

CHAPTER-V

NUMERICAL DIFFERENTIATION & INTEGRATION

5.1 Introduction

Calculus is mathematics of change. Because engineers must continuously deal with systems and processes that change, calculus is an essential tool of the engineering profession. Standing at the heart of calculus are the related mathematical concepts of differentiation and integration. Mathematically, the derivative represents the rate of change of a dependent variable with respect to an independent variable. If y is the dependent variable and x is the independent variable, the first derivative of $y = f(x)$ w.r.t. to x , represented by dy/dx , is given by

$$\frac{dy}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \quad (5.1)$$

The inverse process to differentiation in calculus is integration. Mathematically, integration is represented by

$$I = \int_a^b f(x) dx \quad (5.2)$$

which stands for the integral of the function $f(x)$ w.r.t. the independent variable x , evaluated between the limits $x = a$ to $x = b$. The function $f(x)$ is referred to as the *integrand*.

Non-Computer Methods for Differentiation and Integration

The function to be differentiated or integrated will typically be in one of the following three forms:

1. A simple continuous function such as a polynomial, an exponential, or a trigonometric function.
2. A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
3. A tabulated function where the values of x and $f(x)$ are given at a number of discrete points, as is often the case with experimental or field data.

In the first case, the derivative or integral of a simple function may be evaluated analytically using calculus. For the second case, analytical solutions are often impractical, and sometimes impossible, to obtain. In these instances, as well as in the third case of discrete data, approximate methods must be employed.

A non-computer method for determining derivatives from data is called *equal-area graphical differentiation*. In this method, the (x, y) data are tabulated and, for each interval, a simple divided difference $\Delta y/\Delta x$ is employed to estimate the slope. Then these values are plotted as a stepped curve versus x . Next a smooth curve is drawn that attempts to approximate the area under the stepped curve. That is, it is drawn so that visually, the positive and the negative areas are balanced. The rates at given values of x can then be read from the curve.

In the same spirit, visually oriented approaches were employed to integrate tabulated data and complicated functions in the pre-computer era. A simple intuitive approach is to plot the function on a grid and count the number of boxes that approximate the area. This number multiplied by the area of each box provides a rough estimate of the total area under the curve. This estimate can be refined, at the expense of additional effort, by using a finer grid.

Another commonsense approach is to divide the area into vertical segments, or strips, with a height equal to the function value at the midpoint of each strip. The area of the rectangles can be then calculated and summed to estimate the total area. In this approach, it is assumed that the value at the midpoint provides a valid approximation of the average height of the function for each strip. As with the grid method, refined estimates are possible by using more (and thinner) strips to approximate the integral.

5.2 Numerical differentiation

5.2.1 Lower Order Methods

By truncating the second- and higher-derivatives in the Taylor series

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \dots \quad (5.3)$$

the following formula for approximating the first derivative, called the *first forward difference*, is obtained

$$f'(x) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) = \frac{\Delta f_i}{h} + O(h) \quad (5.4)$$

where Δf_i is referred to as the *first forward difference* and h is called the step size. The entire term $\Delta f/h$ is referred to as a *first finite divided difference*.

Similarly, by truncating the Taylor series between x_{i-1} and x_i ,

$$f(x_i) = f(x_{i-1}) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \dots \quad (5.5)$$

the following formula for approximating the first derivative is obtained

$$f'(x_i) = \frac{f(x_{i-1}) - f(x_i)}{h} + O(h) = \frac{\nabla f_i}{h} + O(h) \quad (5.6)$$

where ∇f_i is referred to as the *first backward difference*.

A third way to approximate the first derivative is to subtract backward Taylor series expansions (between x_{i-1} and x_i) from the forward Taylor series expansion (between x_i and x_{i+1}) resulting in

$$f(x_{i+1}) = f(x_{i-1}) + 2f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \dots \quad (5.7)$$

from which we obtain

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1}))}{2h} - O(h^2) \quad (5.8)$$

The above equation is a *centered difference* representation of the first derivative.

