

Numerical Methods

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Aims

In this lecture, we will . . .

- ▶ discuss Trapezoidal and Simpson's rules for numerical integration.

Numerical Integration

Numerical methods of integration represent a natural alternative whenever conventional methods fail to yield a solution.

Now for numerical integration, we wish to find an approximation to the *definite integral*

$$I(f) = \int_a^b f(x)dx, \quad (1)$$

assuming that $f(x)$ is integrable. If $f(x) \geq 0$ on the given interval $[a, b]$, then geometrically, the integral (1) is equivalent to replacing the *area* under the graph of $f(x)$, the x-axis and between the ordinates $x = a$ and $x = b$.

The *definite integral* (1) may be interpreted as the area under the curve of $y = f(x)$ from a to b as shown by Figure 1.

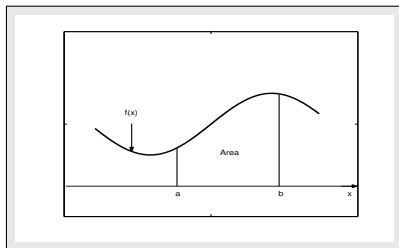


Figure: Definite integral for $f(x)$

An obvious approach is to replace a function $f(x)$ in the integral (1) by an approximating polynomial $p(x)$, that is

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

Numerical integration formulas are derived by integrating interpolation polynomials. Therefore, different interpolation formulas will lead to different numerical integration methods.

Many numerical methods for integration are based on using this interpretation of the integral to derive approximations to it by dividing the interval $[a, b]$ into a number of smaller subintervals. By making simple approximations to the curve $y = f(x)$ in the small subinterval its area may be obtained and on summing all the contributions we obtain an approximation to a integral in the interval $[a, b]$.

Variations of this technique are derived by taking groups of subintervals and fitting different degree polynomials as approximations for each of these groups. The lead of accuracy obtained is dependent on the number of intervals used and the nature the approximation function. There are several methods available in the literature for numerical integration but the most commonly methods may be classified into two groups.

- (a) The *Newton-Cotes formulas* that employ functional values at equally spaced data points.
- (b) The *Gaussian quadrature* formulas that employ unequally spaced data points determined by certain properties of orthogonal polynomials.

Firstly, we shall discuss the Newton-Cotes formulas which has two different types, called, the *closed Newton-Cotes* formulas and the *open Newton-Cotes* formulas. In the first type, we shall discuss in some details the two mostly usable formulas, called the **Trapezoidal rule** and the **Simpson's rule** which can be derived by integrating the Lagrange interpolating polynomials of degree 1 and 2 respectively. In the second type we shall consider some good formulas. The use of the closed Newton-Cotes and other integration formulas of order higher than the Simpson's rule is seldom necessary in most engineering applications and can be use for those cases where extremely high accuracy is required.

Newton-Cotes Formulas

The usual strategy in developing formulas for numerical integration is similar to that for numerical differentiation. We pass a polynomial through points of a function and then integrate this polynomial approximation to a function. This allows us to integrate a function known only as a table of values. Some common formulas based on polynomial interpolation are referred to as the Newton-Cotes formulas.

An $(n + 1)$ -point Newton-Cotes formula for approximating the definite integral (1) is obtained by replacing the integrand $f(x)$ by the n th-degree Lagrange polynomial that interpolates the values of $f(x)$ at equally spaced data points

$$a = x_0 < x_1 < \dots < x_n = b.$$

Note that if the end-points a and b of the given interval $[a, b]$ are in the set of interpolating points; then the Newton-Cotes formulas are called *closed*; otherwise, it is said to be *open*.

Closed Newton-Cotes Formulas

An $(n + 1)$ -point closed Newton-Cotes formula used points $x_i = x_0 + ih$, for, $i = 0, 1, 2, \dots, n$, where $x_0 = a$, $x_n = b$ and $h = \frac{b - a}{n}$, has the form (see Figure 2)

$$\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx \approx \sum_{i=0}^n a_i f(x_i), \quad (2)$$

where

$$a_i = \int_{x_0}^{x_n} L_i(x)dx = \int_{x_0}^{x_n} \prod_{\substack{j=0 \\ j \neq i}}^n \frac{(x - x_j)}{(x_i - x_j)} dx. \quad (3)$$

The following theorem describes the error analysis associated with the above closed Newton-Cotes formulas.

