude and Phase error

We have defined the error in the numerical differentiation in terms of its magnitude. However, as we have seen earlier for periodic functions (section 4.7), we may define the error of approximation in terms of an amplitude error and a phase error. As described in section 4.7, a periodic function may be expressed as the sum of its various harmonics. A non-periodic function may be expressed as a Fourier integral. Hence, it is instructive to look at the error in numerical differentiation of a sinusoidal function sampled at discrete points.

Let the Fourier components of a function be in the form of $f\left(x\right) = A\cos\left(jx + q\right)$ (recall that A is the amplitude and q is the phase angle). We have assumed the function to have a period of 2π and j (=0,1,2,3…) represents the harmonic (for functions with a period T, the analysis is similar with an additional frequency term $\omega=2\pi/T$). Let the function be sampled at an interval

[1] Compare with Eq. (5.16) and note that the h^n term has been removed since there is no single value of h.

of h (we assume that the period is an integer multiple of h although it is not essential to our analysis). The analytical derivatives of the j^th harmonic are obtained as

$$f'(x_i) = -Aj\sin(jx_i + f);\ f''(x_i) = -Aj^2\cos(jx_i + f);...$$

If we use the lowest order central difference scheme to evaluate the first and second derivatives, we get (Table 5.3)

$$f_i' = \frac{f(x_i + h) - f(x_i - h)}{2h} = \frac{A\cos(jx_i + jh + f) - A\cos(jx_i - jh + f)}{2h} = -A\frac{\sin jh}{h}\sin(jx_i + f)$$

and

$$f_i'' = \frac{f(x_i + h) - 2f(x_i) + f(x_i - h)}{h^2} = -A\frac{2(1 - \cos jh)}{h^2}\cos(jx_i + f)$$

A comparison with the exact values shows that there is no phase error in the approximations. The amplitude error depends on h and is conveniently expressed in terms of the *ratio* of the approximate and exact amplitudes as $\frac{\sin jh}{jh}$ for the first derivative and $\frac{2(1-\cos jh)}{j^2h^2}$ for the second derivative. It is easy to verify that this ratio becomes 1 as h tends to zero. Figs. 5.1 and 5.2 show the exact derivatives and their central difference approximations for the fundamental frequency and the second harmonic, respectively. The amplitude error is a function of jh and is plotted in Fig. 5.3.

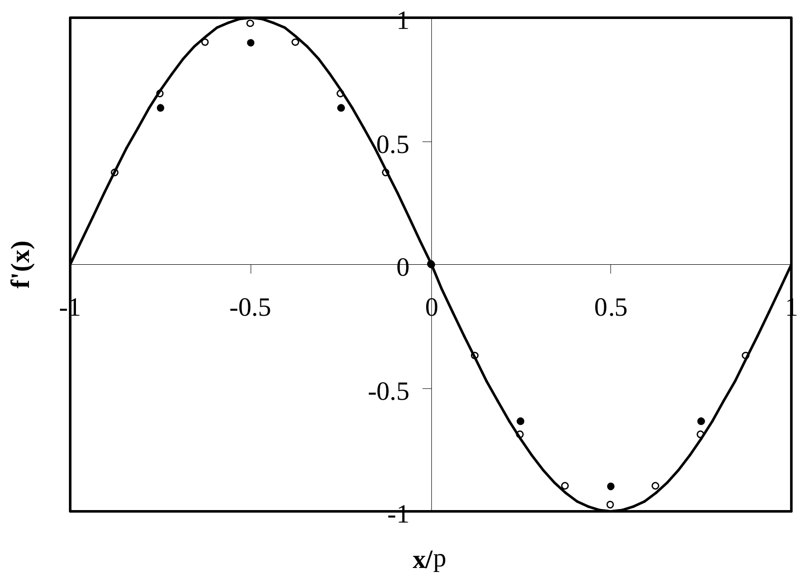

Figure 5.1(a) Analytical and numerical values of the first derivative for the fundamental frequency (j=1). o: h = π/8 •: h = π/4

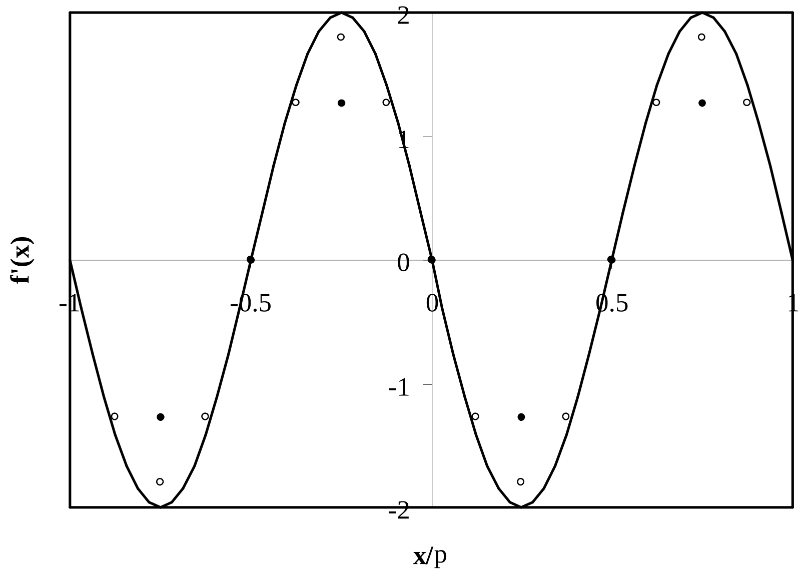

Figure 5.1(b) Analytical and numerical values of the first derivative for the second harmonic (j=2). o: h = π/8 •: h = π/4

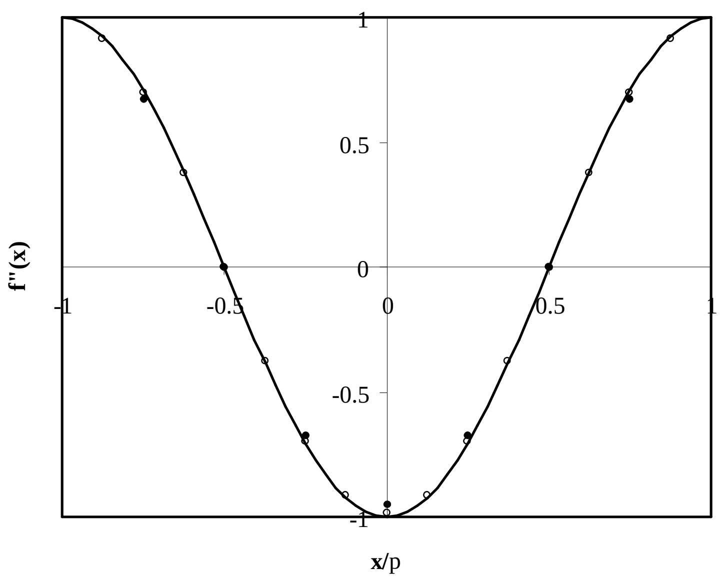

Figure 5.2(a) Analytical and numerical values of the second derivative for the fundamental frequency (j=1). o: h = π/8 •: h = π/4

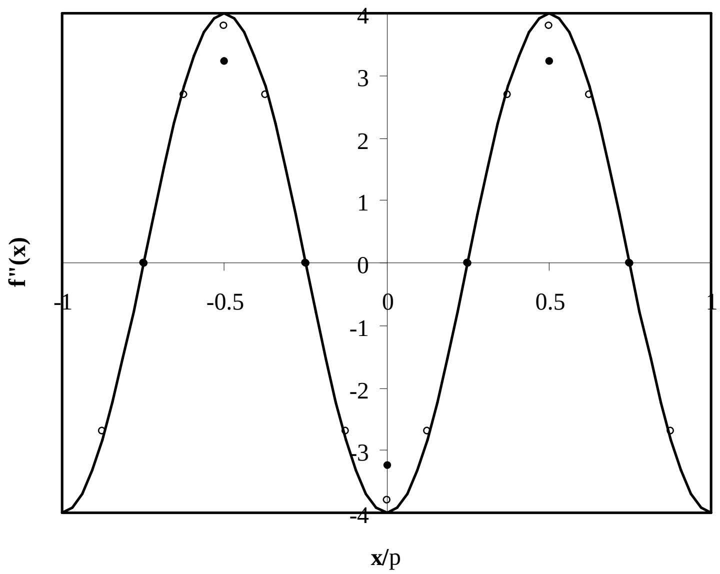

Figure 5.2(b) Analytical and numerical values of the second derivative for the second harmonic (j=2). o: $h = \pi/8$ •: $h = \pi/4$

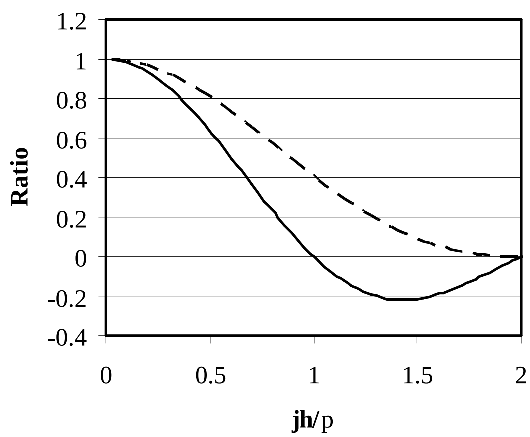

Figure 5.3 Ratio of Numerical and analytical amplitudes. Solid line – first derivative, Dashed line – second derivative

From these figures, it is apparent that the numerical solution is in phase with the exact solution. The increase in the amplitude error with increase in h is also clearly seen.

If, instead of the central difference, we use the forward difference scheme to compute the derivatives (Table 5.1), we get

$$f_i' = \frac{f(x_i+h) - f(x_i)}{h} = \frac{A\cos(jx_i + jh + f) - A\cos(jx_i + f)}{h} = -A\frac{\sin jh/2}{h/2}\sin(jx_i + jh/2 + f)$$

and

$$f_i'' = \frac{f(x_i+2h) - 2f(x_i+h) + f(x_i)}{h^2} = -A\frac{2(1-\cos jh)}{h^2}\cos(jx_i + jh + f)$$

Clearly, now we have a phase error also in addition to the amplitude error. Fig. 5.4 shows the exact and numerical derivatives for the fundamental frequency.

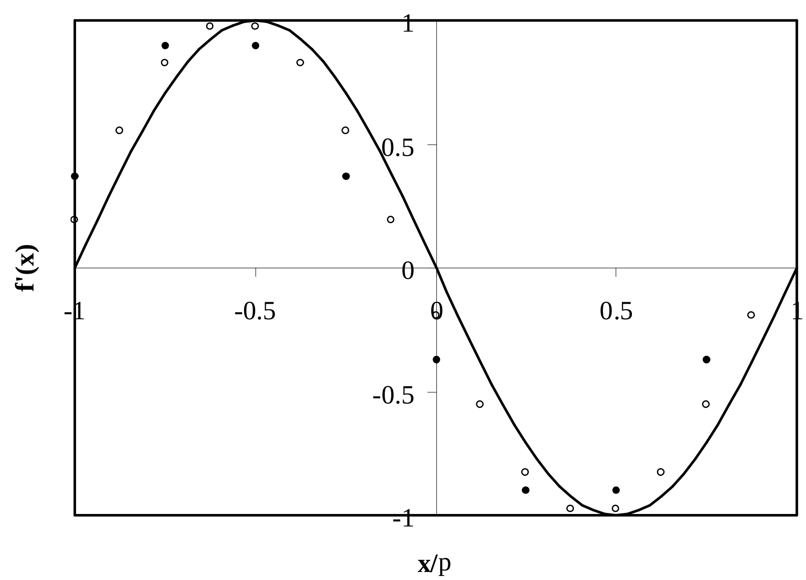

Figure 5.4(a) Analytical and numerical values of the first derivative for the fundamental frequency using forward difference. o: h = π/8 •: h = π/4

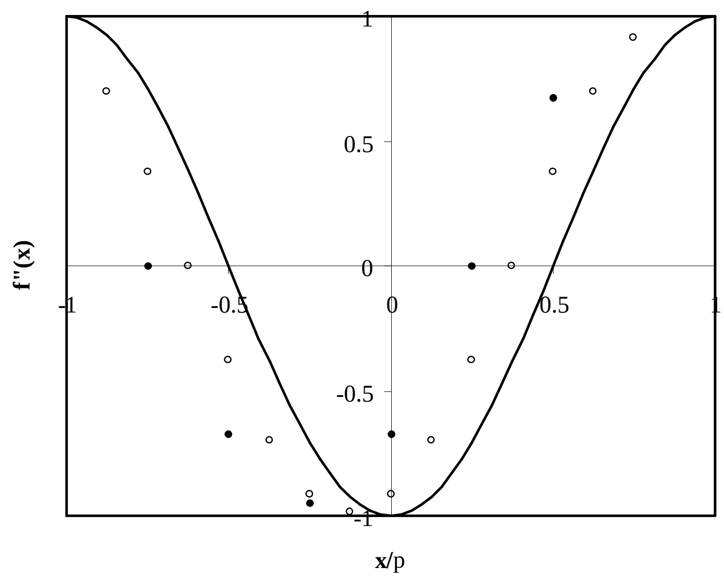

Figure 5.4(b) Analytical and numerical values of the second derivative for the fundamental frequency using forward difference. o: h = $\pi/8$ •: h = $\pi/4$

It should be mentioned that the analysis of amplitude and phase errors is considerably simplified if we use the complex notation of the Fourier series. Here, we have represented the Fourier series in terms of the sine/cosine functions in order to avoid complex algebra. In the next chapter, complex analysis would be used to look at the behaviour of error in the numerical solution of differential equations.