Example Consider the function $f(x) = e^{-x} \sin(x)$

Compute numerical approximations for the $f'(1)$ derivative, using step sizes, $h = 0.1, 0.01, 0.001$

$$f(x) = e^{-x} \sin(x)$$

Using $h = 0.1$

$$f'(1) \approx ((0.296657) - (0.318477)) / (0.2)$$

$$f'(1) \approx (-0.0218198) / (0.2)$$

$$f'(1) \approx -0.109099$$

$$f(x) = e^{-x} \sin(x)$$

Using $h = 0.01$

$$f'(1) \approx ((0.308432) - (0.310648)) / (0.02)$$

$$f'(1) \approx (-0.00221554) / (0.02)$$

$$f'(1) \approx -0.110777$$

```
f[x] = e^-x Sin[x]
Using h = 0.001
f'[1.] ≈ ((0.309449) - (0.30967)) / (0.002)
f'[1.] ≈ (-0.000221587) / (0.002)
f'[1.] ≈ -0.110794
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```
f[x] = e^-x Sin[x]
The true value is:
f'[1] =  $\frac{\text{Cos}[1]}{e} - \frac{\text{Sin}[1]}{e}$ 
f'[1] = -0.110794
```

5.2.2 High-Accuracy Differentiation Formulas

High-accuracy divided difference formulas can be generated by including additional terms from the Taylor series expansion. For example, the forward Taylor series expansion can be written as

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \dots \quad (5.9)$$

which can be solved for

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h^2 + O(h^2) \quad (5.10)$$

The result can be truncated by excluding the second- and higher-derivative terms and were thus left with a final result of

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \quad (5.11)$$

We can retain the second-derivative term by substituting the following approximation of the second derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h) \quad (5.12)$$

into Eq. 5.10 to yield

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2) \quad (5.11)$$

or, collecting terms,

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2) \quad (5.12)$$

Notice that the inclusion of the second-derivative term has improved the accuracy to $O(h^2)$. Similar improved versions can be developed for the backward and centered formulas as well as for the approximations of the higher derivatives. The formulas are given below.

Forward Finite-divided Difference Formulas

First Derivative

Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} \quad O(h)$$

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

Second Derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} \quad O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} \quad O(h^2)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3} \quad O(h)$$

$$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3} \quad O(h^2)$$

Fourth Derivative

$$f^{(4)}(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4} \quad O(h)$$

$$f^{(4)}(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4} \quad O(h^2)$$

Backward Finite-divided Difference Formulas*First Derivative*

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

Error

$$O(h)$$

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

$$O(h^2)$$

Second Derivative

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

$$O(h)$$

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3}))}{h^2}$$

$$O(h^2)$$

Third Derivative

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

$$O(h)$$

$$f'''(x_i) = \frac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4}))}{2h^3}$$

$$O(h^2)$$

Fourth Derivative

$$f^{(4)}(x_i) = \frac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4}))}{h^4}$$

$$O(h)$$

$$f^{(4)}(x_i) = \frac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5}))}{h^4}$$

$$O(h^2)$$

Centered Finite-divided Difference Formulas*First Derivative*

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

$$O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2}))}{12h}$$

$$O(h^4)$$

Second Derivative

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

$$O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2}))}{12h^2}$$

$$O(h^4)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3} \quad O(h^2)$$

$$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3} \quad O(h^4)$$

Fourth Derivative

$$f^{(4)}(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4} \quad O(h^2)$$

$$f^{(4)}(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4} \quad O(h^4)$$

5.3 Newton-Cotes integration formulas

The Newton-Cotes formulas are the most common numerical integration schemes. They are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate:

$$I = \int_a^b f(x) dx \cong \int_a^b f_n(x) dx \quad (5.13)$$

where $f_n(x)$ = a polynomial of the form

$$f_n(x) = a_0 + a_1x + \dots + a_{n-1}x^{n-1} + a_nx^n \quad (5.14)$$

where n is the order of the polynomial.

