Unit - III[rd]

Piecewise Polynomial Interpolation

In order to keep the degree of interpolating polynomials small and also to achieve accurate results, we use piecewise polynomial interpolation. For this, we subdivide the given interval $[a, b]$ into a number of sub-intervals $[x_{i-1}, x_i]$, $i = 1, 2, \ldots, n$ and approximate the function by some lower degree polynomial in each subinterval. That is, we subdivide the given interval $[a, b]$, where $a = x_0 < x_1 < x_2 < \ldots < x_n = b$, into a number of non-overlapping subintervals each containing 2 or 3 or 4 nodal points.

Then, we construct the corresponding linear or quadratic or cubic interpolating polynomials fitting the given data on each subinterval. These polynomials define the piecewise linear or quadratic or cubic interpolating polynomials respectively. For example, for the data $(x_i, f(x_i))$, $i = 0, 1, \ldots, 6$ we can construct the following piecewise linear or quadratic or cubic polynomials.

$x_0 \quad x_1 \quad x_2 \quad x_3 \quad x_4 \quad x_5 \quad x_6$

$f(x_0) \quad f(x_1) \quad f(x_2) \quad f(x_3) \quad f(x_4) \quad f(x_5) \quad f(x_6)$ Piecewise linear polynomial

Piecewise quadratic polynomial

Piecewise cubic polynomial

Piecewise Linear Interpolation :

We have $n+1$ distinct nodal points $x_0, x_1, \dots, x_n$ and want to determine an interpolating polynomial which is linear in each subinterval (x_{i-1}, x_i) and agrees with function $f(x)$ at the $n+1$ nodal points. The subintervals or the line segments are called finite elements in one space dimension and the nodal points are called knots.

For $x \in [x_{i-1}, x_i]$, the linear Lagrange interpolating polynomial gives the piecewise linear interpolating polynomial

$$P_{i,1}(x) = \frac{x - x_i}{x_{i-1} - x_i} f(x_{i-1}) + \frac{x - x_{i-1}}{x_i - x_{i-1}} f(x_i), \quad i = 1, 2, \dots, n \qquad (1)$$

for $x \in [x_i, x_{i+1}]$, we have

$$P_{i+1,1}(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} f(x_i) + \frac{x - x_i}{x_{i+1} - x_i} f(x_{i+1})$$

Define

$$N_i(x) = \begin{cases} 0, & x \le x_{i-1} \\ \dfrac{x - x_{i-1}}{x_i - x_{i-1}}, & x_{i-1} \le x \le x_i \\ \dfrac{x_{i+1} - x}{x_{i+1} - x_i}, & x_i \le x \le x_{i+1} \\ 0, & x \ge x_{i+1} \end{cases} \qquad (2)$$

The function $N_i(x)$ is called a shape function.

Note that the non-zero terms in $N_i(x)$ are the coefficients of $f(x_i)$ in $P_{i,1}(x)$ and $P_{i+1,1}(x)$ respectively. Then, the interpolating polynomial

$$P(x) = \sum_{i=0}^{n} P_{i,1}(x) \qquad (3)$$

which agrees with $f(x)$ at x_i, $i = 0, 1, 2, \dots, n$ and is linear in each subinterval $[x_{i-1}, x_i]$ can be written as

$$P_1(x) = \sum_{i=0}^{n} N_i(x) f(x_i) \qquad (4)$$

The error in the piecewise linear interpolation is given by

$$f(x) - P_{i,1}(x) = \frac{1}{2!}(x - x_{i-1})(x - x_i) f''(\xi_i), \quad x_{i-1} < \xi_i < x_i \qquad (5)$$

<u>Exp.</u> Obtain the piecewise linear interpolating polynomials for the function $f(x)$ defined by the data

x	1	2	4	8
$f(x)$	3	7	21	73

Hence, estimate the values of $f(3)$ and $f(7)$.

<u>Solⁿ</u> For $[1, 2]$, we have

$$P_1(x) = \frac{x-2}{(-1)}(3) + \frac{x-1}{(1)}(7) = 4x - 1$$

For $[2, 4]$, we have

$$P_1(x) = \frac{x-4}{(-2)}(7) + \frac{x-2}{(2)}(21) = 7x - 7$$

For $[4, 8]$, we have

$$P_1(x) = \frac{x-8}{(-4)}(21) + \frac{x-4}{(4)}(73) = 13x - 31$$

$$\Rightarrow \quad P_1(x) = \begin{cases} 4x - 1, & 1 \le x \le 2 \\ 7x - 7, & 2 \le x \le 4 \\ 13x - 31, & 4 \le x \le 8 \end{cases}$$

Hence, $f(3) = 14$. and $f(7) = 60$.