Exercise 5.2

1. Estimate the derivative of the function $f(x)=1+x+2x^2-16x^3+20x^4-3.5x^5$ at x=2 using central difference approximation with two different step sizes of h=0.5 and 1.0. Comment on the error vis-à-vis the step size.
2. Estimate the derivative of the functions exp(-0.1x) and exp(-10x) at x=0 using central difference approximation with a step size of 0.1. Comment on the error vis-à-vis the nature of the function.
3. The velocity of an object, travelling along a straight line, was measured at various times as follows:

Time (min)	0	1	2	3	4	5	6	7	8	9	10
Velocity (cm/min)	0.00	0.65	1.72	3.48	6.39	11.18	19.09	32.12	53.60	89.02	147.41

Estimate the acceleration at 5 minutes using the central difference formulae of order h^4 with step sizes of 1 and 2 min. Use Richardson extrapolation to obtain an $O(h^6)$ estimate from these values.

4. The $O(h^6)$ central difference formula for the first derivative is given by

$$f'(x_i) = -\frac{1}{60}f(x_{i-3}) + \frac{3}{20}f(x_{i-2}) - \frac{3}{4}f(x_{i-1}) + \frac{3}{4}f(x_{i+1}) - \frac{3}{20}f(x_{i+2}) + \frac{1}{60}f(x_{i+3})$$

with an error of $\frac{h^6}{140} f^{vii}(x)$. For the data given in the previous problem, estimate the acceleration at 5 minutes and compare with the estimate of the same order obtained using the Richardson extrapolation. Why are these different?

5. Derive a sixth order accurate finite difference approximation for the first derivative at the point x_i using the function values at the seven points $x_i, x_{i\pm1}, x_{i\pm2}, x_{i\pm4}$ and fitting a 6th degree polynomial. Using this formula, estimate the acceleration for problem 3.
6. For the Fourier component of the form $f(x) = A\cos(jx+q)$, estimate the first and second derivatives using the central difference formulae of order h^4. Obtain the amplitude and/or phase errors and compare with those of the lower order method through a plot similar to Fig. 5.3.

5.3 Numerical Integration

While analytical differentiation of a given function is rather straightforward, the same is not true for integration. A number of times [e.g., exp(-x^2), exp(-x)/x] analytical integration is either not possible or too cumbersome. Even if the function can be analytically integrated, we may require a *weighted integration* (see Tchebycheff polynomial, section 4.3) which may not be performed analytically. In some cases, the function may not be known and only its values at a set of grid points are given. In all such cases, if the integral is desired (e.g., the area enclosed by a curve, distance travelled from velocity measurements) we have to approximate it using numerical techniques (the numerical computation of an integral is also called *quadrature*). As in the case of interpolation, we will discuss both the continuous case (known function) and the discrete case (only function values known at a few points). However, we discuss the discrete case first since the continuous case involves some additional complexities. In all cases we assume that the desired integral is $I = \int_a^b f(x)dx$ but, as we did for interpolation, in some cases we would transform the variable to have the limits cover the standard domain (−1,1).

5.3.1 Discrete case

In this case, the function value is given in tabular form denoted by the set of values {(x_k,f(x_k)), k=0,1,…,n}. The x's may not be equally spaced and do not have to be distinct. We assume, though, that they are *arranged in increasing order of x*. For now, we will also assume that x_0=a and x_n=b so that there is no extrapolation needed for the interpolating polynomial. Sometimes, however, it may be unavoidable to use the so-called *open* formula in which the limit of integration goes beyond the data points given (e.g., $\int_0^1 x^{-1/2}dx$, the function is not defined at the lower limit and its value may be given from, say, x=0.01 to 1. We discuss these improper integrals latter in the chapter). As we did for differentiation, we interpolate the data with piecewise polynomials, which can then be readily integrated. If we use linear interpolation, the interpolating line and its integral are easily obtained. However, for more accurate estimate of the integral, we have to use higher order interpolation. There are a number of ways in which it could be done, as discussed in the previous chapter. For example, we may use

- an n^th degree polynomial passing through all data points (not a very good idea for large n)
- a quadratic, cubic or higher degree spline (computationally intensive)
- a locally-smooth higher order interpolating polynomial typically imposing only C^0 continuity at the common points (preferred option since it requires much smaller computation time[1]).

The desired integral, *I*, can be written as the sum of the function integral over various subintervals. For example, if we use linear interpolation we may write

$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + ... + \int_{x_{i-1}}^{x_i} f(x)dx + ... + \int_{x_{n-1}}^{x_n} f(x)dx \tag{5.23}$$

Again, defining the segment length as $h_i = x_i - x_{i-1}$ for $i = 1,2,...,n$ and using the fact that integration is invariant under a change of origin and the function is assumed to be linear in each segment, the estimated value of the integral, $\tilde{I}$, is written as

$$\tilde{I} = \sum_{i=1}^{n} \int_{0}^{h_i} f(x_{i-1}) + xf[x_{i-1}, x_i]dx = \sum_{i=1}^{n} \frac{f(x_{i-1}) + f(x_i)}{2} h_i \tag{5.24}$$

Since the rightmost quantity in Eq. (5.24) represents the area of a trapezoid formed by joining the function values at x_{i-1} and x_i by a straight line, this method is also called the **Trapezoidal Rule**. Note that we could have written the interpolating polynomial in various alternative forms, but prefer to use the Newton divided difference form since it leads to easier integration and error analysis. We may also estimate the error in each segment, E_i, by (see section 4.4)

$$E_i = I_i - \tilde{I}_i = \int_0^{h_i} x(x-h_i)\, f[x, x_{i-1}, x_i] = \int_0^{h_i} x(x-h_i) \frac{f''(x_i^*)}{2} dx \tag{5.25}$$

where $x_i^* \in (x_{i-1}, x_i)$. Since $x(x-h_i) \le 0$ in the entire interval, we can use the integral mean value theorem to write

$$E_i = \frac{f''(x_i)}{2} \int_0^{h_i} x(x-h_i)dx = -\frac{h_i^3 f''(x_i)}{12} \tag{5.26}$$

in which $x_i \in (x_{i-1}, x_i)$. This indicates that the error[1] for a single segment is $O(h^3)$. The error over the entire domain (a,b) is obtained by summation of individual segment errors. If the data is equidistant, i.e., $h_i = \frac{b-a}{n}\ \forall i$, we may write

---

[1] We did not discuss this option for interpolation or numerical differentiation since in interpolation we wanted continuity of higher derivatives and numerical differentiation tends to magnify small deviations in data. On the other hand, integration tends to dampen the effect of small oscillations.

$$E=\sum_{i=1}^{n}E_i=-\frac{(b-a)^3}{12n^2}\frac{\sum_{i=1}^{n}f''(x_i)}{n}\simeq-\frac{(b-a)^3}{12n^2}\overline{f''}=-\frac{(b-a)h^2\overline{f''}}{12} \qquad (5.27)$$

where $\overline{f''}$ represents the *mean* value of the second derivative of the function over the interval (a,b)[2]. If we assume that this mean value does not change significantly with change in h, we observe that the total error is $O(h^2)$. Thus halving the step size will reduce the error to *roughly*[3] one-fourth (however, see Exercise 5.3.1). As was the case with numerical differentiation, this error may be unacceptable and we again look at various alternatives for improving the accuracy.

Example 5.5: The speed of an object at various times was measured as follows:

Time (s)	0	1	2	3	4	5	6
Speed (cm/s)	0.0000	0.3466	0.3662	0.3466	0.3219	0.2986	0.2780

Estimate the distance travelled by the object at 6 seconds using the trapezoidal rule. First use a step size, h=1 s, and then double this size (h = 2 s).

Solution: With a step size of 1 s, using Eqs. (5.24), the distance (i.e., the integral of the speed) is obtained as

$$\tilde{I}=\sum_{i=1}^{6}\frac{f(x_{i-1})+f(x_i)}{2}h_i=h\left[\frac{f(x_0)}{2}+f(x_1)+f(x_2)+\ldots+f(x_5)+\frac{f(x_6)}{2}\right]=1.819\text{ cm}$$

With double the step size, the estimated distance is

$$\tilde{I}=\sum_{i=1}^{3}\frac{f(x_{i-1})+f(x_i)}{2}h_i=2\times\left[\frac{f(0)}{2}+f(2)+f(4)+\frac{f(6)}{2}\right]=1.654\text{ cm}$$

From Eq. (5.27), we may conclude that the error is roughly four times larger with a step size of 2 s as compared to that for the step size of 1 s. The true value of the distance is, therefore, likely to be a little larger than 1.819 cm.

5.3.1.1 Improving the accuracy

The basic philosophy, again, is to use higher order interpolation schemes but it can be done in a number of different ways:

a. Interpolation followed by integration:

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[1] Similar to the error in numerical differentiation, a dimensional analysis will show that the error in numerical integration will have terms of the form $h^r f^{r-1}(x)$.

[2] We write the equation for error in terms of the mean value of the derivative rather than summation of the derivatives in order to directly compare the error for different schemes (the number of segments may be different for different methods and comparison of the sum would not be meaningful).

[3] Since the mean value of the second derivative changes with h, the error will generally not be *exactly* one-fourth, unless the underlying function, $f(x)$, is a second-degree (*or even third degree*) polynomial.

If we decide to use piecewise[1] quadratic interpolation, we may write[2] (we again use the fact that the integral is not affected by a translation and use $x_{i-2} = -h_{i-1}; x_{i-1} = 0; x_i = h_i$)

$$\begin{aligned}\tilde{I} &= \sum_{i=2,4,6,\ldots,n} \int_{-h_{i-1}}^{h_i} f\left(x_{i-2}\right) + \left(x+h_{i-1}\right) f\left[x_{i-2}, x_{i-1}\right] + x\left(x+h_{i-1}\right) f\left[x_{i-2}, x_{i-1}, x_i\right] dx \\ &= \sum_{i=2,4,6,\ldots,n} \frac{\left(h_{i-1}+h_i\right)\left(2h_{i-1}-h_i\right)}{6h_{i-1}} f\left(x_{i-2}\right) + \frac{\left(h_{i-1}+h_i\right)^3}{6h_{i-1}h_i} f\left(x_{i-1}\right) + \frac{\left(h_{i-1}+h_i\right)\left(-h_{i-1}+2h_i\right)}{6h_i} f\left(x_i\right)\end{aligned} \tag{5.28}$$

and the error as

$$E = \sum_{i=2,4,6,\ldots,n} \int_{-h_{i-1}}^{h_i} x\left(x+h_{i-1}\right)\left(x-h_i\right) f\left[x, x_{i-2}, x_{i-1}, x_i\right] dx \tag{5.29}$$

Unfortunately, we cannot apply the integral mean value theorem directly since $x\left(x+h_{i-1}\right)\left(x-h_i\right)$ does not have a constant sign in the integration domain. For ***equidistant points***, however, following Steffensen (1950) we use integration by parts to get[3]

$$\begin{aligned}E_i &= \int_{-h}^{h} x\left(x+h\right)\left(x-h\right) f\left[x, x_{i-2}, x_{i-1}, x_i\right] dx \\ &= \left[f\left[x, x_{i-2}, x_{i-1}, x_i\right] \int_{-h}^{x} x\left(x+h\right)\left(x-h\right) dx \right]_{-h}^{h} - \int_{-h}^{h} \frac{d\ f\left[x, x_{i-2}, x_{i-1}, x_i\right]}{dx} \int_{-h}^{x} x\left(x+h\right)\left(x-h\right) dx\, dx\end{aligned} \tag{5.30}$$

Note the limits on the integral involving x(x+h)(x-h). While the upper limit of this integral must be x, we could have used any constant lower limit of integration in this term. The value –h is used for convenience as it makes the integral 0 for x=-h as well as x=h. The derivative of the finite divided difference is obtained as:

$$\begin{aligned}\frac{d}{dx} f\left[x, x_{i-2}, x_{i-1}, x_i\right] &= \lim_{e \to 0} \frac{f\left[x+e, x_{i-2}, x_{i-1}, x_i\right] - f\left[x, x_{i-2}, x_{i-1}, x_i\right]}{x+e-x} \\ &= \lim_{e \to 0} f\left[x+e, x, x_{i-2}, x_{i-1}, x_i\right] = f\left[x, x, x_{i-2}, x_{i-1}, x_i\right]\end{aligned} \tag{5.31}$$

Now using the relation between the finite divided difference and the function derivative (see Box 4.3 and note that the relationship is applicable even when some of the points coincide) we get $f\left[x, x, x_{i-2}, x_{i-1}, x_i\right] = \dfrac{f^{iv}\left(x_i^*\right)}{4!}$ in which $x_i^* \in \left(x_{i-2}, x_i\right)$. It is readily seen that

---

[1] As we saw in the previous chapter, with the increase in the number of data points, it may not be a good idea to use a higher order interpolating polynomial passing through *all* data points. The quadratic, cubic, or higher order splines may be used but would typically require more computational time without a commensurate gain in accuracy.