Theorem 1

(Close Newton-Cotes Formulas)

Suppose that $\sum_{i=0}^n a_i f(x_i)$ denotes the $(n+1)$ -point closed Newton-Cotes formula with $x_0 = a$, $x_n = b$, and $h = (b-a)/n$. There exists $\eta(x) \in (a, b)$ for which

$$\int_a^b f(x)dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\eta(x))}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)dt, \quad (4)$$

if n is even and $f \in C^{n+2}[a, b]$. For $f \in C^{n+1}[a, b]$, and n is odd, then

$$\int_a^b f(x)dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\eta(x))}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)dt. \quad (5)$$

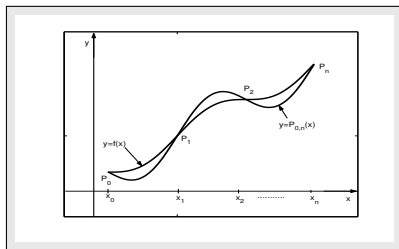


Figure: Close Newton-Cotes approximation

Different numerical integration formulas can be obtained by using the formulas (4) and (5) to approximate the definite integral (1). By using the formula (5) for $n = 1$, we have well-known numerical integration formula, called, the *Trapezoidal rule*. Similarly, by using the formula (4) for $n = 2$, we have one of the best integration rule called, the *Simpson's rule*. We shall discuss the formulation of both these rules and also discuss about their error terms. Later we shall also consider some more closed Newton-Cotes formulas.

Simple Trapezoidal Rule

It is one of the oldest and good numerical method for approximating the definite integral (1). It is based on approximating a function in each subinterval by a straight line.

To derive the **Trapezoidal rule** for one-strip (one interval), let us consider the first degree Lagrange interpolating polynomial with equally spaced data points, that is, $x_0 = a, x_1 = b$ and $h = x_1 - x_0$, then

$$f(x) = p_1(x) = \left(\frac{x - x_1}{x_0 - x_1} \right) f(x_0) + \left(\frac{x - x_0}{x_1 - x_0} \right) f(x_1). \quad (6)$$

Taking integral on both sides of (6) with respect to x between the limits x_0 and x_1 , we have

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

which implies that

$$\begin{aligned} \int_{x_0}^{x_1} f(x) dx &\approx \frac{f(x_0)}{x_0 - x_1} \left[\frac{(x - x_1)^2}{2} \Big|_{x_0}^{x_1} \right] + \frac{f(x_1)}{x_1 - x_0} \left[\frac{(x - x_0)^2}{2} \Big|_{x_0}^{x_1} \right] \\ &\approx \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)], \end{aligned}$$

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

$$\int_{a=x_0}^{b=x_1} f(x) dx \approx T_1(f) = \frac{h}{2} [f(x_0) + f(x_1)]. \quad (7)$$

Then $T_1(f)$ is called the *simple Trapezoidal rule* or the Trapezoidal rule for one trapezoid or one strip and can be used for the approximation of the definite integral (1). The reason for calling this formula the Trapezoidal rule is that when $f(x)$ is a function with positive values, the integral (1) is approximated by the area in the trapezoid, see Figure 3.

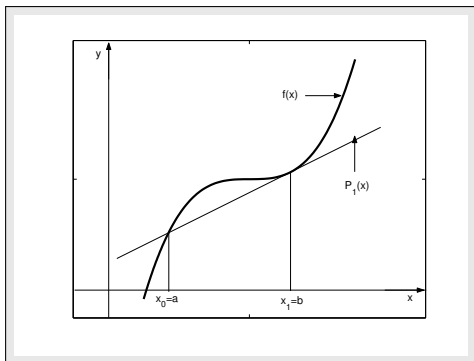


Figure: Simple Trapezoidal rule.

Example 0.1

Approximate the following integral

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

using the simple Trapezoidal rule and compute the absolute error.

