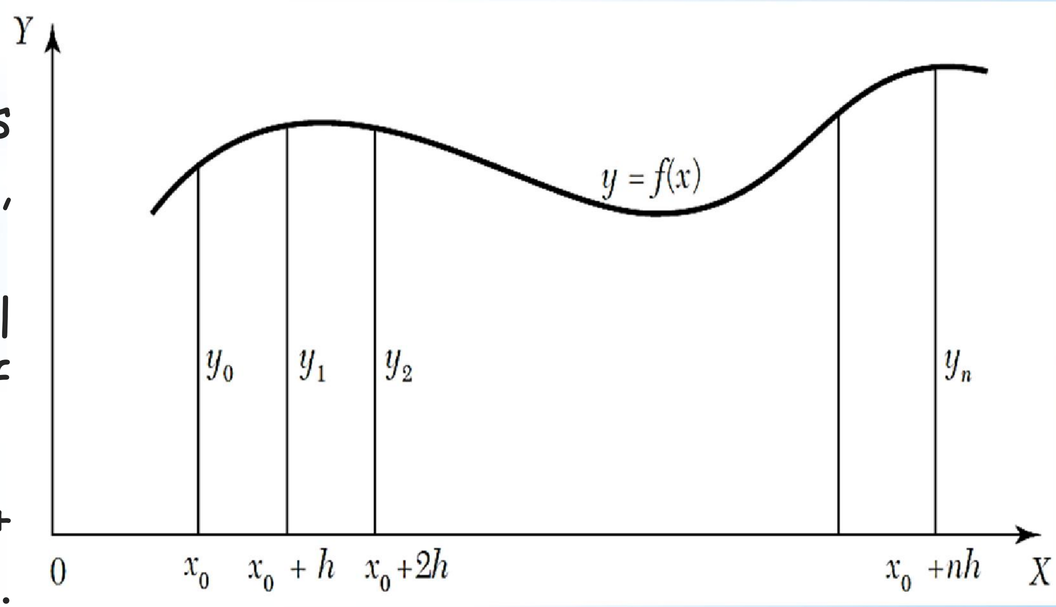
NUMERICAL INTEGRATION

The process of evaluating a definite integral from a set of tabulated values of the integrand f(x) is called numerical integration.

This process when applied to a function of a single variable, is known as quadrature.

Newton-Cotes Quadrature Formula

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



where f(x) takes the values $y_0, y_1, y_2, \ldots\ldots y_n$ for $x = x_0, x_1, x_2, \ldots\ldots. x_n$.

Let us divide the interval (a, b) into n sub-intervals of width h so that

$x_0 = a$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, ……. ., $x_n = x_0 + nh = b$. Then

$$I=\int_{x_0}^{x_{0+nh}} f(x)dx = h\int_0^n f(x_0+rh)dr,$$ Putting $x = x_0 + rh$, $dx = hdr$

$$= h\int_0^n \Big[y_0 + r\Delta y_0 + \frac{r(r-1)}{2!}\Delta^2 y_0 + \frac{r(r-1)(r-2)}{3!}\Delta^3 y_0$$

$$+\frac{r(r-1)(r-2)(r-3)}{4!}\Delta^4 y_0 + \frac{r(r-1)(r-20(r-3)(r-4)}{5!}\Delta^5 y_0$$

$$+\frac{r(r-1)(r-2)(r-3)(r-4)(r-5)}{6!}\Delta^6 y_0 + \dots\Big]dr$$

[by Newton's forward interpolation formula]

Integrating term by term, we obtain

$$\int_{x_0}^{x_0+nh} f(x)dx = nh\Bigg[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0$$

$$+\left(\frac{n^4}{5} - \frac{3n^3}{2} + \frac{11n^2}{3} - 3n\right)\frac{\Delta^4 y_0}{4!} + \left(\frac{n^5}{6} - 2n^4 + \frac{34n^3}{4} - \frac{50n^2}{3} + 12n\right)\frac{\Delta^5 y_0}{5!}$$

