

NUMERICAL INTEGRATION

①

(Given a set of data points $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ of a function $y=f(x)$ where $f(x)$ is not known explicitly, it is required to compute the value of the definite integral

$$I = \int_a^b y dx \quad \text{--- ①}$$

We derive a general formula for numerical integration using Newton's forward difference formula.

Let the interval $[a, b]$ be divided into n equal subintervals such that $a = x_0 < x_1 < \dots, x_n = b$. Clearly, $x_n = x_0 + nh$, where, $h = x_1 - x_0 = x_2 - x_1, \dots, x_n - x_{n-1}$.

Hence, the integral in equation ① becomes

$$I = \int_{x_0}^{x_n} y dx$$

Now, approximating y by Newton's forward difference formula, we obtain,

$$I = \int_{x_0}^{x_n} \left[y_0 + p \Delta y_0 + \frac{p(p-1)}{2} \Delta^2 y_0 + \frac{p(p-1)(p-2)}{6} \Delta^3 y_0 + \dots \right] dx$$

Since, $x = x_0 + ph$, then $dx = h dp$ and hence the above integration becomes

$$I = h \int_0^n \left[y_0 + p \Delta y_0 + \frac{p(p-1)}{2} \Delta^2 y_0 + \frac{p(p-1)(p-2)}{6} \Delta^3 y_0 + \dots \right] dp$$

(2)

Explanation for the change of limit:

we have, $x = x_0 + ph$.

$$\Rightarrow p = \frac{x - x_0}{h}$$

Now, as $x \rightarrow x_0$, $p \rightarrow 0$.

and, as $x \rightarrow x_n$, $p \rightarrow \frac{x_n - x_0}{h}$.

$$\text{i.e. } \frac{x_0 + nh - x_0}{h}$$

$$\therefore p \rightarrow n.$$

So, the new limits become 0 to n.

$$\begin{aligned} \text{Now, } I &= h \left[py_0 + \frac{p^2}{2} \Delta y_0 + \frac{1}{2} \left(\frac{p^3}{3} - \frac{p^2}{2} \right) \Delta^2 y_0 \right. \\ &\quad \left. + \frac{1}{6} \left(\frac{p^4}{4} - 3 \times \frac{p^3}{3} + 2 \times \frac{p^2}{2} \right) \Delta^3 y_0 + \dots \right]_0^n \\ &= h \left[py_0 + \frac{p^2}{2} \Delta y_0 + \frac{p^2(2p-3)}{12} \Delta^2 y_0 + \frac{p^2(p^2-4p+4)}{24} \Delta^3 y_0 + \dots \right]_0^n \\ &= h \left[ny_0 + \frac{n^2}{2} \Delta y_0 + \frac{n^2(2n-3)}{12} \Delta^2 y_0 + \frac{n^2(n^2-4n+4)}{24} \Delta^3 y_0 + \dots \right] \\ &= nh \left[y_0 + \frac{n}{2} \Delta y_0 + \frac{n(2n-3)}{12} \Delta^2 y_0 + \frac{n(n-2)^2}{24} \Delta^3 y_0 + \dots \right] \end{aligned}$$

$$\int_{x_0}^{x_n} y dx = nh \left[y_0 + \frac{n}{2} \Delta y_0 + \frac{n(2n-3)}{12} \Delta^2 y_0 + \frac{n(n-2)^2}{24} \Delta^3 y_0 + \dots \right] \quad (2)$$

From the above general formula, given in equation (2), we can obtain different integration formulae by putting $n=1, 2, 3, \dots$ etc.