Solution. Given $f(x) = \frac{1}{x+1}$ and $h = 1$, so using the simple Trapezoidal rule (7), gives

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

The exact solution of the given integral is

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

is the required absolute error. •

Composite Trapezoidal Rule

It is evident that the Newton-Cotes formulas produce accurate approximations to the definite integral (1) only when the limits a and b are close together, that is, the integration interval is not large. Formulas based on low-degree interpolating polynomials are clearly unsuitable since it is then necessary to use large values of h . Also, note that higher-order Newton-Cotes formulas will not necessarily produce more accurate approximations to the given integral. This difficulty can be avoided by using a piecewise approach; the integration interval is divided into subintervals and low-order formulas are applied on each of these. The corresponding integration rules are said to be in *composite form*, and the most suitable formula of this type make use of the Trapezoidal rule. The interval $[a, b]$ is partitioned into n subintervals (x_{i-1}, x_i) , $i = 1, 2, \dots, n$ with $a = x_0$ and $b = x_n$ of equal width $h = (b - a)/n$ and the rule for a single interval (the simple rule (7)) is applied to each subinterval or a grouping of subintervals (see Figure 4). Since the Trapezoidal rule requires only one interval for application, there is no restriction on the integer n . We define the composite Trapezoidal rule in the form of the following theorem.

Theorem 2

(Composite Trapezoidal Rule)

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

$$\int_{a=x_0}^{b=x_n} f(x)dx \approx T_n(f) = \frac{h}{2} \left[f(a) + 2 \sum_{i=1}^{n-1} f(x_i) + f(b) \right]. \quad (8)$$

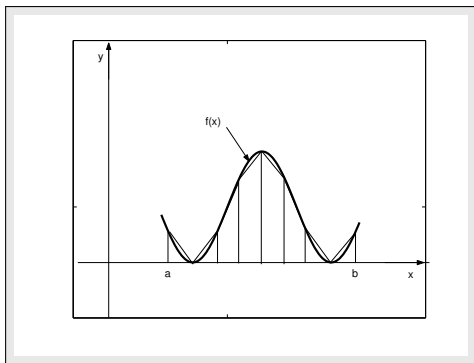


Figure: Composite Trapezoidal rule.

Example 0.2

Evaluate the integral $\int_0^1 e^{4x} dx$ by using the Trapezoidal rule with $n = 1, 2, 4, 8$.

Also compute the corresponding absolute errors.

Solution. For $n = 1$, we use the formula (7) for $h = 1$, as follows

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

For $n = 2$, using the formula (8) and $h = 0.5$, we have

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

For $n = 4$, using the formula (8) and $h = 0.25$, we have

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

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

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

Error Terms for Trapezoidal Rule

We discuss the error for the simple Trapezoidal rule (7) in the form of the following theorem and then we use it to define the error for the composite Trapezoidal rule (8).

Theorem 3

(Error term for Simple Trapezoidal Rule)

Let $f \in C^2[a, b]$, and $h = (b - a)$. The local error that the simple Trapezoidal rule (7) makes in estimating the definite integral (1) is

$$E_{T_1}(f) = -\frac{h^3}{12}f''(\eta(x)), \quad (9)$$

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

Example 0.3

Compute the *local error* for the Trapezoidal rule (7) using the integral

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

Solution. Given $f(x) = \frac{1}{x+1}$ and $[a, b] = [1, 2]$, then the second derivative of the function is

$$f''(x) = \frac{2}{(x+1)^3}.$$

Since the error formula for the simple Trapezoidal rule is

$$E_{T_1}(f) = -\frac{h^3}{12} f''(\eta(x)), \quad \text{where } \eta(x) \in (1, 2).$$

This formula cannot be computed exactly because $\eta(x)$ is not known. But one can bound the error by computing the largest possible value for $|f''(\eta(x))|$.

Bound $|f''(\eta(x))|$ on $[1, 2]$ is

$$M = \max_{1 \leq x \leq 2} \left| \frac{2}{(x+1)^3} \right| = 0.25.$$

Then, for $|f''(\eta(x))| \leq M$, we have

$$|E_{T_1}(f)| \leq \frac{h^3}{12} M.$$

Using $M = 0.25$ and $h = 1$, we get

$$|E_{T_1}(f)| \leq \frac{0.25}{12} = 0.0208.$$

Error Term for Composite Trapezoidal Rule

The *global error* of the Trapezoidal rule (8) equals the sum of n local errors of the Trapezoidal rule (7), that is

$$E_{T_n}(f) = -\frac{h^3}{12}f''(\eta_1(x)) - \frac{h^3}{12}f''(\eta_2(x)) - \cdots - \frac{h^3}{12}f''(\eta_n(x)),$$

which can also be written as

$$E_{T_n}(f) = -\frac{h^3}{12} \sum_{i=1}^n f''(\eta_i(x)), \quad \text{for } \eta_i(x) \in (x_{i-1}, x_i),$$

or

$$E_{T_n}(f) = -\frac{h^3}{12} n f''(\eta(x)),$$


where $f''(\eta(x))$ is the average of the n individual values of the second derivative.