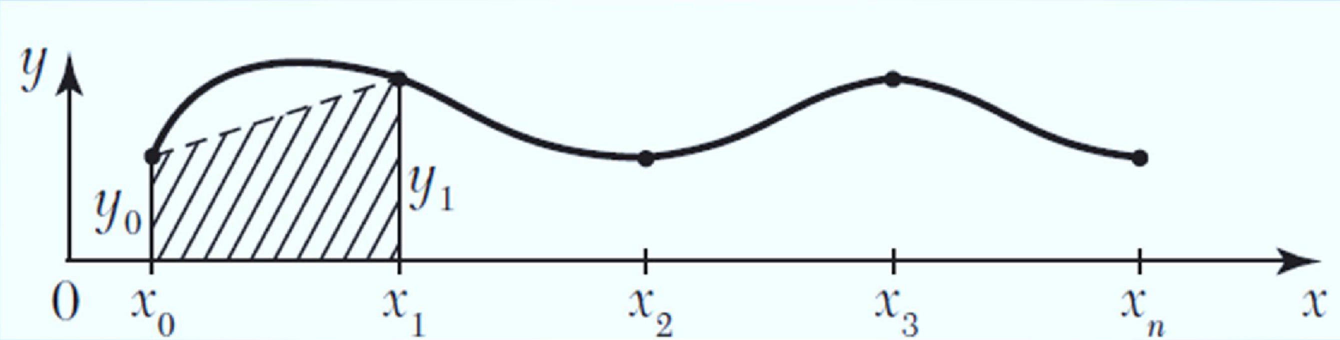
$$+\left(\frac{n^6}{7} - \frac{15n^5}{6} + 17n^4 - \frac{225n^3}{4} + \frac{274n^2}{3} - 60n\right)\frac{\Delta^6 y_0}{6!} + \dots\Bigg]$$

This is known as *Newton-Cotes quadrature formula*.

From this general formula, we deduce the following important quadrature rules by taking $n = 1, 2, 3, \ldots$.

Trapezoidal rule

Putting n = 1 in *Newton-Cotes quadrature formula and* the curve between point (x_0, y_0) and (x_1, y_1) approximate as a straight line i.e., a polynomial of first order so that differences of order higher than first become zero, we get



$$\int_{x_0}^{x_0+h} f(x)dx = h\left(y_0 + \frac{1}{2}\Delta y_0\right) = \frac{h}{2}(y_0 + y_1)$$

Similarly
$$\int_{x_0+h}^{x_0+2h} f(x)dx = h\left(y_1 + \frac{1}{2}\Delta y_1\right) = \frac{h}{2}(y_1 + y_2)$$

....

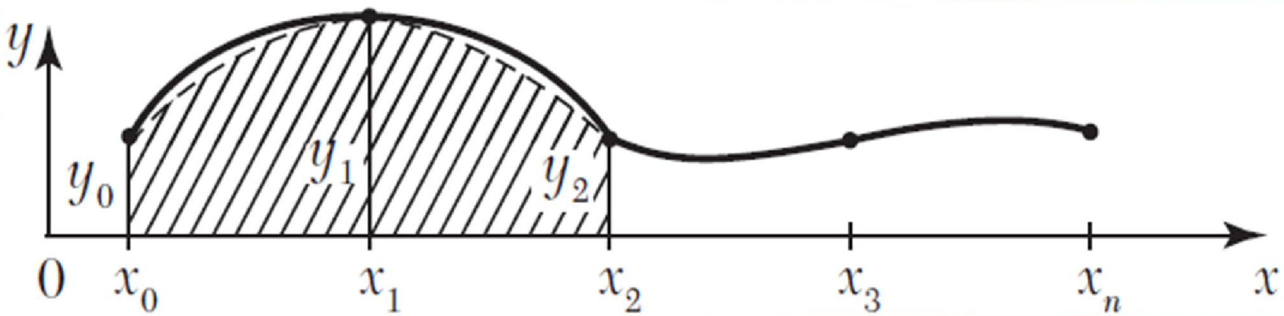
$$\int_{x_0+(n-1)}^{x_0+nh} f(x)dx = \frac{h}{2}(y_{n-1} + yn)$$

Adding these n integrals, we obtain
$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{h}{2}[(y_0 + y_n) + 2(y_1 + y_2 + \cdots + y_{n\text{-}1})]$$

This is known as the trapezoidal rule.

Simpson's one-third rule

Putting n = 2 in cot's formula and the curve through (x_0, y_0), (x_1, y_1), and (x_2, y_2) approximates as a parabola, i.e., a polynomial of the second order so that differences of order higher than the second vanish, we get



$$\int_{x_0}^{x_0+2h} f(x)dx = 2h(y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0) = \frac{h}{3}(y_0 + 4y_1 + y_2)$$

Similarly $$\int_{x_0+2h}^{x_0+4h} f(x)dx = \frac{h}{3}(y_2 + 4y_3 + y_4)$$

....

$$\int_{x_0+(n-2)h}^{x_0+nh} f(x)dx = \frac{h}{3}(y_{n-2} + 4y_{n-1} + y_n),$$ n being even