① Trapezoidal rule:

Setting $n=1$ in the general formula given in equation (2), all differences higher than the first will become zero and we obtain,

$$\int_{x_0}^{x_1} y dx = h \left[y_0 + \frac{1}{2} \Delta y_0 \right]$$

$$= h \left[y_0 + \frac{1}{2} (y_1 - y_0) \right]$$

$$= h \left[y_0 + \frac{1}{2} y_1 - \frac{1}{2} y_0 \right]$$

$$= h \left[\frac{1}{2} y_0 + \frac{1}{2} y_1 \right]$$

$$= \frac{h}{2} (y_0 + y_1)$$

$\because \Delta y_0 = y_1 - y_0$

$$\therefore \int_{x_0}^{x_1} y dx = \frac{h}{2} (y_0 + y_1)$$

Similarly, for the next interval, $[x_1, x_2]$, we obtain

$$\int_{x_1}^{x_2} y dx = \frac{h}{2} (y_1 + y_2)$$

and so on.

For the last interval $[x_{n-1}, x_n]$, we have,

$$\int_{x_{n-1}}^{x_n} y dx = \frac{h}{2} (y_{n-1} + y_n)$$

Combining all the above expressions, we obtain the rule,

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

$$\therefore \int_{x_0}^{x_n} y dx = \frac{h}{2} [y_0 + 2(y_1 + y_2 + \dots + y_{n-1}) + y_n]$$

③

which is known as the trapezoidal rule.

The total error of the trapezoidal formula

is given by

$$E_1 = -\frac{1}{12} h^3 (y_0'' + y_1'' + \dots + y_{n-1}'')$$

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Assuming that $y''(\bar{x})$ is the largest value of the n quantities on the right hand side of eqⁿ ④

we obtain,

$$E_1 = -\frac{1}{12} h^3 n y''(\bar{x}) = -\frac{b-a}{12} h^2 y''(\bar{x}) \left[\because h = \frac{b-a}{n} \right]$$

(2) Simpson's $\frac{1}{3}$ - Rule :

This rule is obtained by putting $n=2$ in eqⁿ (2), and proceeding in the same manner as in the trapezoidal formula derivation, we get,

$$\int_{x_0}^{x_n} y \, dx = \frac{h}{3} [y_0 + 4(y_1 + y_3 + y_5 + \dots + y_{n-1}) + 2(y_2 + y_4 + \dots + y_{n-2}) + y_n]$$

which is the Simpson's $\frac{1}{3}$ - rule or simply Simpson's rule.

The error in this formula is given by.

$$E_2 = -\frac{b-a}{180} h^4 y^{iv}(\bar{x})$$

where $y^{iv}(\bar{x})$ is the largest value of the fourth derivatives.

(3) Simpson's $\frac{3}{8}$ - Rule :

Setting $n=3$ in equation (2) and proceeding the same manner as in the above two methods, we get,

$$\int_{x_0}^{x_n} = \frac{3h}{8} [y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \dots + 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n]$$

which is the Simpson's $3/8$ rule, it is not so accurate as Simpson's rule.

Example: Evaluate $I = \int_0^1 \frac{1}{1+x} dx$,

correct to three decimal places using

(i) trapezoidal rule (ii) Simpson's rule, Take $h=0.5$.

Solution: — Here, $h=0.5$.

$$x_0 = 0, x_1 = 0.5, x_2 = 1.0$$

$$\text{and } y_0 = 1.0000, y_1 = 0.6667,$$

$$y_2 = 0.5000.$$

$$\begin{cases} y = \frac{1}{1+x} \\ \text{at } x_0 = 0, \\ y_0 = \frac{1}{1+0} = 1 \end{cases}$$

(i) Using Trapezoidal rule we have,

$$I = \frac{h}{2} [y_0 + 2y_1 + y_2]$$

$$= \frac{0.5}{2} [1.0000 + 2(0.6667) + 0.5000]$$

$$= 0.70835$$

(ii) Using Simpson's rule we have,

$$I = \frac{h}{3} [y_0 + 4y_1 + y_2] = \frac{0.5}{3} [1.0000 + 4(0.6667) + 0.5]$$

$$= 0.6945.$$

To do: Evaluate the same integral i.e

$$I = \int_0^1 \frac{1}{1+x} dx$$
 correct to three decimal places
using both trapezoidal and Simpson's rules,
taking $h = 0.25$ and 0.125 respectively.