Since $n = \frac{b-a}{h}$, thus the global error in the composite Trapezoidal rule (8) is

$$E_{T_n}(f) = -\frac{h^2}{12}(b-a)f''(\eta(x)), \quad \eta(x) \in (a, b). \quad (10)$$

Hence

$$\int_a^b f(x)dx = \frac{h}{2} \left[f(a) + 2 \sum_{i=1}^{n-1} f(x_i) + f(b) \right] - \frac{h^2}{12}(b-a)f''(\eta(x)), \quad (11)$$

for $\eta(x) \in (a, b)$, is the composite Trapezoidal rule with its error term. 

Note that whereas the simple Trapezoidal rule (7) has a truncation error of order h^3 , the composite Trapezoidal rule (8) has an error of order h^2 . This means that when h is halved and the number of subintervals is doubled the error decreases by a factor of approximately four (assuming that $f''(\eta(x))$ remains fairly constant throughout $[a, b]$). Of course, it is also possible to express the truncation error in terms of n rather than h . Since $h = \frac{b-a}{n}$, it follows that the global truncation error (10) is of order $O(n^2)$.

Example 0.4

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

(a) Compute the approximation of the integral using the composite Trapezoidal rule.

(b) Compute the error bound for your approximation using the formula (10).

(c) Compute the absolute error.

(d) How many subintervals approximate the given integral to an accuracy of at least 10^{-4} using the composite Trapezoidal rule?

Solution. (a) Given $f(x) = \ln(x+1)$, $n = 6$, and so $h = \frac{2-1}{6} = \frac{1}{6}$, then the composite Trapezoidal rule (8) for $n = 6$, can be written as

$$\begin{aligned} T_6(f) &= \frac{1/6}{2} \left[\ln(1+1) + 2 \left(\ln\left(\frac{7}{6} + 1\right) + \ln\left(\frac{8}{6} + 1\right) + \ln\left(\frac{9}{6} + 1\right) \right. \right. \\ &\quad \left. \left. + \ln\left(\frac{10}{6} + 1\right) + \ln\left(\frac{11}{6} + 1\right) \right) + \ln(2+1) \right]. \end{aligned}$$

Hence

$$\int_1^2 \ln(x+1)dx \approx T_6(f) = \frac{1}{12} [0.6932 + 2(4.5591) + 1.0986] = 0.9092.$$

(b) The second derivative of the function can be obtain as

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

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

$$M = \max_{1 \leq x \leq 2} |f''(x)| = \left| \frac{-1}{(x+1)^2} \right| = 0.25.$$

Thus the error formula (10) becomes

$$|E_{T_6}(f)| \leq \frac{(1/6)^2}{12} (0.25) = 0.0006,$$

which is the possible maximum error in our approximation in part (a).

(c) The absolute error $|E|$ in our approximation is given as

$$|E| = |(3 \ln 3 - 2 \ln 2 - 1) - T_6(f)| = |0.9095 - 0.9092| = 0.0003.$$

(d) To find the minimum subintervals for the given accuracy, we use the formula (10) such that

$$|E_{T_n}(f)| \leq \frac{|-(b-a)^3|}{12n^2} M \leq 10^{-4},$$

where $h = (b-a)/n$. Since $M = 0.25$, then solving for n^2 , we obtain

$$n^2 \geq 208.3333, \quad \text{gives} \quad n \geq 14.4338.$$

Hence to get the required accuracy, we need 15 subintervals.

Simple Simpson's Rule

The Trapezoidal rule approximates the area under a curve by the area of trapezoid formed by connecting two points on the curve by straight line. The **Simpson's rule** gives a more accurate approximation since it consists of connecting three points on the curve by second-degree parabola and the area under the parabola to obtain the **approximate area** under the curve, see Figure 5.

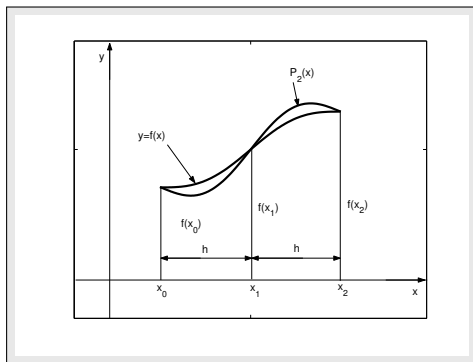


Figure: Simple Simpson's rule.

