Lecture No. 39
Numerical Integration

To evaluate the definite integral of certain functions whose anti derivatives cannot be found easily or in more practical situations the integrand is expressed in tabular form, numerical techniques provide efficient way to approximate the definite integral.

A definite integral $\int_a^b f(x)dx$ can be interpreted as area under the curve $y = f(x)$ bounded by the x-axis and the line $x = a$ and $x = b$. In numerical integration to approximate the definite integral, we estimate the area under the curve by evaluating the integrand $f(x)$ at a set of distinct points $(x_0, x_1, ..., x_n)$, where $x_i \in [a,b]$ for $0 \le i \le n$. Of course, we assume that the function to be integrated is continuous on $[a,b]$.

Integration Methods

The commonly used integration methods can be classified into two groups: the Newton-Cotes formulae that employ functional values at equally spaced points, and the Gaussian quadrature formulae that employ unequally spaced points.

Closed Newton-Cotes Quadrature Formula

The method of integration will be based on interpolation polynomial $P_n(x)$ of degree n appropriate for a given function. When this polynomial $P_n(x)$ is used to approximate $f(x)$ over $[a,b]$, and then the integral of $f(x)$ is approximated by the integral of $P_n(x)$, the resulting formula is called a Newton-Cotes quadrature formula. When the sample points $x_0 = a$ and $x_n = b$ are used, it is called a closed Newton-Cotes formula. Thus the idea of Newton-Cotes formulas is to replace a complicated function or tabulated data with an approximating function that is easy to integrate.

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

where $P_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$

The next result gives the formulae when approximating polynomials of degree n=1, 2 are used.

Theorem

Assume that $x_k = x_0 + kh,$ are equally spaced nodes and $f_k = f(x_k)$. The first two closed Newton-Cotes quadrature formulae:

(1) Trapezoidal Rule $\int_{x_0}^{x_1} f(x)dx \approx \frac{h}{2}\left(f(x_0) + f(x_1) \right)$

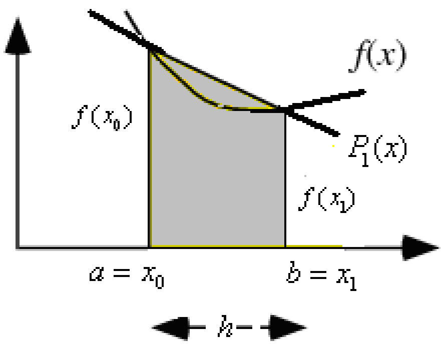
(2) Simpson's Rule $\int_{x_0}^{x_2} f(x)dx \approx \frac{h}{3}\left(f(x_0)+4f(x_1)+f(x_2)\right)$

The Trapezoidal Rule

One of the simplest ways to estimate an integral $I=\int_a^b f(x)dx$ is to employ linear interpolation, i.e., to approximate the curve $y=f(x)$ by a straight line $y=P_1(x)$ also called secant line passing through the points $(a, f(a))$ and $(b, f(b))$ and then to compute the area under the line i.e. area is approximated by the trapezium formed by replacing the curve with its secant line drawn between the end points $(a, f(a))$ and $(b, f(b))$.

Let $a=x_0$, $b=x_1$, and $h=x_1-x_0$. To approximate

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx \approx \int_{x_0}^{x_1} P_1(x)dx$$



Now the area of trapezoid is the product of its altitude and the average length of its parallel sides. The area of trapezoid with altitude x_1-x_0 is