[2] We will assume that n is even. If n is odd, a linear interpolation may be used in the first or last segment. However, it would lead to lower accuracy in the estimate of the integral. A better option would be to use a cubic for the first three or last three segments.

[3] Note that we could divide the integral into two parts ($-h_{i-1}$,0) and (0,h_i) such that the term $x\left(x+h_{i-1}\right)\left(x-h_i\right)$ has the same sign over each of these intervals. The integral mean value theorem could be applied to these individual segments. However, it is readily seen that the presence of opposite signs over these segments would imply that the error cannot be expressed in a usable form.

$\int_{-h}^{h}(x-h)x(x+h)dx = 0$ and $\int_{-h}^{x}(x-h)x(x+h)dx$ is nonnegative for all $x \in (-h,h)$ thus enabling us to use the mean value theorem for integrals. We, therefore, have

$$
\begin{aligned}
E_i &= -\int_{-h}^{h}\frac{f^{iv}(x_i^*)}{4!}\int_{-h}^{x}x(x+h)(x-h)dx\,dx \\
&= -\frac{f^{iv}(x_i)}{4!}\int_{-h}^{h}\frac{(x^2-h^2)^2}{4}dx = -\frac{h^5 f^{iv}(x_i)}{90}
\end{aligned}
$$

in which $x_i \in (x_{i-2}, x_i)$. The estimated integral and total error are given by (Eqs. 5.28 and 5.29)

$$
\begin{aligned}
\tilde{I} &= \frac{h}{3}\sum_{i=2,4,6,\ldots,n}\left[f(x_{i-2})+4f(x_{i-1})+f(x_i)\right] \\
&= \frac{h}{3}\left[f(x_0)+4\sum_{i=1,3,5,\ldots,n-1}f(x_i)+2\sum_{i=2,4,6,\ldots,n-2}f(x_i)+f(x_n)\right]
\end{aligned}
\qquad (5.32)
$$

and

$$
E = \sum_{i=2,4,6,\ldots,n} -\frac{h^5 f^{iv}(x_i)}{90} = -\frac{(b-a)^5}{180n^4}\frac{\sum_{i=2,4,6,\ldots,n} f^{iv}(x_i)}{n/2} = -\frac{(b-a)^5\,\overline{f}^{iv}}{180n^4} \qquad (5.33)
$$

where $\overline{f}^{iv}$ represents the *mean* value of the fourth derivative of the function over the interval (a,b). If we assume that this mean value does not change significantly with change in *h*, we observe that the total error is *O(h^4)* (see Box 5.1 for general error expression). Also note that, although we derived the formula with a quadratic interpolation, the integral would be exact even if *f(x)* is a cubic polynomial[1] since the fourth derivative will be identically zero. This implies that once we perform a quadratic interpolation through 3 equidistant points, and then draw the cubic interpolating polynomial utilizing an additional (equidistant) point, the net area between these two curves would be zero, no matter what the function value is at the additional point[2]! Eq. (5.32) is commonly called **Simpson's[3] one-third** rule because of the presence of the h/3 term.

Box 5.1: **Error in integral using polynomial approximation**

Steffensen (1950) lists general expressions for the error in even- and odd-degree polynomial interpolation.

---

[1] Sometimes, we say that the ***degree of precision*** of the quadrature scheme is 3 to indicate that *all* 3rd degree polynomials would be exactly integrated but there is some 4th degree polynomial which cannot be exactly integrated.

[2] An easier to visualize simile is that of using a constant value to integrate a linear function. If we choose the constant value at the midpoint of the interval, any straight line passing through this point will result in the same area since the difference in area before and after the midpoint cancel out each other.

[3] After Simpson (1743) but proposed earlier by Cavalieri (1639), Gregory (1668), Newton (1676).

For an even (say, 2m) degree polynomial interpolation using 2m+1 equidistant points located at $0, \pm h, \pm 2h, ..., \pm mh$, the error in estimation of $\int_{-mh}^{mh} f(x)\,dx$ is given by

$$\frac{2h^{2m+3} f^{2m+2}(x)}{(2m+2)!} \int_0^m x^2 \left(x^2-1\right)\left(x^2-4\right)...\left(x^2-m^2\right) dx$$

in which $x \in (-mh, mh)$

For an odd (say, 2m+1) degree polynomial using 2m+2 equidistant points located at $\pm\frac{h}{2}, \pm\frac{3h}{2}, ..., \pm\frac{(2m+1)h}{2}$, the error is expressed as

$$\frac{2h^{2m+3} f^{2m+2}(x)}{(2m+2)!} \int_0^{m+\frac{1}{2}} \left(x^2-\frac{1}{4}\right)\left(x^2-\frac{9}{4}\right)...\left(x^2-\left(m+\frac{1}{2}\right)^2\right) dx$$

in which $x \in \left(-\left(m+\frac{1}{2}\right)h, \left(m+\frac{1}{2}\right)h\right)$.

For example, the error in the use of the odd degree polynomial with m=0 (linear interpolation, trapezoidal rule) is obtained as $\frac{2h^3 f''(x)}{2} \int_0^{1/2} \left(x^2-\frac{1}{4}\right) dx = -\frac{h^3 f''(x)}{12}$ and that in even degree polynomial with m=1 (quadratic interpolation, Simpson's rule) is obtained as $\frac{2h^5 f^{iv}(x)}{24} \int_0^1 x^2\left(x^2-1\right) dx = -\frac{h^5 f^{iv}(x)}{90}$.

b. Using the finite difference formula:

Combining the trapezoidal rule estimate over two consecutive segments and using the finite difference approximation of the second derivative[1], we may write an improved estimate of the integral over the interval (x_{i-2}, x_i) as

$$\int_{x_{i-2}}^{x_i} f(x)\,dx \simeq \tilde{I}_i = h\frac{f(x_{i-2})+f(x_{i-1})}{2} + h\frac{f(x_{i-1})+f(x_i)}{2} - 2\frac{h^3}{12}\frac{f(x_{i-2})-2f(x_{i-1})+f(x_i)}{h^2} \quad (5.34)$$

[1] For simplicity, we assume that the points are equidistant. For unequal spacing, the finite difference approximation of the second derivative becomes somewhat complicated.

in which the first two terms on the r.h.s. are the trapezoidal rule estimates and the third term is the sum of errors in *both* segments. It is seen that this again results in the Simpson's 1/3 rule.

c. Method of undetermined coefficients:

Assuming an expression of the form

$$\tilde{I}_i = c_{i-2} f(x_{i-2}) + c_{i-1} f(x_{i-1}) + c_i f(x_i) \tag{5.35}$$

in which the c's are undetermined coefficients, we require that the integral be exact for all polynomials of 2nd degree. Taking the function as f(x)=1, x, and x^2, respectively, we obtain three linear equations which can be solved to obtain the coefficients:

$$\begin{aligned} &c_{i-2} + c_{i-1} + c_i = h_{i-1} + h_i \\ &-h_{i-1}.c_{i-2} + 0.c_{i-1} + h_i.c_i = \frac{-h_{i-1}^2 + h_i^2}{2} \\ &h_{i-1}^2.c_{i-2} + 0.c_{i-1} + h_i^2.c_i = \frac{h_{i-1}^3 + h_i^3}{3} \end{aligned} \tag{5.36}$$

which results in the same equation as (5.32) for equidistant points[1].

d. Richardson's extrapolation:

From Eq. (5.27), the error in estimate of integral using the trapezoidal rule is equal to $-\frac{(b-a)\bar{f}''h^2}{12}$. If we use a step size of *2h*, and assume that the mean value of second derivative is more or less same, the error term should be four times that for the step size of *h*. As before, a new and probably more accurate, value is obtained as

$$\tilde{I}_i \simeq \frac{4\left[\frac{h}{2}\left\{f(x_{i-2}) + 2f(x_{i-1}) + f(x_i)\right\}\right] - \frac{2h}{2}\left[f(x_{i-2}) + f(x_i)\right]}{3} \tag{5.37}$$

in which the first term on the r.h.s. represents the trapezoidal rule estimate for the l.h.s. using step size *h*, and the second term represents the same with step size of *2h*. It is easy to see that we again get the Simpson's rule and the error, as shown earlier, is $O(h^4)$. One may then combine two estimates of $O(h^4)$ (e.g., one using step sizes of *h* and *2h*, and the other using *2h* and *4h*) to obtain an $O(h^6)$ estimate and so on. Romberg proposed a general recursive form for this extrapolation well-suited for computer implementation which may be written as

$$\tilde{I}_{h,k+2} \simeq \frac{2^k \tilde{I}_{h,k} - \tilde{I}_{2h,k}}{2^k - 1} \tag{5.38}$$

in which $\tilde{I}_{h,k}$ represents the estimate of *I* of accuracy $O(h^k)$ with step size of *h*. Thus, starting from trapezoidal rule estimates, $O(h^2)$, for step sizes h, 2h, 4h, and 8h, successive estimates could be obtained from

---

[1] If the points are equidistant, it may be better to write Eq. (5.35) as

$$\tilde{I}_i = h\left[c_{i-2} f(x_{i-2}) + c_{i-1} f(x_{i-1}) + c_i f(x_i)\right]$$

$$\tilde{I}_{h,4} = \frac{4\tilde{I}_{h,2} - \tilde{I}_{2h,2}}{3}; \quad \tilde{I}_{2h,4} = \frac{4\tilde{I}_{2h,2} - \tilde{I}_{4h,2}}{3}; \quad \tilde{I}_{4h,4} = \frac{4\tilde{I}_{4h,2} - \tilde{I}_{8h,2}}{3}$$

$$\tilde{I}_{h,6} = \frac{16\tilde{I}_{h,4} - \tilde{I}_{2h,4}}{15}; \quad \tilde{I}_{2h,6} = \frac{16\tilde{I}_{2h,4} - \tilde{I}_{4h,4}}{15}$$

$$\tilde{I}_{h,8} = \frac{64\tilde{I}_{h,6} - \tilde{I}_{2h,6}}{63}$$

with the final result of $O(h^8)$ accuracy! This algorithm, known as the **Romberg Integration**, is thus a very powerful technique for performing numerical integration with very high accuracy using only a few lower accuracy estimates[1]. However, for unevenly spaced data it is not directly applicable.

Example 5.6: For the problem described in Example 5.5, estimate the distance travelled by the object at 6 seconds using the Simpson's 1/3 rule.

Solution: Using Eq. (5.32), the distance is obtained as

$$\tilde{I} = \frac{h}{3}\left[f(t_0) + 4\sum_{i=1,3,5} f(t_i) + 2\sum_{i=2,4} f(t_i) + f(t_6) \right] = 1.874 \text{ cm}$$

Going back to Example 5.5, our assertion, that the true value of the distance should be a little larger than 1.819 cm, seems to be valid. Also note that the Richardson extrapolation of values obtained in Example 5.5 provide us the estimate (4x1.819-1.654)/3 cm, i.e., 1.874 cm, the same as the Simpson's rule.