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

$$\begin{aligned} f(x) = p_2(x) &= \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \\ &+ \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2). \end{aligned}$$

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

$$\begin{aligned} \int_{x_0}^{x_2} f(x) dx &\approx \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} \int_{x_0}^{x_2} (x - x_1)(x - x_2) dx \\ &+ \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} \int_{x_0}^{x_2} (x - x_0)(x - x_2) dx \\ &+ \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)} \int_{x_0}^{x_2} (x - x_0)(x - x_1) dx, \end{aligned}$$

which implies that

$$\int_a^b f(x) dx \approx \frac{f(x_0)}{2h^2} I_1 + \frac{f(x_1)}{-h^2} I_2 + \frac{f(x_2)}{2h^2} I_3,$$

where

$$I_1 = \int_{x_0}^{x_2} (x - x_1)(x - x_2) dx; \quad I_2 = \int_{x_0}^{x_2} (x - x_0)(x - x_2) dx; \quad I_3 = \int_{x_0}^{x_2} (x - x_0)(x - x_1) dx.$$

Solving above three integrals by using *integration by parts*, we obtain the values of I_1, I_2 and I_3 as follows

$$I_1 = \frac{2h^3}{3}, \quad I_2 = -\frac{4h^3}{3}, \quad I_3 = \frac{2h^3}{3}.$$

By using these values, we have

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

Simplifying, gives

$$\int_a^b f(x)dx \approx S_2(f) = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]. \quad (12)$$

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

Example 0.5

Approximate the following integral

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

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

Solution. Since $f(x) = \frac{1}{x+1}$ and $h = (2-1)/2 = 0.5$, then by using Simpson's rule (12), we have

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

Hence

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

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

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

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

Example 0.6

Use simple Simpson's rule to show that

$$\int_1^{1.6} \frac{2}{x} dx < 1 < \int_1^{1.7} \frac{2}{x} dx.$$

Solution. Given $f(x) = \frac{2}{x}$ and take $h = (1.6 - 1)/2 = 0.3$, then by using Simpson's rule (12), we have

$$S_2(f) = \frac{0.3}{3} [f(1) + 4f(1.3) + f(1.6)] = (0.1)[2 + 6.1538 + 1.25] = 0.9404.$$

Now taking $h = (1.7 - 1)/2 = 0.35$, then by using Simpson's rule (12), we have

$$S_2(f) = \frac{0.35}{3} [f(1) + 4f(1.35) + f(1.7)] = (0.1167)[2 + 5.9260 + 1.1764] = 1.0623.$$

Hence

$$0.9404 < 1 < 1.0623,$$

the required result. •

Example 0.7

Let f be defined by

$$f(x) = \begin{cases} x^2 - x + 1, & \text{if } 0 \leq x \leq 1, \\ 2x - 1, & \text{if } 1 \leq x \leq 2. \end{cases}$$

Approximate the integral $\int_0^2 f(x)dx$ by using Simpson's rule with $n = 2$.

Solution. Since one can know that

$$\int_0^2 f(x)dx = \int_0^1 f(x)dx + \int_1^2 f(x)dx,$$

and we are given

$$\int_0^2 f(x)dx = \int_0^1 (x^2 - x + 1)dx + \int_1^2 (2x - 1)dx.$$

First we find the approximation of the first integral on the right hand side of above equation for $n = 2$, using the formula (12) and $h = 0.5$, we have

$$I_1(f) \approx \frac{0.5}{3} [f(0) + 4f(0.5) + f(1)] \approx \frac{0.5}{3} [1 + 3 + 1] \approx 0.8333.$$

Now we find the approximation of the second integral on the right hand side of above equation for $n = 2$, using the formula (12) and $h = 0.5$, we have

$$I_2(f) \approx \frac{0.5}{3} [f(1) + 4f(1.5) + f(2)] \approx \frac{0.5}{3} [1 + 8 + 3] \approx 2.0000.$$

Hence

$$\int_0^2 f(x)dx = I_1(f) + I_2(f) \approx 0.8333 + 2.000 = 2.83333,$$

the required approximation of the given integral. •

Composite Simpson's Rule

Just as with the simple Trapezoidal rule (7), the simple Simpson's rule (12) can be improved by dividing the integration interval $[a, b]$ into a number of subintervals of equal width h ; where $h = \frac{b-a}{n}$. Since the simple Simpson's rule (12) requires a interval consisting of three points (pair of strips). In practice, we usually take more than three points and add the separate results for the different pairs of strips (see Figure 6). Since the simple Simpson's rule requires a pair of strips for application, so there is restriction on the integer n , which must be even. We define the *composite Simpson's rule* in the form of the following theorem.