$$(x_1-x_0)\left(\frac{f(x_0)+f(x_1)}{2}\right)$$

$$=\frac{h}{2}\left(f(x_0)+f(x_1)\right)$$

Thus $\int_{x_0}^{x_1} f(x)dx \approx \frac{h}{2}\left(f(x_0)+f(x_1)\right)$

Note: the error term involved in trapezoidal rule is

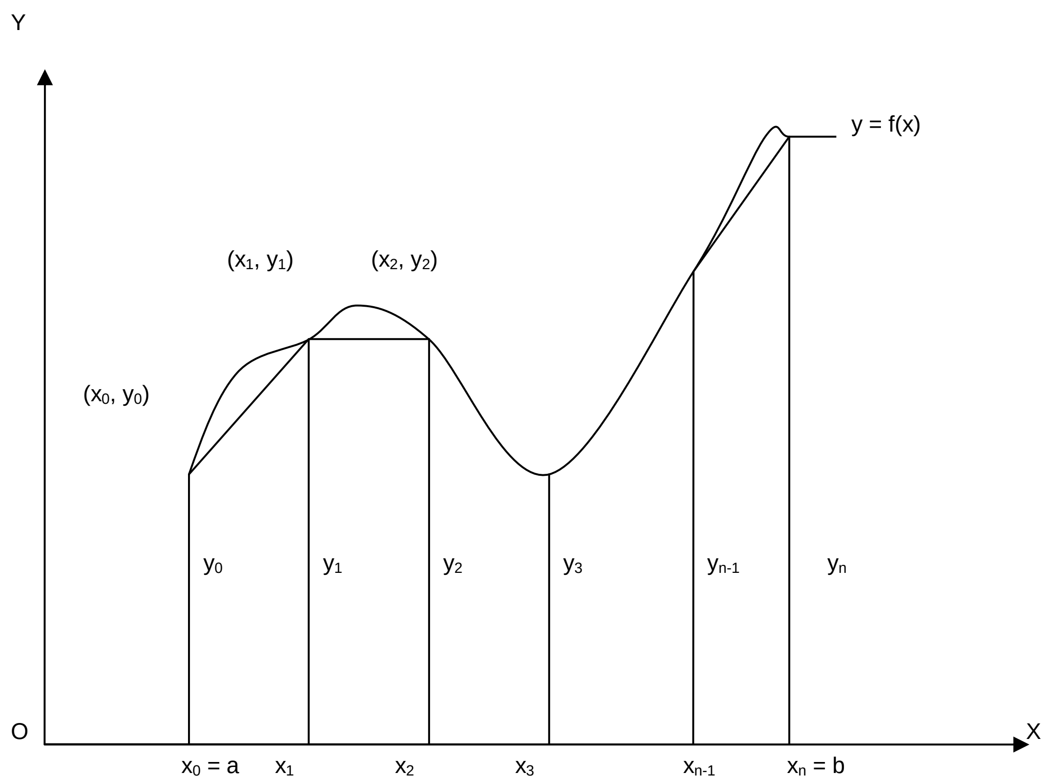
$$=-\frac{h^3}{12}f''(\xi), \quad \xi\in[x_0,x_1]$$

Thus the trapezoidal rule with error term is

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}\left(f(x_0)+f(x_1)\right)-\frac{h^3}{12}f''(\xi)$$

The Trapezoidal Rule (Composite Form)

In order to evaluate the definite integral $I = \int_a^b f(x)dx$ we divide the interval $[a,b]$ into n sub-intervals, each of size $h = \dfrac{b-a}{n}$ and denote the sub-intervals by $[x_0, x_1],[x_1, x_2], \ldots,[x_{n-1}, x_n]$, such that $x_0 = a,\ x_n = b,$ and $x_k = x_0 + kh,\ k = 1, 2, \ldots, n$ and then use the trapezoidal rule on each subinterval



Thus, we can write the above definite integral as a sum. Therefore,

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

The area under the curve in each sub-interval is approximated by a trapezium. The integral I, which represents an area between the curve $y = f(x)$, the x-axis and the ordinates at $x = x_0,\ x = x_n$ is obtained by adding all the trapezoidal areas in each sub-interval. Now, using the trapezoidal rule into equation:

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(y_0 + y_1) - \frac{h^3}{2} y''(\xi)$$

We get

$$I = \int_{x_0}^{x_n} f(x)dx = \frac{h}{2}(y_0 + y_1) - \frac{h^3}{2} y''(\xi_1) + \frac{h}{2}(y_1 + y_2) - \frac{h^3}{12} y''(\xi_2)$$
$$+ \cdots + \frac{h}{2}(y_{n-1} + y_n) - \frac{h^3}{12} y''(\xi_n)$$