Other techniques for obtaining a more accurate formula use higher order interpolation and then perform the necessary integration. Two different philosophies could be applied at this time:

(i) as we did in *a* above, we use more points to perform the higher order interpolation and then integrate this polynomial over the domain covered by *all* these points

(ii) we use more points to obtain the higher order interpolating polynomial and then integrate it over *a single segment*.

The first procedure is commonly known as the **Newton-Cotes** method (examples being the trapezoidal rule and the Simpson's rule) while the second is similar to **Adams** method. We describe below these techniques using the third order interpolating polynomial.

5.3.1.2 *Newton-Cotes Method*

We write[2] (we again use the fact that the integral is not affected by a translation and consider, for simplicity, the points to be equally spaced with $x_{i-3} = -h; x_{i-2} = 0; x_{i-1} = h; x_i = 2h$)

[1] Therefore, one really does not need to remember the higher accuracy formulae, only the trapezoidal rule will do!

[2] Assuming that *n* is a multiple of 3. If not, the first (or last) 2 or 4 segments could be evaluated using the quadratic interpolation.

$$\tilde{I} = \sum_{i=3,6,9,\ldots,n} \int_{-h}^{2h} f\left(x_{i-3}\right) + \left(x+h\right) f\left[x_{i-3}, x_{i-2}\right] + x\left(x+h\right) f\left[x_{i-3}, x_{i-2}, x_{i-1}\right] + x\left(x^2 - h^2\right) f\left[x_{i-3}, x_{i-2}, x_{i-1}, x_i\right] dx$$

$$= \frac{3h}{8} \sum_{i=3,6,9,\ldots,n} \left[f\left(x_{i-3}\right) + 3f\left(x_{i-2}\right) + 3f\left(x_{i-1}\right) + f\left(x_i\right) \right] \quad (5.39)$$

which is known as the Simpson's[1] three-eighths rule with the error given by (see Box 5.1)

$$\begin{aligned} E &= \sum_{i=3,6,9,\ldots,n} \int_{-h}^{2h} x\left(x^2 - h^2\right)\left(x - 2h\right) \frac{f^{iv}\left(x_i^*\right)}{4!} dx = -\frac{3}{80} h^5 \sum_{i=3,6,9,\ldots,n} f^{iv}\left(x_i\right) \\ &= -\frac{\left(b-a\right)^5 \overline{f}^{iv}}{80n^4} \end{aligned} \quad (5.40)$$

A comparison with Eq. (5.33) shows that Simpson's 1/3 and 3/8 rules have the same order of accuracy (h^4) but the 1/3 rule is more accurate even though it is based on a lower degree polynomial[2]! Thus a better interpolating polynomial may not necessarily lead to a more accurate integral. The 3/8 rule may be useful, however, if the number of segments is odd. In that case, the 3/8 rule may be applied to the first (or last) three segments and the 1/3 rule may be applied to the remaining (even in number) segments. Fig. 5.5 shows a graphical representation of the estimates of the integral obtained using the trapezoidal rule, Simpson's 1/3 rule and Simpson's 3/8 rule.

Fig. 5.5 Newton-Cotes methods

5.3.1.3 *Adams Method*

In the Newton-Cotes method, we use an interpolating polynomial over multiple segments and then integrate it over all those segments. As we know from our discussions on interpolation, the error of interpolation is likely to be small in the centre of the interval and large near the ends. We would, therefore, expect that in the three-segment case discussed in the previous paragraph, the interpolant would be much better over the middle segment and not-so-good over the corner segments. It would thus appear that a better accuracy may be obtained if we perform the integration only over the middle segment[3]. In case of evolving data (e.g., real-

[1] Proposed much earlier by Newton (1676).
[2] If we use different h, e.g., by dividing (b-a) into two segments for the 1/3 rule and three segments for the 3/8 rule, the 3/8 rule will be found to be more accurate. However, we feel that a true comparison should be based on the same set of grid points. If we have, say, 6 segments and we use 3 applications of 1/3 rule OR 2 applications of 3/8 rule, the 1/3 rule will have smaller error (assuming, of course, that the fourth derivative does not change much).
[3] As we will see, it does not lead to a more accurate integral. The reason, as before, is that a better interpolant does not necessarily mean a more accurate integral.

time analysis of velocity data to obtain distance travelled), as new measurements become available, we would like to have updated estimates of the integral. However, if want to apply the three-segment Newton-Cotes method, we have to wait for further measurements to get all three segments before we could apply the 3/8 rule. It may be desirable to develop a technique in which as we add more points, the incremental integral could be easily obtained. It becomes even more desirable if the function value at any point depends on the value of integral at the previous times (we will discuss this in the chapter on differential equations). The Adams method addresses these issues as described next.

In Adams method, we write the integral as the sum of integrals over each segment, expressed as (we take $x_{i-2} = -h; x_{i-1} = 0; x_i = h; x_{i+1} = 2h$)

$$\tilde{I} = \sum_{i=1,2,\ldots,n} \tilde{I}_i = \sum_{i=1,2,3,\ldots,n} \int_0^h f\left(x_{i-2}\right) + \left(x+h\right) f\left[x_{i-2}, x_{i-1}\right] + x\left(x+h\right) f\left[x_{i-2}, x_{i-1}, x_i\right] + x\left(x^2 - h^2\right) f\left[x_{i-2}, x_{i-1}, x_i, x_{i+1}\right] dx \tag{5.41}$$

and the error over a segment is given by $E_i = \int_0^h \left(x+h\right) x \left(x-h\right)\left(x-2h\right) f\left[x, x_{i-2}, x_{i-1}, x_i, x_{i+1}\right] dx$.

Thus, while the grid points x_{i-2}, x_{i-1}, x_i, and x_{i+1} are used to generate the 3rd degree interpolating polynomial, the integration is performed only over one segment[1]. The resulting expression for the integral and the error over a segment are [note that the integral mean value theorem is used to evaluate the error since $\left(x+h\right) x \left(x-h\right)\left(x-2h\right)$ is nonnegative throughout the interval (0,h) and, as before, Box 4.3 has been used to relate the derivative and the divided difference]

$$\begin{aligned} \tilde{I}_i &= \frac{h}{24}\left[-f\left(x_{i-2}\right) + 13 f\left(x_{i-1}\right) + 13 f\left(x_i\right) - f\left(x_{i+1}\right)\right] \\ E_i &= \frac{11 h^5 f^{iv}\left(x_i\right)}{720} \end{aligned} \tag{5.42}$$

Disregarding the fact that Eq. (5.42) is not applicable for i=1 and n, we may estimate the error in the value of the integral as

$$E = \frac{11 h^5}{720} \sum_{i=1}^{n} f^{iv}\left(x_i\right) \simeq \frac{11\left(b-a\right)^5 \bar{f}^{iv}}{720 n^4} \tag{5.43}$$

A comparison with Eq. (5.40) shows that the error is larger (and of opposite sign) than that in the Simpson's 3/8 rule. Adams methods are, therefore, generally not used for numerical integration. They are quite useful, though, for numerical solution of differential equations as discussed in Chapter 6. Fig. 5.6 graphically represents the difference between the Newton-Cotes and Adams methods.

[1] We may perform the integral over the first, middle, or the last segment. Here we use the middle segment assuming that the interpolation would be more accurate over the central portion of the data points used. For an evolving data, we would typically perform the integral over the last segment. Also, note that for the first and the last segments of the entire data set the "central integral" formula will not be directly applicable since there is no data corresponding to x_{-1} and x_{n+1}.

Fig. 5.6 Difference between Newton-Cotes and Adams methods

Table 5.4 lists some of the Newton-Cotes formulae and their error.

Table 5.4 Newton-Cotes formulae

No. of segments	Common Name	**Formula***	**Error**
1	Trapezoidal rule	$\frac{h}{2}\left[f(x_0)+f(x_1)\right]$	$-\frac{h^3 f''}{12}$
		$\frac{(b-a)}{2n}\left[f(x_0)+2\sum_{i=1}^{n-1} f(x_i)+f(x_n)\right]$	$-\frac{(b-a)^3 \bar{f}''}{12n^2}$
2	Simpson's 1/3 rule	$\frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right]$	$-\frac{h^5 f^{iv}}{90}$
		$\frac{(b-a)}{3n}\left[f(x_0)+4\sum_{i=1,3,..}^{n-1} f(x_i)+2\sum_{i=2,4,..}^{n-2} f(x_i)+f(x_n)\right]$	$-\frac{(b-a)^5 \bar{f}^{iv}}{180n^4}$
3	Simpson's 3/8 rule	$\frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right]$	$-\frac{3h^5 f^{iv}}{80}$
		$\frac{3(b-a)}{8n}\left[f(x_0)+3\sum_{i=1,2,4,5,7,8,..}^{n-1} f(x_i)+2\sum_{i=3,6,9,..}^{n-3} f(x_i)+f(x_n)\right]$	$-\frac{(b-a)^5 \bar{f}^{iv}}{80n^4}$
4	Boole's rule (sometimes mistyped as Bode's rule)	$\frac{2h}{45}\left[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\right]$	$-\frac{8h^7 f^{vi}}{945}$
		Too long to list ?	$-\frac{2(b-a)^7 \bar{f}^{vi}}{945n^6}$

* First line shows the formula and error for the first interval and the second line shows the same for the entire interval (b-a). It has been assumed that *n* is exactly divisible by the number of segments for each formula.

Example 5.7: The speed of an object at various times was measured as follows:

Time (s)	0	1	2	3	4
Speed (cm/s)	0.0000	0.3466	0.3662	0.3466	0.3219

Estimate the distance travelled by the object at 4 seconds using the Boole's rule. Also estimate the distance by using (i) two applications of the Simpson's 1/3 rule, (ii) trapezoidal rule over the first segment and the 3/8 rule over next three, and (iii) 3/8 rule over the first three segments and trapezoidal rule over the last segment.

Solution: Using the Boole's rule, the distance is obtained as

$$d_4 = \frac{2}{45}\left[7\times 0 + 32\times 0.3466 + 12\times 0.3662 + 32\times 0.3466 + 7\times 0.3219\right] \text{ cm} = 1.281 \text{ cm}$$

Using two applications of the Simpson's 1/3 rule, we get

$$d_4 = \frac{(4-0)}{3\times 4}\left[0 + 4(0.3466 + 0.3466) + 2(0.3662) + 0.3219\right] \text{cm} = 1.276 \text{ cm}$$

Using trapezoidal rule over the first segment and 3/8 over the remaining three, we get

$$d_4 = \frac{1}{2}(0 + 0.3466) + \frac{3}{8}\left[0.3466 + 3\times 0.3662 + 3\times 0.3466 + 0.3219\right] \text{ cm} = 1.226 \text{ cm}$$

Using 3/8 rule over the first three segments and trapezoidal rule over the last, we get

$$d_4 = \frac{3}{8}\left[0 + 3\times 0.3466 + 3\times 0.3662 + 0.3466\right] + \frac{1}{2}(0.3466 + 0.3219) \text{ cm} = 1.266 \text{ cm}$$

We expect the Boole's rule to be the most accurate and the 1/3 rule to be a little less accurate. The other two methods would have a still lower accuracy because of the use of the trapezoidal rule for one segment. The results show that, *for this problem*, the application of the trapezoidal method over the last segment is "probably" more accurate than its application over the first segment.

From this discussion it is obvious that, for a given set of function values, one could obtain its integral over the range ($a=x_0$, $b=x_n$) to a desired accuracy using the Newton-Cotes **closed** (because the range of given data encloses the limits of integration) formulae[1]. Occasionally, however, we may be required to evaluate the integral over limits extending beyond the range of data. For example, having measured the velocity of an object at time 0, 1, 2, and 3 minutes, we want to predict where it would be at t=4 min. Clearly, it involves some extrapolation and therefore should be avoided as far as possible. However, for evaluating improper integrals (discussed latter in this chapter) and for obtaining a first estimate (discussed in Chapter 6 on ordinary differential equations), formulae based on extrapolation are quite useful. In such cases, **open** (both the upper and lower limits extend beyond the given data) or **semi-open** (either the lower or the upper limit extends beyond the data) formulae have to be used. These are based on obtaining the interpolating polynomial, extrapolating it to the limits of integration and then performing the integration.