The integral can be approximated by one polynomial or using a series of polynomials applied piecewise to the function or data over segments of constant length.

Closed and open forms of the Newton-Cotes formulas are available. The closed forms are those where the data points at the beginning and end of the limits of integration are known. The open forms have integration limits that extend beyond the range of the data. In this sense, they are akin to extrapolation. Open Newton-Cotes formulas are not generally used for definite integration. However, they are utilized for evaluating improper integrals and for the solution of ordinary differential equations.

5.3.1 The Trapezoidal Rule

The trapezoidal rule is the first of the Newton-Cotes closed integration formulas. It corresponds to the case where the polynomial in Eq. 5.13 is first-order:

$$I = \int_a^b f(x)dx \cong \int_a^b f_1(x)dx \quad (5.15)$$

The straight line passing through the two points $(a, f(a))$ and $(b, f(b))$ is given by

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \quad (5.16)$$

The area under this straight line is an estimate of the integral of $f(x)$ between the limits a and b :

$$I = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx \quad (5.17)$$

The result of the integration is

$$I = (b - a) \frac{f(a) + f(b)}{2} \quad (5.18)$$

which is called the *trapezoidal rule*.

Error of the Trapezoidal Rule

When we employ the integral under a straight line to approximate the integral under the curve, we obviously can incur an error that may be substantial. An estimate of the local truncation error of a single application of the trapezoidal rule is

$$E_t = -\frac{1}{12} f''(\xi)(b - a)^3 \quad (5.19)$$

where ξ lies somewhere in the interval from a to b .

Multiple-Application of Trapezoidal Rule

One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from a to b into a number of segments and apply the method to each segment. The areas of the individual segments can then be added to yield the integral for the entire interval. The resulting equations are called *multiple-application*, or *composite, integration formulas*.

Considering $n + 1$ equally spaced base points $(x_0, x_1, x_2, \dots, x_n)$, and n segments of equal width:

$$h = \frac{b - a}{n} \quad (5.20)$$

If a and b are designated as x_0 and x_n , respectively, the total integral can be represented as

$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \dots + \int_{x_{n-1}}^{x_n} f(x)dx \quad (5.21)$$

Substituting the trapezoidal rule for each interval yields

$$I = h \frac{f(x_0) + f(x_1)}{2} + h \frac{f(x_1) + f(x_2)}{2} + \dots + h \frac{f(x_{n-1}) + f(x_n)}{2} \quad (5.22)$$

or, grouping terms,

$$I = \frac{h}{2} \left[f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right] \quad (5.23)$$

or, using Eq. 5.20 to express Eq. 5.23 in the following form,

$$I = \underbrace{(b - a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}}_{\text{Average Height}} \quad (5.24)$$

Because the summation of the coefficients of $f(x)$ in the numerator divided by $2n$ is equal to 1, the average height represents a weighted average of the function values. According to Eq. 5.24, the interior points are given twice the weight of the two end points $f(x_0)$ and $f(x_n)$.

An error for the multiple-application trapezoidal rule can be obtained by summing the individual errors for each segment to give

$$E_t = -\frac{(b-a)}{12n^3} \sum_{i=1}^n f''(\xi_i) \quad (5.25)$$

where $f''(\xi_i)$ is the second derivative at a point ξ_i located in segment i . This result can be simplified by estimating the mean or the average value of the second derivative for the entire interval as

$$\bar{f}'' \cong \frac{\sum_{i=1}^n f''(\xi_i)}{n} \quad (5.26)$$

Therefore $\sum f''(\xi_i) \cong n\bar{f}''$ and Eq. 5.25 can be rewritten as

$$E_a = -\frac{(b-a)^3}{12n^2} \bar{f}'' \quad (5.27)$$

Thus, if the number in the bracket is doubled, the truncation error will be quartered. Note that Eq. 5.27 is an approximate error because the approximate nature of Eq. 5.26.