Where $x_{k-1} < \xi < x_k$, for $k = 1, 2, ..., n-1$.
Thus, we arrive at the result

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n) + E_n$$

Where the error term En is given by

$$E_n = -\frac{h^3}{12}[y''(\xi_1) + y''(\xi_2) + \cdots + y''(\xi_n)]$$

Equation represents the trapezoidal rule over $[x_0, x_n]$, which is also called the composite form of the trapezoidal rule. The error term given by Equation:

$$E_n = -\frac{h^3}{12}[y''(\xi_1) + y''(\xi_2) + \cdots + y''(\xi_n)]$$
$$= -\frac{h^3}{12}\sum_{k=1}^{n} y''(\xi_k), \quad \xi_k \in (x_{k-1}, x_k)$$

is called the global error.
However, if we assume that $y''(x)$ is continuous over $[x_0, x_n]$ then there exists some ξ in $[x_0, x_n]$ such that and $x_n = x_0 + nh$ and the maximum error incurred in the approximate value obtained by trapezoidal rule is

$$E_n = -\frac{h^3 M}{12n^2} \quad \text{where} \quad M = \max\left| f''(\xi) \right|, \quad \xi \in [x_0, x_n]$$

Example (The Trapezoidal Rule):

Evaluate the integral $I = \int_0^1 \frac{dx}{1+x^2}$, by using Trapezoidal rule, take $h = \frac{1}{4}$.

Solution

At first, we shall tabulate the function as

x	0	1/4	1/2	3/4	1
$y = \frac{1}{1+x^2}$	1	0.9412	0.8000	0.6400	0.5000

Using trapezoidal rule, and taking $h = \frac{1}{4}$

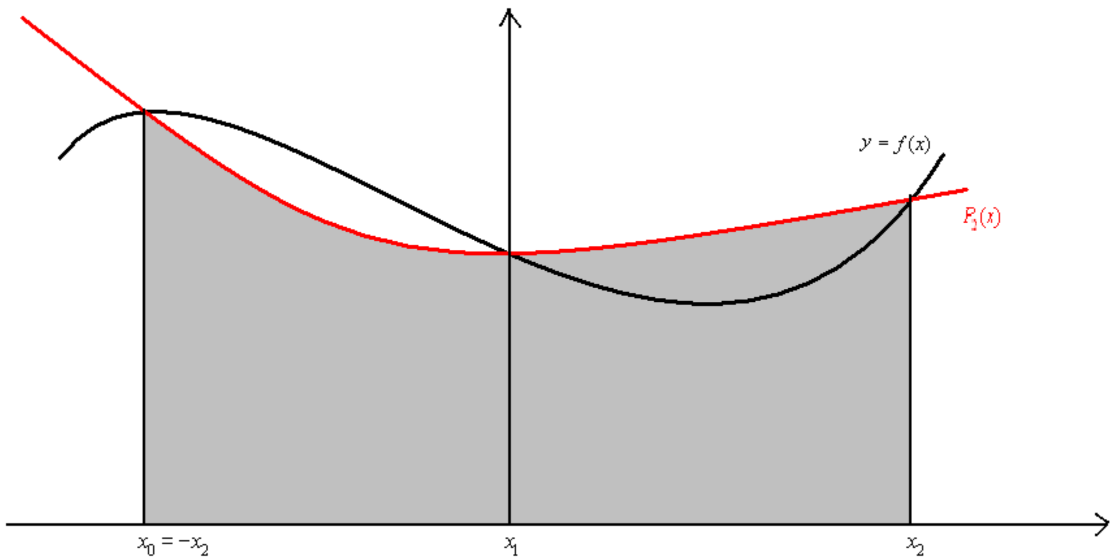
$$I = \int_0^1 \frac{dx}{1+x^2},$$
$$= \frac{h}{2}[y_0 + 2(y_1 + y_2 + y_3) + y_4]$$
$$= \frac{1}{8}[1 + 2(0.9412 + 0.8000 + 0.6400) + 0.5000]$$
$$= \frac{1}{8}[1 + 2(2.3812) + 0.5000]$$
$$= \frac{1}{8}[1 + 2(2.3812) + 0.5000]$$
$$= \frac{1}{8}[6.2624]$$
$$= 0.7828$$