5.3.1.4 Open and semi-open Formulae

[1] It should be emphasized that we have *ignored round-off errors*. If these are included, a higher order method for integration (or differentiation) may show larger *total error* than that of a smaller order method. In practice, therefore, methods of very high order are not used.

Suppose we want to evaluate $I = \int_a^b f(x)dx$ with the function values given in tabular form $\{(x_k, f(x_k)),\ k=0,1,\ldots,n\}$[1] in such a way that $a<x_0$ and/or $b>x_n$. We may use the closed formulae discussed in the previous section to evaluate the integral over the range (x_0,x_n). However, since the function value is not known at a and/or b, we will have to extrapolate the function beyond the given data in order to perform the integral at either ends. For simplifying the presentation **we assume that** $\boldsymbol{a=x_0}$ **and** $\boldsymbol{b=x_n+h}$ where $h\left(=\frac{x_n-x_0}{n}\right)$ is the spacing of the data points (in other words, we discuss the *semi-open* formulae). The extension to the case when the lower limit also extends beyond the data points or when the distance between the limits and the endmost data points is not equal to h, is straightforward, though tedious.

After using a few data points near the end for extrapolation, we could use the Newton-Cotes philosophy and perform the integration over the interval spanning all these points and the upper limit, b. Or, we could use the Adams method to perform the integration only over the interval (x_n,b). If we use the same (k^{th}) degree polynomial to perform the "closed" integration[2] over (x_0,x_{n-k-1}) and the "semi-open" integration over (x_{n-k},b), there would be no difference in the results from the Newton-Cotes and Adams method. It is sometimes argued that the integrals over the end segments could be performed using a technique which is *one order lower* than that used for other segments since the summation of errors in the non-corner segments effectively lowers its order by one[3]. However, we use the same degree of polynomial interpolation for the end-segments as for the rest of the domain and describe the Adams method below.

Using linear interpolation, the trapezoidal rule could be used to obtain the integral over the range (x_0,x_n). Using the function values at x_{n-1} and x_n, we extrapolate to b and obtain

$$\int_{x_n}^{b} f(x)dx \simeq \frac{h}{2}\left[3f(x_n) - f(x_{n-1})\right] \tag{5.44}$$

and

$$\tilde{I} = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-2} f(x_i) + f(x_{n-1}) + 4f(x_n)\right] \tag{5.45}$$

If the lower limit of the integral is $a=x_0-h$ (i.e., the corresponding open formula), the coefficient of $f(x_0)$ in Eq. (5.45) would also be equal to 4 and that of $f(x_1)$ will be equal to 1[4]. The error of integration in the extrapolated segment is given by

---

[1] We assume that the x's are equally spaced and arranged in increasing order of x.
[2] Using the appropriate Newton-Cotes formula described in the previous section.
[3] For example, a single application of trapezoidal rule has accuracy $O(h^3)$ but the overall error over a given interval is $O(h^2)$.
[4] However, if n=1, it may be readily verified that both $f(x_0)$ and $f(x_1)$ would have a coefficient equal to 3. The error over the entire interval is equal to $\frac{3}{4}h^3 f''(x)$ where $a<x<b$. We believe that the semi-open formulae are more useful than the open formulae because of their use in the solution of differential equations. Hence we do not list the open formulae. The interested reader may refer to Davis and Rabinowitz for further details.

$$E=\int_h^{2h} x\left(x-h\right)\frac{f''\left(x^*\right)}{2!}dx=\frac{5h^3 f''\left(x\right)}{12} \tag{5.46}$$

with $x\in\left(x_{n-1},b\right)$. Interpolation with different order polynomials leads to similar formulae, some of which are listed in Table 5.5.

Table 5.5 Semi-open integration formulae[1]

Extrapolating Polynomial	**Formula***	**Error+**
Constant	$hf\left(x_n\right)$	$\frac{h^2 f'}{2}$
	$h\left[\sum_{i=0}^{n} f(x_i)\right]$	
Linear	$\frac{h}{2}\left[-f(x_{n-1})+3f(x_n)\right]$	$\frac{5h^3 f''}{12}$
	$\frac{h}{2}\left[f(x_0)+2\sum_{i=1}^{n-2} f(x_i)+f(x_{n-1})+4f(x_n)\right]$	
Quadratic	$\frac{h}{12}\left[5f(x_{n-2})-16f(x_{n-1})+23f(x_n)\right]$	$\frac{9h^4 f'''}{24}$
	$\frac{h}{3}\left[f(x_0)+4\sum_{i=1,3,..}^{n-3} f(x_i)+2\sum_{i=2,4,..}^{n-4} f(x_i)+\frac{13}{4}f(x_{n-2})+0.f(x_{n-1})+\frac{27}{4}f(x_n)\right]$	

* The first line gives the integral from x_n to b and the second line from x_0 to b.
\+ The derivatives are evaluated at some point in the appropriate interval, which is (x_{n-k},b) for k^{th} degree polynomial interpolation. The error is over the extrapolated segment only. The error over the entire interval is not listed as, for sufficiently large n, it would be similar to the corresponding closed formulae.

Most of the formulae we have discussed in this section have been derived for evenly spaced points. Extension to data with irregular spacing is conceptually similar but rather tedious. Fortunately, most practical problems would involve measurements at regular intervals and the Romberg's algorithm would probably be the best. Sometimes though we would not be able to avoid irregular intervals (e.g., if the function is rapidly varying in some portion, we may have to take very frequent measurements there to capture its behaviour). We hope that the material covered here would enable the reader to extend these methods to such cases and move on to the other important application of numerical integration: that for a given function.

Example 5.8: The speed of an object at various times was measured as follows:

Time (s)	0	1	2	3	4

[1] Recall that all the data points are equidistant and the "open" interval is beyond x_n at the same distance. Moreover, for quadratic (and higher) extrapolating polynomial, we assume that *n* is a multiple of the degree of the extrapolating polynomial so that the number of segments enables us to apply the closed formula from x_0 to x_n.

Speed (cm/s)	0.0000	0.3466	0.3662	0.3466	0.3219

Estimate the distance travelled by the object at 5 seconds using the constant, linear, and quadratic extrapolating polynomials.

Solution: Note that the distance is to be estimated at a time which is beyond the range of data. Hence, open formulae need to be used. From Table 5.5, the distance is estimated for various extrapolations as:

Constant: $h\left[\sum_{i=0}^{4} f\left(t_i\right)\right]=1\times\left(0.0000+0.3466+0.3662+0.3466+0.3219\right)$ cm = 1.381 cm.

Linear: $\frac{h}{2}\left[f\left(t_0\right)+2\sum_{i=1}^{2} f\left(t_i\right)+f\left(t_3\right)+4f\left(t_4\right)\right]$ cm = 1.530 cm.

Quadratic: $\frac{h}{3}\left[f\left(t_0\right)+4f\left(t_1\right)+\frac{13}{4}f\left(t_2\right)+0.f\left(t_3\right)+\frac{27}{4}f\left(t_4\right)\right]$ cm = 1.583 cm

We, therefore, expect the true value of the distance to be a little larger than 1.583 cm.

5.3.2 Continuous case

If we are asked to integrate a known function, f(x), over a finite interval (a,b), and the function is such that it is not possible (or very difficult) to integrate it analytically, we could use any of the methods discussed for the discrete case to approximate the integral since the function values could be generated at will at any point in the domain[1]. Romberg integration would work very well since the points could be chosen to be evenly spaced [One may also think of fitting a polynomial to the given function by, say, using the Legendre polynomials and then integrating this polynomial. However, this would require the integration of the given function (see section 4.3) which is not available!]. Since the function evaluation is generally time consuming, we would like to achieve maximum accuracy with minimum number of function evaluations[2]. We discuss in this section the techniques known as ***Gauss Quadrature***, which introduce additional degrees of freedom in the formulation by not fixing the location of the grid points *a priori*. As before, there are a number of ways in which the technique could be described and some of these are listed below:

a. The method of undetermined coefficients (*and ordinates*):

As before, we assume an expression of the form

$$\tilde{I}=\sum_{i=0}^{n} c_i^* f\left(x_i\right) \tag{5.47}$$

[1] We assume that the function could be readily computed at all points in the domain. Improper integrals for which either the integration limits extend to infinity or the function becomes infinite (even indeterminate values of the form 0/0 cannot be evaluated *by the computer*) at one of the limits, are discussed in the next section.

[2] This is an additional complexity compared to the discrete case, where the function values are given at some points and the matter of function evaluation did not arise.

in which the c*'s are undetermined coefficients, and x's are (yet to be determined) ordinates at which we would evaluate the function values[1]. Since there are 2n+2 degrees of freedom, we could specify that the integral be exact for all polynomials of degree 2n+1. Taking the function as $f(x) = 1, x, x^2, ..., x^{2n+1}$, respectively, we obtain 2n+2 nonlinear equations which can be solved to obtain the coefficients and the ordinates. For example, using two points (n=1), the 4 equations are

$$\begin{aligned} c_0^* + c_1^* &= b - a \\ c_0^* x_0 + c_1^* x_1 &= \frac{b^2 - a^2}{2} \\ c_0^* x_0^2 + c_1^* x_1^2 &= \frac{b^3 - a^3}{3} \\ c_0^* x_0^3 + c_1^* x_1^3 &= \frac{b^4 - a^4}{4} \end{aligned} \tag{5.48}$$

At this stage, it is convenient to transform the variable x in such a way that the range of integration becomes (-1,1) instead of (a,b) (see section 4.3). In the rest of this section, we would use the transformed variable, z, only. We then have[2]

$$\begin{aligned} &\int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f(z)dz \simeq \frac{b-a}{2}\tilde{I}_z \\ &\text{where, } \tilde{I}_z = \sum_{i=0}^{n} c_i f(z_i) \simeq \int_{-1}^{1} f(z)dz \end{aligned} \tag{5.49}$$

and the corresponding equations as (obtained by using $f(z) = 1, z, z^2, ..., z^{2n+1}$, respectively)

$$\begin{aligned} c_0 + c_1 &= 2 \\ c_0 z_0 + c_1 z_1 &= 0 \\ c_0 z_0^2 + c_1 z_1^2 &= \frac{2}{3} \\ c_0 z_0^3 + c_1 z_1^3 &= 0 \end{aligned} \tag{5.50}$$

from which, $c_0 = c_1 = 1; z_0 = -\frac{1}{\sqrt{3}}, z_1 = \frac{1}{\sqrt{3}}$. A rough estimate of the error in $\tilde{I}_z$ may be obtained by assuming it to be proportional to $f^{2n+2}(x)$ in which $x \in (-1,1)$. For example, taking $f(z) = z^4$ (therefore $f^{iv}(x) = 24$),

$$E_z = I_z - \tilde{I}_z = \left[\frac{z^5}{5}\right]_{-1}^{1} - \sum_{i=0}^{1} c_i z_i^4 = \frac{2}{5} - \frac{2}{9} = \frac{8}{45} = \frac{f^{iv}(x)}{135} \tag{5.51}$$

---

[1] At this stage we could have changed the notation to use the range of i from 1 to m, with m indicating the number of points at which the function is evaluated. However, in keeping with the discussion till now, we prefer to follow the range 0 to n. The reader should keep in mind that the number of points are (n+1).

[2] Recall that $x = \frac{b+a}{2} + \frac{b-a}{2}z$. Also, we assume that the z's are arranged in the increasing order such that z_0 is the smallest and z_n largest.

The error in $\tilde{I}$ will, of course, be $\frac{b-a}{2}$ times this error.

Equations (5.50) are nonlinear (since both c and z are unknown) and consequently a little difficult to solve for large *n*. Therefore, we describe another alternative, which leads to simpler determination of the weights and ordinates.