NB: In the multiple-application of the trapezoidal formula, the error decreases as the number of segments n increases. However, the rate of decrease of error is gradual. (Doubling the number of segments quarters the error.) In the subsequent sections, we will develop higher-order formulas that are more accurate and that converge more quickly on the true integral as the segments are increased.

Example Numerically approximate the integral $\int_0^2 (2 + \cos[2\sqrt{x}]) dx$

by using the trapezoidal rule with $m = 1, 2, 4, 8,$ and 16 subintervals.

For $m = 1$

$$5 + \cos[2\sqrt{2}]$$

$$4.04864$$

For $m = 2$

$$\frac{1}{2} (5 + 2(2 + \cos[2]) + \cos[2\sqrt{2}])$$

$$3.60817$$

$$\frac{1}{4} (5 + 2(2 + \cos[2]) + 2(2 + \cos[\sqrt{2}]) + \cos[2\sqrt{2}] + 2(2 + \cos[\sqrt{6}]))$$

For $m = 4$

3.4971

For $m = 8$

$$\frac{1}{8} (5 + 2 (2 + \cos[1]) + 2 (2 + \cos[2]) + 2 (2 + \cos[\sqrt{2}]) + \cos[2\sqrt{2}] + 2 (2 + \cos[\sqrt{3}]) + 2 (2 + \cos[\sqrt{5}]) + 2 (2 + \cos[\sqrt{6}]) + 2 (2 + \cos[\sqrt{7}]))$$

3.46928

For $m = 16$

$$\frac{1}{16} \left(5 + 2 (2 + \cos[1]) + 2 (2 + \cos[2]) + 2 \left(2 + \cos\left[\sqrt{\frac{3}{2}}\right] \right) + 2 \left(2 + \cos\left[\frac{1}{\sqrt{2}}\right] \right) + 2 \left(2 + \cos\left[\frac{3}{\sqrt{2}}\right] \right) + 2 (2 + \cos[\sqrt{2}]) + \cos[2\sqrt{2}] + 2 \left(2 + \cos\left[\sqrt{\frac{5}{2}}\right] \right) + 2 (2 + \cos[\sqrt{3}]) + 2 \left(2 + \cos\left[\sqrt{\frac{7}{2}}\right] \right) + 2 (2 + \cos[\sqrt{5}]) + 2 \left(2 + \cos\left[\sqrt{\frac{11}{2}}\right] \right) + 2 (2 + \cos[\sqrt{6}]) + 2 \left(2 + \cos\left[\sqrt{\frac{13}{2}}\right] \right) + 2 (2 + \cos[\sqrt{7}]) + 2 \left(2 + \cos\left[\sqrt{\frac{15}{2}}\right] \right) \right)$$

3.46232

5.3.2 Simpson's Rules

Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomial to connect the points. For example, if there is an extra point midway between $f(a)$ and $f(b)$, the three points can be connected with a parabola. If there are two points equally spaced between $f(a)$ and $f(b)$, the four points can be connected with a third-order polynomial. The formulas that result from taking the integrals under these polynomials are called *Simpson's rules*.

i. Simpson's 1/3 Rule

Simpson's 1/3 rule results when a second-order interpolating polynomial is substituted into Eq. 5.13:

$$I = \int_a^b f(x)dx \cong \int_a^b f_2(x)dx \quad (5.28)$$

If a and b are designated as x_0 and x_2 and $f_2(x)$ is represented by a second-order Lagrange polynomial, the integral becomes

$$I = \int_x^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_1) + \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_2) \right] dx \quad (5.29)$$

After integration and algebraic manipulation, the following formula results

$$I \cong \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] \quad (5.30)$$

where, for this case, $h = (b - a)/2$. This equation is known as *Simpson's 1/3 rule*.

Simpson's 1/3 rule can also be expressed in the following format

$$I \cong \underbrace{(b - a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}}_{\text{Average Height}} \quad (5.31)$$

where $a = x_0$, $b = x_2$, and x_1 = the point midway between a and b , which is given by $(b + a)/2$. Notice that, according to the above equation, the middle point is weighted two-thirds and the two end points by one-sixth.