But the closed form solution to the given integral is

$$\int_0^1 \frac{dx}{1+x^2} = \left[\tan^{-1} x\right]_0^1$$
$$= \frac{\pi}{4} = 0.7854$$

Simpson's 1/3 Rule

The trapezoidal rule tries to simplify integration by approximating the function to be integrated by a straight line or a series of straight line segments. In Simpson's rule we try to approximate by a series of parabolic segments, hoping that the parabola will more closely match a given curve $y = f(x)$, than would the straight line in the trapezoidal rule. To estimate $I = \int_a^b f(x)dx$, the curve $y = f(x)$, is approximated by a parabola $y = P_2(x)$ passing through three points $(x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2))$ and then the area under the parabolic segment is computed. We assume that x_1 coincides with the origin so that $x_0 = -x_2$ and parabola is $P_2(x) = ax^2 + bx + c$



$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx \approx \int_{x_0}^{x_2} P_2(x)dx$$

$$a = x_0,\ x_1 = x_0 + h \ \ and \ \ x_2 = x_0 + 2h = b$$

$$\int_{x_0}^{x_2} P_2(x)dx = \int_{-x_2}^{x_2} P_2(x)dx$$

$$= \int_{-x_2}^{x_2} (ax^2 + bx + c)dx$$

$$= \frac{ax^3}{3}\Bigg|_{-x_2}^{x_2} + \frac{bx^2}{2}\Bigg|_{-x_2}^{x_2} + cx\Big|_{-x_2}^{x_2}$$

$$= \frac{ax^3}{3}\Bigg|_{-x_2}^{x_2} + \frac{bx^2}{2}\Bigg|_{-x_2}^{x_2} + cx\Big|_{-x_2}^{x_2}$$

$$= \frac{ax_2^{\ 3}}{3} + \frac{ax_2^{\ 3}}{3} + \frac{bx_2^{\ 2}}{2} - \frac{bx_2^{\ 2}}{2} + cx_2 + cx_2$$

$$= \frac{2ax_2^{\ 3}}{3} + 2cx_2$$

$$= \frac{x_2}{3}(2ax_2^{\ 2} + 6c) \qquad ....(1)$$

We also have

$$h = x_1 - x_0 = 0 - (-x_2) = x_2$$
$$f(x_0) = f(-x_2) = ax_2^{\,2} - bx_2 + c = ah^2 - bh + c$$
$$f(x_1) = f(0) = c$$
$$f(x_2) = ax_2^{\,2} + bx_2 + c = ah^2 + bh + c$$
$$f(x_0) + f(x_2) = 2ah^2 + 2c$$

and so

$$f(x_0) + 4f(x_1) + f(x_2) = 2ah^2 + 6c$$

Substituting this in the area formula (1), we have

$$\int_{x_0}^{x_2} P_2(x)dx = \frac{h}{3}(2ah^2 + 6c)$$
$$= \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right)$$

Thus $\int_{x_0}^{x_2} f(x)dx \approx \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right)$

Note: the error term involved in Simpson's 1/3 rule is

$$= -\frac{h^5}{90} f^{(iv)}(\xi), \quad \xi \in [x_0, x_1]$$

Thus the Simpson's 1/3 rule with error term is

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right) - \frac{h^5}{90} f^{(iv)}(\xi)$$