Since the polynomials used for obtaining the equations are arbitrary, we may use

$$\begin{aligned} f(z) &= 1, (z-z_0), (z-z_0)(z-z_1), \ldots, (z-z_0)(z-z_1)\ldots(z-z_n), \\ & z(z-z_0)(z-z_1)\ldots(z-z_n), \ldots, z^n(z-z_0)(z-z_1)\ldots(z-z_n) \end{aligned} \tag{5.52}$$

as the 2n+2 polynomials and obtain the following equations:

$$\begin{aligned}
&\sum_{i=0}^{n} c_i = \int_{-1}^{1} 1 dz = 2 \\
&\sum_{i=1}^{n} c_i (z_i - z_0) = \int_{-1}^{1} (z - z_0) dz = -2z_0 \\
&\sum_{i=2}^{n} c_i (z_i - z_0)(z_i - z_1) = \int_{-1}^{1} (z - z_0)(z - z_1)\, dz = \frac{2}{3} + 2z_0 z_1 \\
&. \\
&. \\
&c_n (z_n - z_0)(z_n - z_1)\ldots(z_n - z_{n-1}) = \int_{-1}^{1} \prod_{i=0}^{n-1} (z - z_i) dz \\
&0 = \int_{-1}^{1} \prod_{i=0}^{n} (z - z_i) dz \\
&0 = \int_{-1}^{1} z \prod_{i=0}^{n} (z - z_i) dz \\
&. \\
&. \\
&0 = \int_{-1}^{1} z^n \prod_{i=0}^{n} (z - z_i) dz
\end{aligned} \tag{5.53}$$

It should be noted that:

- The last *n+1* equations do not involve the coefficients *c* and could be solved for the ordinates, *z*. The first equation involves all c*'s*, the second does not have c_0 (since the function has a factor z-z_0), the third does not have c_0 and c_1,…, and the (n+1)th equation involves only c_n (and the ordinates). Therefore, once the ordinates are obtained, the coefficients can be sequentially obtained starting from the (n+1)th equation.

- The last n+1 equations are still nonlinear in the ordinates. However, if we define $\prod_{i=0}^{n}(z-z_i)=\sum_{i=0}^{n+1}\alpha_i z^i$, we obtain a set of n+1 *linear* equations in α as[1]

$$\int_{-1}^{1}\prod_{i=0}^{n}(z-z_i)dz=\sum_{i=0}^{n+1}\frac{1-(-1)^{i+1}}{i+1}\alpha_i=0$$
$$\sum_{i=0}^{n+1}\frac{1-(-1)^{i+2}}{i+2}\alpha_i=0$$
$$.\qquad (5.54)$$
$$.$$
$$\sum_{i=0}^{n+1}\frac{1-(-1)^{i+n+1}}{i+n+1}\alpha_i=0$$

which could be solved to obtain the α's (recall that $\alpha_{n+1}=1$) and the roots of the equation $\sum_{i=0}^{n+1}\alpha_i z^i=0$ would give the required ordinates[2].

- For each equation for α, half[3] of the terms would be zero. Thus instead of solving a single set of n+1 equations, we would only need to solve two sets of (n+1)/2 equations. For example, for 4 points (n=3), we obtain the following equations:

---

[1] It is easy to see that $\alpha_{n+1}=1, \alpha_n=-\sum_{i=0}^{n} z_i$ and $\alpha_0=(-1)^{n+1}\prod_{i=0}^{n} z_i$. The actual relationships are, however, not important.

[2] Another technique for linearizing uses manipulations on the original system of equations (5.53). On multiplying the first equation by α_0, i.e., z_0z_1, the second by α_1, i.e., $-(z_1+z_2)$, and adding them to the third equation, we get $\alpha_0=-\frac{1}{3}$. Doing the same operation on the second, third, and fourth equations, we get $\alpha_1=0$ leading to the equation $z^2-\frac{1}{3}=0$ and, therefore, $z_0=-\frac{1}{\sqrt{3}}, z_1=\frac{1}{\sqrt{3}}$. For a general case, similar manipulation leads to the same set of *n+1* equations as Eq. (5.54).

[3] For odd n. If n is even, one set of equations would have n/2 nonzero terms while the other set will have n/2+1 nonzero terms.

$$
\begin{aligned}
&c_0 + c_1 + c_2 + c_3 = 2 && (i)\\
&c_1(z_1 - z_0) + c_2(z_2 - z_0) + c_3(z_3 - z_0) = -2z_0 && (ii)\\
&c_2(z_2 - z_0)(z_2 - z_1) + c_3(z_3 - z_0)(z_3 - z_1) = \frac{2}{3} + 2z_0 z_1 && (iii)\\
&c_3(z_3 - z_0)(z_3 - z_1)(z_3 - z_2) = -\frac{2}{3}(z_0 + z_1 + z_2) - 2z_0 z_1 z_2 && (iv)\\
&2a_0 + \frac{2}{3}a_2 + \frac{2}{5} = 0 && (v)\\
&\frac{2}{3}a_1 + \frac{2}{5}a_3 = 0 && (vi)\\
&\frac{2}{3}a_0 + \frac{2}{5}a_2 + \frac{2}{7} = 0 && (vii)\\
&\frac{2}{5}a_1 + \frac{2}{7}a_3 = 0 && (viii)
\end{aligned}
\qquad (5.55)
$$

From the sixth and eighth equations, $a_1 = a_3 = 0$ and from the fifth and seventh equations, $a_2 = -\frac{6}{7}, a_0 = \frac{3}{35}$. The ordinates are therefore obtained by solving $z^4 - \frac{6}{7}z^2 + \frac{3}{35} = 0$ as $z_{0,3} = \mp\sqrt{\frac{3}{7} + \sqrt{\frac{24}{245}}} = \mp 0.86114$ and $z_{1,2} = \mp\sqrt{\frac{3}{7} - \sqrt{\frac{24}{245}}} = \mp 0.33998$. The coefficients are then sequentially obtained starting from the fourth equation as
$c_3 = 0.3479, c_2 = 0.6521, c_1 = 0.6521, c_0 = 0.3479$

- An important observation could be made from the last n+1 equations in (5.53) that the n+1th degree polynomial $\prod_{i=0}^{n}(z - z_i)$ is orthogonal[1] to all polynomials of order n (and lower). It indicates, and it will be further established in the next subsections, that the ordinates would be the zeroes of the Legendre polynomial of order n+1.

This method, though simple to use, is not as efficient as those described next. Hence we will not discuss it further.

b. Based on Hermite Interpolation:

In section 4.5, we discussed the problem of interpolating when the function value *as well as* its derivative(s) is known at a few grid points. Let us assume that the function, and its first derivative, is known at *n+1* points: $z_0, z_1, z_2 \ldots, z_n$ in the interval (-1,1). Using the Hermite interpolation we could write the interpolating polynomial of degree 2n+1 as (see section 4.5)

$$f_{2n+1}(z) = \sum_{i=0}^{n}\left[H_{i,0}\, f(z_i) + H_{i,1}\, f'(z_i)\right] \qquad (5.56)$$

where the H's are polynomials in z (with maximum degree 2n+1) and are given by

[1] You may want to review section 4.3 on orthogonal polynomials.

$$H_{i,0} = \left[1 - 2(z - z_i) L_i'(z_i)\right]\left[L_i(z)\right]^2$$
$$H_{i,1} = (z - z_i)\left[L_i(z)\right]^2 \qquad (5.57)$$

L(z) denoting the Lagrange polynomial[1]. Clearly, if we want a quadrature scheme of the form, Eq. (5.49), which is exact for this 2n+1-degree polynomial, we must have

$$\sum_{i=0}^{n} c_i f(z_i) = \int_{-1}^{1} \sum_{i=0}^{n} \left[H_{i,0} f(z_i) + H_{i,1} f'(z_i)\right] dz$$

This implies that we should choose the z's in such a way that $\int_{-1}^{1} H_{i,1}(z)\,dz = 0\ \forall i$ (thereby making the coefficients of the derivative terms in the integral vanish) and the coefficients would be given by $c_i = \int_{-1}^{1} H_{i,0}(z)\,dz \quad \forall i$. This provides us with a methodology to find out the ordinates, z_i, and then, $H_{i,0}$, from which the coefficients of the quadrature formula are obtained. Using the definition of the Lagrange polynomials and the fact that these are polynomials of order *n*, it is obvious from Eq. (5.57) that for the coefficients $H_{i,1}$ to vanish from the quadrature formula, it is sufficient[2] that the (n+1)th order polynomial $\prod_{i=0}^{n}(z - z_i)$ is orthogonal to *all* polynomials of inferior order, i.e., order n or lower. As we have seen in the previous chapter, this condition is satisfied by the Legendre polynomial, $P_{n+1}(z)$, and its zeroes would be the required ordinates of the quadrature scheme.

c. Based on Orthogonal polynomials:

Let $f_{2n+1}(z)$ be a polynomial of order (2n+1) passing through the function values at all the grid points. We may then write

$$f_{2n+1}(z) = \sum_{i=0}^{n} L_i(z)\, f(z_i) + p_n(z) \prod_{i=0}^{n} (z - z_i) \qquad (5.58)$$

in which the first term on the r.h.s. is the n^{th} degree polynomial interpolating function in the Lagrange form, $p_n(z)$ is an arbitrary n^{th} degree polynomial, and we have used the condition that the second term on the r.h.s. must be a polynomial of degree (2n+1) and must vanish at all the grid points (since the first term, by itself, interpolates the function at all grid points). Now, writing[3]

$$\int_{-1}^{1} f(z)\,dz \simeq \sum_{i=0}^{n} W_i f(z_i) \qquad (5.59)$$

where the weights are defined by

---

[1] Recall that $L_i(z) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{z - z_j}{z_i - z_j}$

[2] It can be shown that it is also *necessary*.

[3] Since the coefficients c, which we have used in the previous subsections, may be thought of as a weight assigned to each function value, we would now replace them by the commonly used symbol, W.

$$W_i = \int_{-1}^{1} L_i(z)\,dz \tag{5.60}$$

it is seen that the quadrature would be exact for all polynomials of order (2n+1) if

$$\int_{-1}^{1} p_n(z) \prod_{i=0}^{n} (z - z_i)\,dz = 0 \tag{5.61}$$

for *all* n^th degree polynomials, $p_n(z)$. Thus, the term $\prod_{i=0}^{n}(z - z_i)$ should be orthogonal to all n^th degree polynomials, and we again reach the conclusion that the quadrature points should be the zeroes of the Legendre polynomial of order (n+1). This form of the quadrature scheme is, therefore, commonly called the ***Gauss-Legendre*** quadrature. The weights are then obtained from Eq. (5.59) as $\int_{-1}^{1} L_i(z)\,dz$ and turn out to be the same as $\int_{-1}^{1} H_{i,0}\,dz$ in the previous method.

Though we had obtained a rough estimate of the error in approximating the integral using the method of undetermined coefficient with two quadrature points, it would be appropriate at this stage to provide an expression for the error in general case.

Using Eq. (4.51) for the remainder term in interpolation using the Hermite polynomials, we obtain the error in numerical integration as

$$E_z = I_z - \tilde{I}_z = \int_{-1}^{1} \frac{f^{2n+2}(x^*)}{(2n+2)!} \prod_{i=0}^{n} (z - z_i)^2\,dz \tag{5.62}$$

Applying the integral mean value theorem, we get $E_z = \frac{f^{2n+2}(x)}{(2n+2)!} \int_{-1}^{1} \prod_{i=0}^{n} (z - z_i)^2\,dz$. Now using the facts that z_i are zeroes of $P_{n+1}(z)$, and the coefficient of the leading term in $P_n(z)$ is $\frac{(2n)!}{2^n (n!)^2}$ (see section 4.3), we get $\prod_{i=0}^{n} (z - z_i)^2 = \left\{ \frac{2^{n+1}\left[(n+1)!\right]^2 P_{n+1}(z)}{(2n+2)!} \right\}^2$. Using the inner product relationship $\int_{-1}^{1} P_n(z) P_n(z)\,dz = \frac{2}{2n+1}$ (see section 4.3), we finally obtain

$$E_z = \frac{2^{2n+3}\left[(n+1)!\right]^4}{(2n+3)\left[(2n+2)!\right]^3} f^{2n+2}(x) \tag{5.63}$$

Note that for n=1, $E_z = \frac{f^{iv}(x)}{135}$, which was obtained earlier using the method of undetermined coefficients. The weights, abscissas, and error for a few values of n are listed in Table below.

Table 5.6 Weights, abscissas, and error for Gauss-Legendre quadrature

n*	Abscissa	Weights	Error

0	0.00000	2.0000	$\frac{f''(x)}{3}$
1	± 0.57735	1.0000	$\frac{f^{iv}(x)}{135}$
2	0.00000	0.88889	$\frac{f^{vi}(x)}{15750}$
	± 0.77460	0.55556	
3	± 0.33998	0.65215	$\frac{f^{(8)}(x)}{3472875}$
	± 0.86114	0.34785	
4	0.00000	0.56889	$\frac{f^{(10)}(x)}{1237732650}$
	± 0.53847	0.47863	
	± 0.90618	0.23693	

*: Recall that the number of quadrature points is n+1.