It can be shown that a single-segment application of Simpson's 1/3 rule has a truncation error of

$$E_t = -\frac{1}{90} h^5 f^{(4)}(\xi) \quad (5.32)$$

or, because $h = (b - a)/2$,

$$E_t = -\frac{(b - a)^5}{2880} f^{(4)}(\xi) \quad (5.33)$$

where ξ lies somewhere in the interval from a to b . Thus, Simpson's 1/3 rule is more accurate than the trapezoidal rule.

Multiple Application of Simpson's 1/3 Rule

Just as with the trapezoidal rule, Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width:

$$h = \frac{b - a}{n} \quad (5.34)$$

The total integration can be represented as

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \dots + \int_{x_{n-2}}^{x_n} f(x)dx \quad (5.35)$$

Substituting Simpson's 1/3 rule for the individual integral yields

$$I \cong 2h \frac{f(x_0) + 4f(x_1) + f(x_2)}{6} + 2h \frac{f(x_2) + 4f(x_3) + f(x_4)}{6} + \dots + 2h \frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6} \quad (5.36)$$

or, combining terms, and using Eq. 5.34,

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4 \sum_{i=1,3,5}^{n-1} f(x_i) + 2 \sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}_{\text{Average Height}} \quad (5.37)$$

An error estimate for the multiple-application Simpson's rule is obtained in the same fashion as for the trapezoidal rule by summing the individual errors for the segments and averaging the derivative to yield

$$E_a = -\frac{(b-a)^5}{180n^4} \bar{f}^{(4)} \quad (5.38)$$

where $\bar{f}^{(4)}$ is the average fourth derivative for the interval.

Example Numerically approximate the integral $\int_0^2 (2 + \cos[2\sqrt{x}]) dx$

by using Simpson's rule with $m = 1, 2, 4,$ and 8 .

For $m = 1$

$$\frac{1}{3} (5 + 4(2 + \cos[2]) + \cos[2\sqrt{2}])$$

$$3.4613498419$$

For $m = 2$

$$\frac{1}{6} (5 + 2(2 + \cos[2]) + 4(2 + \cos[\sqrt{2}]) + \cos[2\sqrt{2}] + 4(2 + \cos[\sqrt{6}]))$$

$$3.46008250981$$

For $m = 4$

$$\frac{1}{12} (5 + 4(2 + \cos[1]) + 2(2 + \cos[2]) + 2(2 + \cos[\sqrt{2}]) + \cos[2\sqrt{2}] + 4(2 + \cos[\sqrt{3}]) + 4(2 + \cos[\sqrt{5}]) + 2(2 + \cos[\sqrt{6}]) + 4(2 + \cos[\sqrt{7}]))$$

$$3.46000297964$$

For $m = 8$

$$\frac{1}{24} \left(5 + 2(2 + \cos[1]) + 2(2 + \cos[2]) + 4 \left(2 + \cos\left[\sqrt{\frac{3}{2}}\right] \right) + 4 \left(2 + \cos\left[\frac{1}{\sqrt{2}}\right] \right) + 4 \left(2 + \cos\left[\frac{3}{\sqrt{2}}\right] \right) + 2(2 + \cos[\sqrt{2}]) + \cos[2\sqrt{2}] + 4 \left(2 + \cos\left[\sqrt{\frac{5}{2}}\right] \right) + 2(2 + \cos[\sqrt{3}]) + 4 \left(2 + \cos\left[\sqrt{\frac{7}{2}}\right] \right) + 2(2 + \cos[\sqrt{5}]) + 4 \left(2 + \cos\left[\sqrt{\frac{11}{2}}\right] \right) + 2(2 + \cos[\sqrt{6}]) + 4 \left(2 + \cos\left[\sqrt{\frac{13}{2}}\right] \right) + 2(2 + \cos[\sqrt{7}]) + 4 \left(2 + \cos\left[\sqrt{\frac{15}{2}}\right] \right) \right)$$