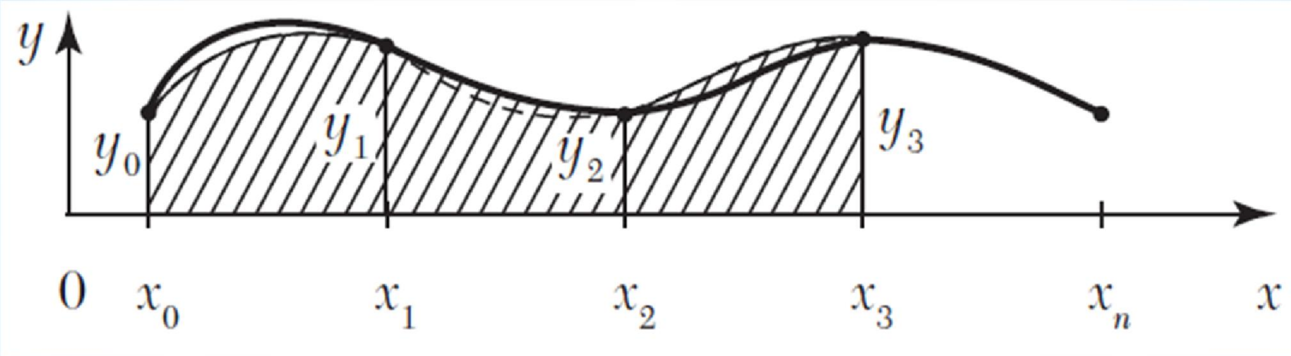
Adding all these integrals, we have when n is even

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{h}{3}[(y_0+y_n)+4(y_1+y_3+\ldots+y_{n-1})+2(y_2+y_4+\ldots y_{n-2})]$$

This is known as the Simpson's one-third rule or simply Simpson's rule and is most commonly used.

Simpson's three-eighth rule

Putting n = 3 in cot's formula and the curve through points (x_i, y_i): i = 0, 1, 2, 3 as a polynomial of the third order so that differences above the third order vanish, we get



$$\int_{x_0}^{x_0+3h} f(x)dx = 3h\left(y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0\right)$$

$$= \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + y_3)$$

Similarly

$$\int_{x_0+3h}^{x_0+5h} f(x)dx = \frac{3h}{8}(y_3 + 3y_4 + 3y_5 + y_6)$$

and so on

Adding all such expressions from x_0 to $x_0 + nh$, where n is a multiple of 3, we obtain

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{3h}{8}[(y_0 + y_n) + 3(y_1 + y_2 + y_4 + y_5 + \cdots + y_{n-1})$$
$$+2(y_3 + y_6 + \cdots + y_{n-3})]$$

Gaussian Quadrature

All methods described previously are based on equally spaced data. Therefore, if n points are considered, an (n-1)st degree polynomial can be fitted to the data points are integrated.

$$I = \int_a^b f(x)dx = \sum_{i=1}^{n} w_i f(x_i)$$

x_i are the location at which function f(x) is known and w_i are weighting factor.

When a known function is to be integrated, an additional degree of freedom exist.

If n points are used, 2n parameters are available (x_i and w_i) so it is possible to fit a polynomial of degree (2n-1).

Gaussian quadrature is integration method which uses the same number of functional values but with different spacing and yields better accuracy by choosing the value of x_i appropriately and w_i.

Gauss simplify the development of formula

$$I = \int_{-1}^{1} f(t)dt = \sum_{i=1}^{n} c_i f(t_i)$$

For two points t_1 and t_2 and weighting factor c_1 and c_2

So 4 parameter fit the polynomial up to degree 3 such as f(t) = 1, t, t^2, t^3.

$$I[f(t) = 1] = \int_{-1}^{1} dt = 2 = c_1(1) + c_2(1) = c_1 + c_2$$

$$I[f(t) = t] = \int_{-1}^{1} tdt = 0 = c_1(t_1) + c_2(t_2)$$

$$I[f(t) = t^2] = \int_{-1}^{1} t^2dt = 2/3 = c_1({t_1}^2) + c_2({t_2}^2)$$

$$I[f(t) = t^3] = \int_{-1}^{1} t^3dt = 0 = c_1({t_1}^3) + c_2({t_2}^3)$$

Solve the equations for t_1, t_2, c_1, c_2

$$t_1 = \frac{-1}{\sqrt{3}},\ t_2 = \frac{1}{\sqrt{3}}\quad c_1 = c_2 = 1$$

$$I = \int_{-1}^{1} f(t)dt = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

Guassian quadrature parameter

No. of Points n	t_i	c_i	Order
2	-1/$\sqrt{3}$ 1/$\sqrt{3}$	1 1	3
3	-$\sqrt{0.6}$ 0 $\sqrt{0.6}$	5/9 8/9 5/9	5
4	-0.8611363116 -0.3399810436 0.3399810436 0.8611363116	0.3478548451 0.6521451549 0.6521451549 0.3478548451	7

In general, the limits of the integral $\int_a^b f(x)dx$ are changed to -1 to 1 by means of the transformation

Transform from x space to t space

x = m t + p

Integration limit x = a   t = -1

x = b   t = 1

Put into transformation equ.

a = m(-1) + p   b = m(1) + p

Find m and p

m = (b-a)/2   p = (b+a)/2

x = [(b-a)/2] t + [(b+a)/2]

$$I = \int_a^b f(x)dx = \int_{-1}^{1} f(mt+p)mdt = \frac{(b-a)}{2}\sum_{i=1}^{n} c_i f(t_i)$$