or

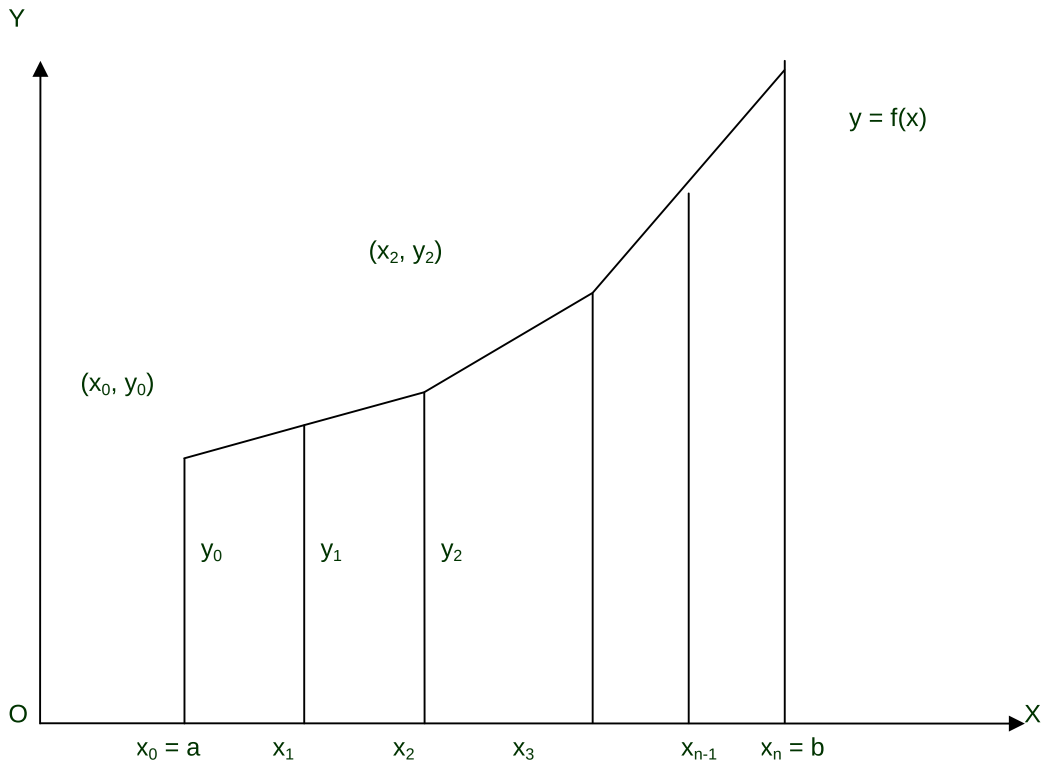
$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(y_0 + 4y_1 + y_2) - \frac{h^5}{90} y^{(iv)}(\xi)$$

Simpson's 1/3 Rule (Composite Form)

In deriving equation,

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(y_0 + 4y_1 + y_2) - \frac{h^5}{90} y^{(iv)}(\xi)$$

Geometrically, this equation represents the area between the curve $y = f(x)$, the x-axis and the ordinates at $x = x_0$ and x_2 after replacing the arc of the curve between (x_0, y_0) and (x_2, y_2) by an arc of a quadratic polynomial as in the figure.



In Simpson's 1/3 rule, we have used two sub-intervals of equal width. In order to get a composite formula, we shall divide the interval of integration [a, b] into an even number of sub intervals say 2N, each of width (b – a)/2N, thereby we have

$$x_0 = a, x_1, \ldots, x_{2N} = b \text{ and } x_k = x_0 + kh, \quad k = 1, 2, \ldots, (2N-1)$$

Thus, the definite integral I can be written as

$$I = \int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{2N-2}}^{x_{2N}} f(x)dx$$

Applying Simpson's 1/3 rule as in equation

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(y_0 + 4y_1 + y_2) - \frac{h^5}{90} y^{(iv)}(\xi)$$

to each of the integrals on the right-hand side of the above equation, we obtain

$$I = \frac{h}{3}[(y_0 + 4y_1 + y_2) + (y_2 + 4y_3 + y_4) + \cdots$$
$$+ (y_{2N-2} + 4y_{2N-1} + y_{2N})] - \frac{N}{90} h^5 y^{(iv)}(\xi)$$

That is

$$\int_{x_0}^{x_{2N}} f(x)dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + \cdots + y_{2N-1}) + 2(y_2 + y_4 + \cdots + y_{2N-2}) + y_{2N}] + \text{Error term}$$

This formula is called composite Simpson's 1/3 rule. The error term E, which is also called global error, is given by

$$E = -\frac{N}{90}h^5 y^{(iv)}(\xi) = -\frac{x_{2N} - x_0}{180}h^4 y^{(iv)}(\xi)$$

for some ξ in $[x_0, x_{2N}]$.