Theorem 4

(Composite Simpson's Rule)

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

$$\int_a^b f(x)dx \approx S_n(f) = \frac{h}{3} \left[f(a) + 2 \sum_{i=1}^{n/2-1} f(x_{2i}) + 4 \sum_{i=1}^{n/2} f(x_{2i-1}) + f(b) \right]. \quad (13)$$

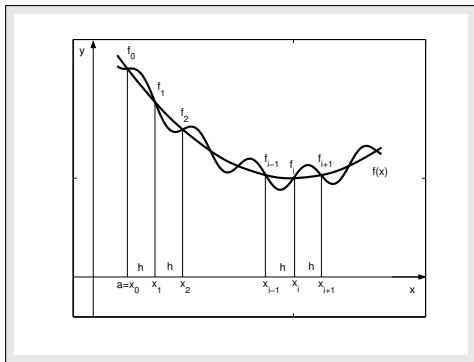


Figure: Composite Simpson's Rule.

Example 0.8

Let f be defined by

$$f(x) = \begin{cases} x^2 - x + 1, & \text{if } 0 \leq x \leq 1, \\ 2x - 1, & \text{if } 1 \leq x \leq 2. \end{cases}$$

Approximate the integral $\int_0^2 f(x)dx$ by using Simpson's rule with $n = 4$.

Solution. Since one can know that

$$\int_0^2 f(x)dx = \int_0^1 f(x)dx + \int_1^2 f(x)dx,$$

and we are given

$$\int_0^2 f(x)dx = \int_0^1 (x^2 - x + 1)dx + \int_1^2 (2x - 1)dx = I_1(f) + I_2(f).$$

First we find the approximation of the first integral on the right hand side of above equation for $n = 4$, using the formula (13) and $h = 0.25$, we have

$$I_1(f) \approx \frac{0.5}{3} [f(0) + 4(f(0.25) + f(0.75)) + 2f(0.5) + f(1)] \approx \frac{0.25}{3} [8] \approx 0.8333.$$

Now we find the approximation of the second integral on the right hand side of above equation for $n = 4$, using the formula (13) and $h = 0.25$, we have

$$I_2(f) \approx \frac{0.5}{3} [f(1) + 4(f(1.25) + f(1.75)) + 2f(1.5) + f(2)] \approx \frac{0.25}{3} [24] \approx 2.0000.$$

Hence

$$\int_0^2 f(x)dx = I_1(f) + I_2(f) \approx 0.8333 + 2.000 = 2.83333,$$

the required approximation of the given integral. •

Example 0.9

Suppose that $f(1) = 0.5$, $f(1.2) = 0.9$, $[f(1.25) + f(1.75)] = \alpha$, $f(1.5) = 1.5$, $f(1.6) = 1.65$, $f(1.95) = 1.95$ and $f(2) = 2$. Find the approximate value of α if the best composite Simpson's rule gives the value, 1.35, for the integral $\int_1^2 f(x) dx$.

Solution. Since we need the equally spaced data points, so we can take $x_0 = 1, x_1 = 1.25, x_2 = 1.5, x_3 = 1.75$ and $x_4 = 2$, gives $n = 4$, so $h = \frac{2-1}{4} = 0.25$. By using the composite formula (13) for $n = 4$, we have

$$\int_1^2 f(x) dx \approx \frac{0.25}{3} [f(1) + 4[f(1.25) + f(1.75)] + 2f(1.5) + f(2)].$$

Now using the given values, we obtain

$$1.35 \approx \frac{1}{12} [0.5 + 4(\alpha) + 2(1.5) + 2], \quad \text{or} \quad 12(1.35) - 5.5 \approx 4\alpha,$$

gives $\alpha \approx 2.675$. •

Error Terms for Simpson's Rule

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

Firstly: Error Term for Simple Simpson's Rule

Theorem 5

(Error Term for Simple Simpson's Rule)