Eq. (5.60) expresses the weights in a very simple form but it is quite cumbersome to evaluate. We could express the weights in a form more suitable from computational point of view by writing [see Eq. 4.22)]

$$L_i(z) = \frac{\prod_{j=0}^{n}(z-z_j)}{(z-z_i)\left[\frac{d}{dz}\left\{\prod_{j=0}^{n}(z-z_j)\right\}\right]_{z=z_i}} = \frac{P_{n+1}(z)}{(z-z_i)P'_{n+1}(z_i)}$$

since z_j are the zeroes of $P_{n+1}(z)$ implying that $P_{n+1}(z) = C_{n+1}\prod_{j=0}^{n}(z-z_j)$, with C_{n+1} denoting the coefficient of the leading term, z^{n+1}. Using the Christoffel-Darboux identity[1], we get

$$\int_{-1}^{1}\frac{P_{n+1}(z)}{(z-z_i)}dz = \frac{C_{n+1}\langle P_n, P_n\rangle}{C_n P_n(z_i)}\sum_{j=0}^{n}\frac{P_j(z_i)\int_{-1}^{1}P_j(z)dz}{\langle P_j, P_j\rangle} \quad (5.64)$$

From the orthogonality of Legendre polynomials, and since $P_0(z)$=1, the rightmost integral above will vanish except for j=0. From the expressions for the leading

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[1] For any set of orthogonal polynomials, $f_i(x)$, we have $\sum_{j=0}^{n}\frac{f_j(x)f_j(x^*)}{\langle f_j, f_j\rangle} = \frac{f_{n+1}(x)f_n(x^*) - f_n(x)f_{n+1}(x^*)}{\frac{C_{n+1}}{C_n}\langle f_n, f_n\rangle(x-x^*)}$ in which $\langle\cdot\rangle$ indicates the inner product. For the particular case in which x* are the zeroes of $f_{n+1}(x)$, represented by x_i, i=0,1,…,n, we have $\sum_{j=0}^{n}\frac{f_j(x)f_j(x_i)}{\langle f_j, f_j\rangle} = \frac{C_n f_{n+1}(x)f_n(x_i)}{C_{n+1}\langle f_n, f_n\rangle(x-x_i)}$. Applying it to the Legendre polynomials, we get $\frac{P_{n+1}(z)}{(z-z_i)} = \frac{C_{n+1}\langle P_n, P_n\rangle}{C_n P_n(z_i)}\sum_{j=0}^{n}\frac{P_j(z)P_j(z_i)}{\langle P_j, P_j\rangle}$.

coefficient, we have $\frac{C_{n+1}}{C_n}=\frac{\frac{(2n+2)!}{2^{n+1}\left[(n+1)!\right]^2}}{\frac{(2n)!}{2^n(n!)^2}}=\frac{2n+1}{n+1}$ and since $\langle P_n,P_n\rangle=\frac{2}{2n+1}$, we get $\int_{-1}^{1}\frac{P_{n+1}(z)}{(z-z_i)}dz=\frac{2}{(n+1)P_n(z_i)}$ and

$$W_i=\int_{-1}^{1}L_i(z)\,dz=\frac{1}{P'_{n+1}(z_i)}\int_{-1}^{1}\frac{P_{n+1}(z)}{(z-z_i)}dz=\frac{2}{(n+1)P_n(z_i)P'_{n+1}(z_i)} \tag{5.65}$$

or, using the relation between Legendre polynomials and derivative[1],

$$W_i=\frac{2}{\left(1-z_i^2\right)\left[P'_{n+1}(z_i)\right]^2}=\frac{2\left(1-z_i^2\right)}{\left[(n+1)P_n(z_i)\right]^2} \tag{5.66}$$

Note that we have treated *all* the ordinates and weights to be adjustable. Sometimes the problem may demand that some of the ordinates or weights be fixed *a priori*. Generally, by assigning one parameter we would lose an order of accuracy from the *2n+1* obtainable from *n* free points[2]. Therefore, it is not very common to do so. However, if it is important to use the function value at one or both end points, Radau and Lobatto quadrature schemes, respectively, could be used. Similarly, if we constrain all weights to be equal, we get Tchebycheff quadrature scheme. We do not discuss these here and refer the interested reader to ….

A number of times, we may be interested in evaluating the integral using multiple applications of the quadrature scheme with increasing number of points to study the convergence properties. Table 5.6 clearly shows that there are no common points when we move from n=2 to n=3 or n=4. Thus we will not be able to re-use any of the previously computed function values. Since the function evaluation may be time-consuming, it would be more efficient to devise a scheme which would be able to utilise some, if not all, of the function values evaluated earlier. Kronrod (1964) proposed one such scheme which starts from, say n_1, points and adds n_1+1 points in such a way that the new abscissa include all n_1 of the old points, the free parameters being the n_1+1 new abscissas and $2n_1$+1 weights. These quadrature schemes, known as the Gauss-Kronrod scheme, are not discussed here.

Sometimes, instead of integral of the function, we require the integral of the function multiplied by some weighting function, *w(x)*. For example, in minimax approximation of a function (see section 4.3), we require integrals of the form $\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}dx$. One option in this case would be to treat *w(x)f(x)* as another function, say, *g(x)* and then apply the Gauss

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[1] The relationship is $\left(1-z^2\right)P'_n(z)=nP_{n-1}(z)-nzP_n(z)$. Using n+1 in place of n, and noting that z_i are zeroes of $P_{n+1}(z)$, we get $(n+1)P_n(z_i)=\left(1-z_i^2\right)P'_{n+1}(z)$.

[2] But not always. For example, if the prescribed ordinate coincides with one of the zeroes of $P_{n+1}(z)$, we still get the same accuracy.

Legendre quadrature to this function. However, *g(x)* may not be as well-behaved as f(x) and it is preferred to use a weighted-Gauss-quadrature[1]. These may be written in the general form

$$\int_{-1}^{1} w(z)f(z)\,dz = \sum_{i=0}^{n} W_i f(z_i) + E_z \tag{5.67}$$

with

$$W_i = \int_{-1}^{1} w(z)L_i(z)\,dz \tag{5.68}$$

and

$$E_z = \frac{f^{2n+2}(x)}{(2n+2)!}\int_{-1}^{1} w(z)\prod_{i=0}^{n}(z-z_i)^2\,dz \tag{5.69}$$

z_i being zeroes of the (n+1)[th] order polynomial from the set of polynomials orthogonal over (-1,1) with respect to weight w(z). The choice $w(z) = \left(1-z^2\right)^{-1/2}$ leads to the Gauss-Tchebycheff quadrature and is described next. Some other weighting functions are mentioned in the section on improper integrals.

Example 5.9: For four point Gauss-Legendre quadrature, obtain the location of the quadrature points and the associated weights. Use this scheme to estimate $\int_0^1 \exp\left(x-x^2\right)dx$.

Solution: For four quadrature points (n=3), the quadrature points would be located at the zeroes of $P_4(z)$, and are, therefore, obtained from (see Eq. 4.11)

$$35z^4 - 30z^2 + 3 = 0$$

Thus, we get $z^2 = \frac{30 \pm \sqrt{900-420}}{70} = 0.7415557, 0.1155871$. The quadrature points are then obtained as $\pm 0.86114, \pm 0.33998$.

The weight for the point 0.86114 is obtained from Eq. (5.66) as

$$\frac{2\left(1-0.86114^2\right)}{\left[4P_3(0.86114)\right]^2} = \frac{0.51689}{\left[4\left(\frac{5}{2}0.86114^3 - \frac{3}{2}0.86114\right)\right]^2} = 0.34785$$

We may use the alternative expression to find the weight as

$$\frac{2}{\left(1-0.86114^2\right)\left[P_4'(0.86114)\right]^2} = \frac{2}{0.25844\left[\frac{35}{2}0.86114^3 - \frac{15}{2}0.86114\right]^2} = 0.34785$$

The other weights are found similarly and are as listed in Table 5.6. To estimate the integral $\int_0^1 \exp\left(x-x^2\right)dx$, we first convert it to the standard domain (-1,1) by

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[1] Apparently, Gauss had not considered the weighted schemes, which were later studied by Christoffel. The weights, W, are therefore sometimes called the Christoffel numbers.

defining $z = 2x - 1$ and the integral becomes $\frac{1}{2}\int_{-1}^{1} \exp\left(\frac{z+1}{2} - \left(\frac{z+1}{2}\right)^2\right) dz$. The estimate of this integral is obtained as $\tilde{I}_z = \sum_{i=0}^{3} W_i \exp\left[\frac{z_i+1}{2} - \left(\frac{z_i+1}{2}\right)^2\right] = 2.3692$. Hence the original integral is estimated as 2.369/2=1.1846.

Gauss-Tchebycheff quadrature

We have seen (section 4.3) that the Tchebycheff polynomials are orthogonal over (-1,1) for weight function $1/\sqrt{1-z^2}$. Therefore, for the weighted quadrature scheme with a weight of $1/\sqrt{1-z^2}$, the quadrature points would be at the zeroes of $T_{n+1}(z)$ given by (see section 4.3)

$$z_i = \cos\left[\frac{2n-2i+1}{n+1}\frac{p}{2}\right] \qquad i = 0,1,2,\ldots,n \tag{5.70}$$

and the weights are given by (Eq. 4.22 has been used as was done in the derivation of Eq. 5.65)

$$W_i = \int_{-1}^{1} w(z) L_i(z)\, dz = \frac{1}{T'_{n+1}(z_i)} \int_{-1}^{1} \frac{w(z) T_{n+1}(z)}{(z - z_i)} dz \tag{5.71}$$

Following the same methodology as for Gauss-Legendre quadrature, we get[1]

$$W_i = \frac{C_{n+1}\langle T_n, T_n\rangle}{C_n T_n(z_i) T'_{n+1}(z_i)} = \frac{2^n \frac{p}{2}}{2^{n-1}(n+1)} = \frac{p}{n+1} \tag{5.72}$$

showing that all the weights are same! Similarly, the error is obtained as

$$E_z = \frac{f^{2n+2}(x)}{(2n+2)!}\int_{-1}^{1} w(z)\left[\frac{T_{n+1}(z)}{C_{n+1}}\right]^2 dz = \frac{p}{2^{2n+1}(2n+2)!} f^{2n+2}(x) \tag{5.73}$$

Note that all the weights turn out to be equal. However, they were not constrained to do so *a priori*. Hence there is no loss of order of precision normally associated with fixing one or more abscissas or weights.

We could compare the errors in Gauss-Legendre (GL) and Gauss-Tchebycheff (GT) schemes but it would not be meaningful since they integrate different functions: f(z) and $f(z)/\sqrt{1-z^2}$, respectively. For evaluating $\int_{-1}^{1} f(z)\, dz$, it would appear to be advantageous to use the GT scheme if the function involves the factor $1/\sqrt{1-z^2}$. The following example illustrates these points.

[1] We have used the fact that if z_i are the zeroes of $T_{n+1}(z)$, then $T_n(z_i) = -\sqrt{1-z_i^2}$ and $T'_{n+1}(z_i) = -\frac{n+1}{\sqrt{1-z_i^2}}$

Example 5.10: Compare the results obtained from the four point (n=3) Gauss-Legendre and Gauss-Tchebycheff quadrature schemes for estimating the integrals (i) $\int_{-1}^{1} 1\, dz$, (ii) $\int_{-1}^{1} \frac{1}{\sqrt{1-z^2}}\, dz$, (iii) $\int_{-1}^{1} \exp(z)\, dz$, and (iv) $\int_{-1}^{1} \frac{\exp(z)}{\sqrt{1-z^2}}\, dz$.