$$3.45999800397$$

ii. Simpson's 3/8 Rule

In a similar manner to the derivation of the trapezoidal and Simpson's 1/3 rule, a third-order Lagrange polynomial can be fit to four points and integrated:

$$I = \int_a^b f(x)dx \cong \int_a^b f_3(x)dx \tag{5.39}$$

to yield

$$I \cong \frac{3h}{8} \frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8} \tag{5.40}$$

where $h = (b - a)/3$. This equation is called *Simpson's 3/8 rule* because h is multiplied by $3/8$. It is the third Newton-Cotes closed integration formula. The $3/8$ rule can also be expressed in the following form:

$$I \cong \underbrace{(b - a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}}_{\text{Average Height}} \tag{5.41}$$

Thus, the two interior points are given weight's are given weights of three-eighths, whereas the end points are weighted with one-eighth. Simpson's $3/8$ rule has an error of

$$E_t = -\frac{(b - a)^5}{6480} f^{(4)}(\xi) \tag{5.42}$$

Simpson's $1/3$ rule is usually the method of preference because it attains third-order accuracy with three points rather than the four points required for the $3/8$ version. However, the $3/8$ rule has utility when the number of segments is odd.

Summary of the Newton-Cotes integration formulas is given below.

Segments (n)	Points	Name	Formula	Truncation Error
1	2	Trapezoidal rule	$(b - a) \frac{f(x_0) + f(x_1)}{2}$	$-(1/12)h^3 f''(\xi)$
2	3	Simpson's 1/3 rule	$(b - a) \frac{f(x_0) + 4f(x_1) + f(x_2)}{6}$	$-(1/90)h^5 f^{(4)}(\xi)$
3	4	Simpson's 3/8 rule	$(b - a) \frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}$	$-(3/80)h^5 f^{(4)}(\xi)$

Example Numerically approximate the integral $\int_0^2 (2 + \cos[2\sqrt{x}]) dx$

by using Simpson's 3/8 rule with $m = 1, 2, 4$.

For $m = 1$

$$\frac{1}{4} \left(5 + 3 \left(2 + \cos \left[2\sqrt{\frac{2}{3}} \right] \right) + \cos[2\sqrt{2}] + 3 \left(2 + \cos \left[\frac{4}{\sqrt{3}} \right] \right) \right)$$

3.46059898098

For $m = 2$

$$\frac{1}{8} \left(5 + 2(2 + \cos[2]) + 3 \left(2 + \cos \left[2\sqrt{\frac{2}{3}} \right] \right) + 3 \left(2 + \cos \left[2\sqrt{\frac{5}{3}} \right] \right) + \cos[2\sqrt{2}] + 3 \left(2 + \cos \left[\frac{2}{\sqrt{3}} \right] \right) + 3 \left(2 + \cos \left[\frac{4}{\sqrt{3}} \right] \right) \right)$$

3.46003538318

For $m = 3$

$$\frac{1}{16} \left(5 + 2(2 + \cos[2]) + 3 \left(2 + \cos \left[\sqrt{\frac{2}{3}} \right] \right) + 3 \left(2 + \cos \left[2\sqrt{\frac{2}{3}} \right] \right) + 3 \left(2 + \cos \left[2\sqrt{\frac{5}{3}} \right] \right) + 2(2 + \cos[\sqrt{2}]) + \cos[2\sqrt{2}] + 3 \left(2 + \cos \left[\frac{2}{\sqrt{3}} \right] \right) + 3 \left(2 + \cos \left[\frac{4}{\sqrt{3}} \right] \right) + 3 \left(2 + \cos \left[\sqrt{\frac{10}{3}} \right] \right) + 3 \left(2 + \cos \left[\sqrt{\frac{14}{3}} \right] \right) + 2(2 + \cos[\sqrt{6}]) + 3 \left(2 + \cos \left[\sqrt{\frac{22}{3}} \right] \right) \right)$$

3.46000003113