Let $f \in C^4[a, b]$, and $h = (b - a)/2$. The local error that the Simpson's rule makes in estimating the definite integral (1) is

$$E_{S_2}(f) = -\frac{h^5}{90} f^{(4)}(\eta(x)), \quad (14)$$

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

Example 0.10

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

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

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

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

Since the error formula for the Simpson's rule is

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

or

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

This formula cannot be computed exactly because $\eta(x)$ is not known. But one can bound the error by computing the largest possible value for $|f^{(4)}|$. Bound $|f^{(4)}|$ on $[1, 2]$ is

$$M = \max_{1 \leq x \leq 2} = \left| \frac{24}{(x+1)^5} \right| = 0.75.$$

Then for $|f^{(4)}(\eta(x))| \leq M$, we have

$$|E_{S_2}(f)| \leq \frac{h^5}{90} M.$$

Taking $M = 0.75$ and $h = 0.5$, we get

$$|E_{S_2}(f)| \leq \frac{(0.03125)}{90} (0.75) = 0.0003.$$

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

Error Terms for Simpson's Rule

Secondly: Error Term for Composite Simpson's Rule

Since the composite Simpson's rule (13) requires that the given interval $[a, b]$ is divided into even number of subintervals and each application of the simple Simpson's rule requires two subintervals, therefore, the global error of the composite Simpson's rule (13) is the sum of $\frac{n}{2}$ local truncation error of the simple

Simpson's rule with $n = \frac{b-a}{h}$, that is,

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

which implies that

$$E_{S_n}(f) = -\frac{h^5}{90}\left(\frac{n}{2}\right) \left[\frac{\sum_{i=1}^{n/2} f^{(4)}(\eta_i(x))}{n/2} \right].$$

Thus by using the Intermediate Value Theorem, we have

$$E_{S_n}(f) = -\frac{(b-a)}{180}h^4 f^{(4)}(\eta(x)), \quad (15)$$

for $\eta(x) \in (a, b)$ and $nh = b - a$. Then the formula (15) is known as the *global error* of the Simpson's rule. •

Example 0.11

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

- (a) Find the approximation of the give integral using the composite Simpson's rule.
(b) Compute the error bound for the approximation using the formula (15).
(c) Compute the absolute error.
(d) How many subintervals approximate the given integral to an accuracy of at least 10^{-4} using the composite Simpson's rule ?

Solution. (a) Given $f(x) = \ln(x+1)$, $n = 6$, and so $h = \frac{2-1}{6} = \frac{1}{6}$, then the composite Simpson's rule (13) for $n = 6$, can be written as

$$\begin{aligned} S_6(f) &= \frac{1/6}{3} \left[\ln(1+1) + 4\left(\ln\left(\frac{7}{6}+1\right)\right) + \ln\left(\frac{9}{6}+1\right) + \ln\left(\frac{11}{6}+1\right) \right] \\ &+ \left[2\left(\ln\left(\frac{8}{6}+1\right)\right) + \ln\left(\frac{10}{6}+1\right) \right] + \ln(2+1). \end{aligned}$$

Hence

$$\int_1^2 \ln(x+1)dx \approx S_6(f) = \frac{1}{18} \left[0.6932 + 4(2.7309) + 2(1.8281) + 1.0986 \right] = 0.9095.$$

(b) Since the fourth derivative of the function is

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

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

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

Thus the error formula (15) becomes

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

which is the possible maximum error in our approximation in part (a).

(c) The absolute error $|E|$ in our approximation is given as

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

(d) To find the minimum subintervals for the given accuracy, we use the error formula (15) which is

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

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

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

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

Example 0.12

Determine the number of subintervals n required to approximate

$$I(f) = \int_0^2 \frac{1}{x+4} dx,$$

with an error less than 10^{-4} using Simpson's rule.

Solution. we have to use the error formula (15) which is

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

Given the integrand is $f(x) = \frac{1}{x+4}$, and we have $f^{(4)}(x) = \frac{24}{(x+4)^5}$. The maximum value of $|f^{(4)}(x)|$ on the interval $[0, 2]$ is $3/128$, and thus $M = \frac{3}{128}$. Using the above error formula, we get

$$\frac{3}{(90 \times 128)} h^4 \leq 10^{-4}, \quad \text{or} \quad h \leq \frac{2}{5} \sqrt[4]{15} = 0.7872.$$

Since $n = \frac{2}{h} = \frac{2}{0.7872} = 2.5407$, so the number of even subintervals n required is $n \geq 4$.

Summary

In this lecture, we ...

- ▶ discussed Trapezoidal and Simpson's rules for numerical integration.