Solution: The quadrature points and weights for the Gauss-Legendre (GL) scheme are listed in Table 5.6. The weights for the Gauss-Tchebycheff (GT) scheme are all equal (=π/4) and the quadrature points are obtained from Eq. (5.70) as $\pm 0.92388, \pm 0.38268$. The estimates of the integrals are obtained below:

(i) For $\int_{-1}^{1} 1\, dz$

GL : f(z)=1, $\tilde{I} = \sum_{i=0}^{3} W_i \times 1 = 2$, which is the exact value of the integral

GT : $f(z) = \sqrt{1-z^2}$, $\tilde{I} = \sum_{i=0}^{3} W_i \times \sqrt{1-z_i^2} = 2.052$

(ii) For $\int_{-1}^{1} \frac{1}{\sqrt{1-z^2}}\, dz$

GL : $f(z) = 1 \big/ \sqrt{1-z^2}$, $\tilde{I} = \sum_{i=0}^{3} W_i \times \frac{1}{\sqrt{1-z_i^2}} = 2.755$

GT : $f(z) = 1, \tilde{I} = \sum_{i=0}^{3} W_i \times 1 = p$, which is the exact value of the integral

(iii) For $\int_{-1}^{1} \exp(z)\, dz$ (the exact value of the integral is 2.350)

GL : $f(z) = \exp(z)$, $\tilde{I} = \sum_{i=0}^{3} W_i \times \exp(z_i) = 2.350$

GT : $f(z) = \exp(z)\sqrt{1-z^2}$, $\tilde{I} = \sum_{i=0}^{3} W_i \times \exp(z_i)\sqrt{1-z_i^2} = 2.435$

(ii) For $\int_{-1}^{1} \frac{\exp(z)}{\sqrt{1-z^2}}\, dz$ (the exact value of the integral is 3.938)

GL : $f(z) = \exp(z) \big/ \sqrt{1-z^2}$, $\tilde{I} = \sum_{i=0}^{3} W_i \times \frac{\exp(z_i)}{\sqrt{1-z_i^2}} = 3.376$

GT : $f(z) = 1, \tilde{I} = \sum_{i=0}^{3} W_i \times \exp(z_i) = 3.977$

5.3.3 Improper Integrals

Till now, we have made the tacit assumption that the integral to be evaluated using a numerical scheme is *proper*, i.e., it has finite limits and the integrand is defined and continuous at all points in the interval[1]. The good thing about a proper integral is that it will always converge. As is clear from this definition, an *improper integral* would be one in which either the limit(s) of the integral is/are at $\pm\infty$ or the function to be integrated is undefined/discontinuous at any point in the interval. However, it is not clear whether an improper integral will converge or not. As it turns out, it may converge in some cases and diverge in others. Obviously, if the integral diverges, there is no point in using a numerical method to estimate its value. Therefore, we will assume that the improper integrals to be evaluated numerically converge (see Box 5.2 for some theorems which are helpful in checking the convergence of an improper integral).

Box 5.2: Convergence of improper integrals

Some easily verifiable results are:

The p-integral, $\int_1^\infty \frac{1}{x^p} dx$ converges for p>1 (and diverges otherwise)

$\int_0^1 \frac{1}{x^p} dx$ converges for p<1 (and diverges otherwise)

$\int_0^\infty e^{\alpha x} dx$ converges for $\alpha<0$ (and diverges otherwise)

For other improper integrals, comparison tests are used to establish their convergence. To apply these tests, it is helpful to note the absolute convergence property (if $\int_a^b \left| f(x) \right| dx$ converges then so does $\int_a^b f(x) dx$).

Comparison test (also called Direct Comparison or Standard Comparison):

Over the interval [a,b) or (a,b][2], if f and g are continuous and $0 \le f(x) \le g(x)$ for all x in the interval, then $\int_a^b f(x) dx$ converges if $\int_a^b g(x) dx$ converges (and $\int_a^b g(x) dx$ diverges if $\int_a^b f(x) dx$ diverges).

[1] For numerical integration we may be able to get around the more restrictive condition of the function being continuous at all points in the interval by suitable subdivision of the interval.
[2] Here a could be $-\infty$ or finite and b could be ∞ or finite.

Limit Comparison test

Over the interval [a,b) or (a,b], if f and g are continuous and $f(x) > 0$ and $g(x) > 0$ for all x in the interval, such that $\lim_{x \to b^- \text{ or } a^+} \frac{f(x)}{g(x)} = L$ then:

If $0 < L < \infty$, $\int_a^b f(x)dx$ converges *if and only if* $\int_a^b g(x)dx$ converges.

If L=0, $\int_a^b f(x)dx$ converges if (note the absence of *only if*) $\int_a^b g(x)dx$ converges.

If L=∞, $\int_a^b f(x)dx$ diverges if $\int_a^b g(x)dx$ diverges.

Once we know that an improper integral converges, we should look at the ways to evaluate it numerically. If the limits are finite and the integral is improper because the integrand is not defined at one of the limits (or some point within the interval), e.g. $\int_0^1 x^{-1/2}dx$ in which the integrand is not defined at the lower limit; we may use one of the semi-open methods (see section 5.3.1.4) to estimate the integral. If we are not averse to using irregularly spaced grid points, the Gauss-Legendre quadrature is likely to be the best open method for evaluating such integrals (in case the singularity lies within the interval and not at one of the ends, we may partition the integral into two parts at the singularity and separately evaluate each part).

Sometimes a change of variable may eliminate the singularity. For example, $\int_0^1 \frac{f(x)}{x^p}dx$ could be converted to $\frac{1}{p}\int_0^1 y^{\frac{1}{p}-2} f\left(y^{1/p}\right)dy$ by substituting $y=x^p$ (clearly, p should be equal to or smaller than ½ for this to work). Another option could be to truncate the interval of integration if it is ensured that the resulting error would be within permissible limits. For example, if in the integral above, $\left|f(x)\right| \le 1$ over the entire interval and assuming that p is less than 1, it can be shown that $\int_0^e \frac{f(x)}{x^p}dx \le \int_0^e \frac{1}{x^p}dx = \frac{e^{1-p}}{1-p}$. This suggests that we may choose an appropriate ε and approximate the given improper integral as the proper integral $\int_{e}^{1} \frac{f(x)}{x^p} dx$.

The reader is referred to Davis and Rabinowitz for a detailed discussion.

Example 5.11: Evaluate $\int_{0}^{1} \frac{1}{\sqrt{1-x^2}} dx$ using semi-open (quadratic with h=0.2) and 5-point Gauss-Legendre quadrature.

Solution: It is observed that the integrand is undefined at the upper limit of the integral. The first step would, therefore, be to see whether the integral converges or not. It is readily seen that over the interval (0,1), $\frac{1}{\sqrt{1-x^2}} = \frac{1}{\sqrt{1+x}\sqrt{1-x}} \leq \frac{1}{\sqrt{1-x}}$ and

both $f(x) = \frac{1}{\sqrt{1-x^2}}$ and $g(x) = \frac{1}{\sqrt{1-x}}$ are nonnegative. Also, $\int_{0}^{1} \frac{1}{\sqrt{1-x}} dx$ is equivalent

to $\int_{0}^{1} \frac{1}{\sqrt{x}} dx$, which converges (see Box 5.2, here p=1/2). Hence the comparison test shows that the given improper integral converges (it is easy to see that the true value is π/2, i.e., 1.571).

Using quadratic semi-open formula (Table 5.5), with h=0.2 (i.e., n=4), we get

$$\tilde{I} = \frac{0.2}{3}\left[f(0) + 4f(0.2) + \frac{13}{4} f(0.4) + 0.f(0.6) + \frac{27}{4} f(0.8) \right] = 1.325$$

Using 5-point Gauss-Legendre (with the transformation z=2x-1 to convert the range into the standard range), we get

$$\tilde{I}_z = 0.56889 f_z(0) + 0.47863\left[f_z(-0.53847) + f_z(0.53847) \right] + 0.23693\left[f_z(-0.90618) + f_z(0.90618) \right]$$
$$= 2.8254$$

Hence the original integral is estimated as 2.8254/2=1.413.

If either or both limits of the integral are not finite (but the value of the integral is bounded), we could use several options to first convert it into a proper integral and then numerically evaluate it. Probably the simplest option would be a substitution of variable. For example, a substitution y=exp(-x) changes the limits (0,∞) into (0,1) with the only constraint that the resulting integrand in y should be bounded over the entire interval. The truncation of the interval, as discussed for the case of integrands with singularity, may also work for some functions. The weighted Gauss-quadrature (Eq. 5.67) for finite integration interval could be extended to infinite intervals through the Gauss-Laguerre formula (0, ∞) and the Gauss-Hermite formula (-∞, ∞) which use the weights exp[-z] and exp[-z^2], respectively. We will, however, not discuss these here.

Example 5.12: Evaluate $\int_{0}^{\infty} \frac{e^{-x}}{1+x^2} dx$.

Solution: Using the comparison test, since $\frac{e^{-x}}{1+x^2} \le e^{-x}$ and $\int_0^\infty e^{-x}dx$ converges (Box 5.2), $\int_0^\infty \frac{e^{-x}}{1+x^2}dx$ also converges.

Now substituting z=2exp(-x)-1, $\int_0^\infty \frac{1}{1+x^2}dx = \int_{-1}^{1} \frac{dz}{2\left[1+\left(\ln\frac{z+1}{2}\right)^2\right]}$. Using four point Gauss-Legendre quadrature, we get

$$\tilde{I} = \sum_{i=0}^{3} W_i \times \frac{1}{2\left[1+\left(\ln\frac{z_i+1}{2}\right)^2\right]} = 0.6291$$

Exercise 5.3

1. Estimate the integral of a 4th degree polynomial over (0,2) using the trapezoidal rule with step sizes of 1 and 2 and comment on the effect of the step size on the error. Use three different polynomials: (a) $1+2x+x^2+2x^3-x^4$, (b) $6+7x+9x^2+8x^3-5x^4$, and (c) $10+20x+60x^2+41x^3-25x^4$.
2. A function is sampled at equidistant points as shown in the table below:

x	0	1	2	3	4	5	6	7	8	9	10	11	12
f(x)	1.000	1.564	2.266	3.115	4.125	5.307	6.672	8.232	10.000	11.986	14.203	16.662	19.375

Estimate the integral $\int_0^{12} f(x)dx$ using the Simpson's 1/3 and 3/8 rules.

3. Assuming that the data in exercise 2 at x=12 is not sampled, estimate the same integral using a semi-open method with quadratic extrapolation.
4. If it is known that the actual function is $f(x)=1+\frac{x}{2}+\left(\frac{x}{4}\right)^2+\left(\frac{x}{8}\right)^3$, obtain the errors of estimation of the methods used in exercise 2 and 3 and comment on the accuracy.
5. Use the 5 point Gauss-Legendre and Gauss-Tchebycheff quadratures to estimate the above integral.
6. Estimate the following integrals using the semi-open method with quadratic extrapolation, 4 point Gauss-Legendre quadrature and 6 point Gauss-Tchebycheff quadrature:

   (i) $\int_0^1 \frac{dx}{\sqrt{1-x}}$

(ii) $\int_0^1 \frac{dx}{x^{0.1}+x^{0.9}}$ (note that the semi-open method requires extrapolation at the lower limit and the formulae given in Table 5.5 would need appropriate modification)

7. Estimate the following integrals using coordinate transformation and then applying the 5 point Gauss-Legendre quadrature:

   (i) $\int_0^\infty e^{-x^2} dx$ (ii) $\int_1^\infty \frac{dx}{x^{1.1}+x^{1.9}}$

5.4 Summary

In this chapter, various methods for estimating the derivatives or integral of a given function (either as a function or as discretely sampled values) have been described. Use of the Taylor's series to estimate the derivative from discrete data was described first and the concept of forward, backward, and central difference was introduced. Different techniques of improving the accuracy of the estimate by incorporating more data points were described. Amplitude and phase errors in the estimation of derivatives of periodic functions were briefly described to lay the background for their more extensive use in the solution of differential equations. Numerical integration was discussed, first for a function sampled at discrete points and then for a continuous function. For the discrete case, numerical integration using a piecewise linear approximation of the function was discussed first. The improvement in accuracy by using higher order approximations was described next. Both the Newton-Cotes and the Adams methods were described to achieve the improvement in accuracy. The Adams method was described briefly and a more detailed description would follow in the next chapter where these methods find better use in the solution of differential equations. Open and semi-open integration formulae were discussed to account for the cases where the range of integration extends beyond the range of observed data. Numerical integration of a given function was then discussed with the emphasis placed on the use of orthogonal polynomials. Various forms of the Gauss quadrature schemes were described. Finally, numerical integration of improper integrals, which either had the range of integration going to infinity or the function value becoming infinite at some point in the range, was discussed.

The methods described in this chapter may be used to solve differential equations either by replacing the derivative by a *difference* of function values or by re-casting the equation in terms of an integral. In the next two chapters we describe various techniques of solution of ordinary and partial differential equations which will borrow heavily from the material discussed in this (and the previous) chapter. Note that partial differential equations would need expressions for the numerical differentiation of a function of two (or more) variables, which have not been discussed in this chapter. However, the extension of the single-variable technique to multiple variables is relatively straightforward and would be described as needed in Chapter 7. Similarly, numerical integral of multiple integrals has not been discussed in this chapter but follows a philosophy similar to that of the single variable case.