Example (Simpson's 1/3 Rule):

Estimate the value of $\int_1^5 \ln x dx$ using Simpson's 1/3 rule. Also, obtain the value of h, so that the value of the integral will be accurate up to five decimal places.

Solution Let for number of sub-intervals $2N = 8$, and $x_{2N} = 5$, $x_0 = 1$

$$h = \frac{x_{2N} - x_0}{2N}$$

$$= \frac{5-1}{8} = 0.5$$

k	$x_k = x_0 + kh$	$y = f(x) = \ln x$
1	$x_1 = 1+1*0.5 = 1.5$	$y_1 = f(x_1) = \ln x_1 = \ln 1.5 = 0.4055$
2	$x_2 = 1+2*0.5 = 2$	$y_2 = f(x_2) = \ln x_2 = \ln 2.0 = 0.6931$
3	$x_3 = 1+3*0.5 = 2.5$	$f(x_3) = 0.9163$
4	$x_4 = 3.0$	$y_4 = 1.0986$
5	$x_5 = 3.5$	$f(x_5) = 1.2528$
6	$x_6 = 4.0$	1.3863
7	$x_7 = 4.5$	1.5041
8	$x_8 = 5$	1.6094

Now using Simpson's 1/3 rule,

$$\int_1^5 \ln x dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5 + y_7) + 2(y_2 + y_4 + y_6) + y_8]$$

$$= \frac{0.5}{3}[0 + 4(0.4055 + 0.9163 + 1.2528 + 1.5041)$$

$$+ 2(0.6931 + 1.0986 + 1.3863) + 1.6094]$$

$$= \frac{0.5}{3}[0 + 4(4.0786) + 2(3.178) + 1.6094]$$

$$= \frac{0.5}{3}(24.2798) = 4.0466$$

The error in Simpson's rule is given by

$$E = -\frac{x_{2N} - x_0}{180} h^4 y^{(iv)}(\xi)$$

(ignoring the sign)

Since

$$y = \ln x, y' = \frac{1}{x}, y'' = -\frac{1}{x^2}, y''' = \frac{2}{x^3}, y^{(iv)} = -\frac{6}{x^4}$$

$$\underset{1 \le x \le 5}{Max} \quad y^{(iv)}(x) = 6,$$

$$\underset{1 \le x \le 5}{Min} \quad y^{(iv)}(x) = 0.0096$$

Therefore, the error bounds are given by

$$\frac{(0.0096)(4)h^4}{180} < E < \frac{(6)(4)h^4}{180}$$

If the result is to be accurate up to five decimal places, then

$$\frac{24h^4}{180} < 10^{-5}$$

That is, $h^4 < 0.000075$ or $h < 0.09$. It may be noted that the actual value of integrals is

$$\int_1^5 \ln x dx = [x \ln x - x]_1^5 = 5 \ln 5 - 4 = 4.0472$$

Example (Simpson's 1/3 Rule):

Evaluate the integral $I = \int_0^1 \frac{dx}{1+x^2}$, by using Simpson's 1/3 rule, take $h = \frac{1}{4}$.

Solution

At first, we shall tabulate the function as

X	0	¼	½	¾	1
$y = 1/ 1+x^2$	1	0.9412	0.8000	0.6400	0.5000

Using Simpson's 1/3 rule, and taking $h = \frac{1}{4}$, we have

$$I = \int_0^1 \frac{dx}{1+x^2},$$

$$= \frac{h}{3}\left[y_0 + 4(y_1 + y_3) + 2y_2 + y_4\right]$$

$$= \frac{1}{12}\left[1 + 4(0.9412 + 0.6400) + 2(0.8000) + 0.5000\right]$$

$$= \frac{1}{12}\left[1 + 4(1.5812) + 1.6 + 0.5000\right]$$

$$= \frac{1}{12}\left[9.4248\right]$$

$$= 0.7854$$

Exercise

Evaluate the following integrals by using
(i) Trapezoidal rule
(ii) Simpson's 1/3 rule

1. $\int_0^4 x^2 dx, \quad h = 1/2$
2. $\int_1^3 \frac{1}{x} dx, \quad h = 1/5$