Spline: A spline is a sufficiently smooth polynomial function that is piecewise defined and possesses a high degree of smoothness at the places where the polynomial pieces connect.

or A spline function of degree n with knots (nodes) x_i, $i = 0, 1, \dots, n$ is a function $F(x)$ satisfying the properties

(i) $F(x_i) = f(x_i)$, $i = 0, 1, \dots, n$

(ii) $F(x)$ is a polynomial of degree n on each subinterval $[x_{i-1}, x_i]$, $1 \le i \le n$.

(iii) $F(x)$ and its first $(n-1)$ derivatives are continuous on (a, b) where $a = x_0 < x_1 < x_2 < \dots < x_n = b$.

Spline Interpolation: spline interpolation is a form of interpolation where the interpolant is spline.

Note: Linear spline interpolation is same as linear piecewise interpolation.

Cubic Spline Interpolation:

A cubic spline satisfies the following properties

(i) $F(x_i) = f(x_i)$, $i = 0, 1, \dots, n$

(ii) $F(x)$ is a polynomial of degree 3 on each $[x_{i-1}, x_i]$, $1 \le i \le n$

(iii) $F(x)$, $F'(x)$ and $F''(x)$ are continuous on (a, b).

Let $f'(x_i) = m_i$ and $f''(x_i) = M_i$.

Note: Quadratic splines have disadvantages and are not used commonly. Cubic splines have no disadvantages like quadratic splines and are used commonly.

On each subinterval $[x_{i-1}, x_i]$, we approximate $f(x)$ by a cubic polynomial as

$$f(x) = P_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i, \; i = 1, 2, \ldots, n.$$

So, we have $4n$ unknowns a_i, b_i, c_i, d_i, $i = 1, 2, \ldots, n$ to be determined. Using the continuity of $f(x)$, $f'(x)$ and $f''(x)$ we have the following equations for $i = 1, 2, \ldots, n-1$

ⓐ Continuity of $f(x)$:

$$\left.\begin{aligned} &\text{On } [x_{i-1}, x_i]: \; P_i(x_i) = f_i = a_i x_i^3 + b_i x_i^2 + c_i x_i + d_i \\ &\text{On } [x_i, x_{i+1}]: \; P_{i+1}(x_i) = f_i = a_{i+1} x_i^3 + b_{i+1} x_i^2 + c_{i+1} x_i + d_{i+1} \end{aligned}\right\} \quad (6)$$

ⓑ Continuity of $f'(x)$:

$$3a_i x_i^2 + 2b_i x_i + c_i = 3a_{i+1} x_i^2 + 2b_{i+1} x_i + c_{i+1} \quad (7)$$

ⓒ Continuity of $f''(x)$:

$$6a_i x_i + 2b_i = 6a_{i+1} + 2b_{i+1} \quad (8)$$

At the end points x_0 and x_n, we have the interpolatory conditions

$$f_0 = a_1 x_0^3 + b_1 x_0^2 + c_1 x_0 + d_1 \quad (9)$$

$$f_n = a_n x_n^3 + b_n x_n^2 + c_n x_n + d_n \quad (10)$$

We have $4n-2$ equations from (6) to (10). We need 2 more equations to obtain the polynomials uniquely. In most cases, we prescribe $f''(x)$ at the two end points i.e.

$$f''(x_0) = M_0 = p \text{ and } f''(x_n) = M_n = q \quad (11)$$

The end conditions, $M_0 = 0$, $M_n = 0$, lead to a natural spline. Here, p and q may be non-zero.

If the above two conditions (11) are imposed, then we have $4n$ equations in $4n$ unknowns. We can write these equations in matrix form and can obtain solution. This method is called direct method. Any other alternative method may also be used to obtain the cubic spline interpolation.

An Alternate Method :

Since $f(x)$ is to be a piecewise cubic polynomial, $f''(x)$ is a linear function of x in the interval $[x_{i-1}, x_i]$.

Thus, we can write

$$f''(x) = \frac{x_i - x}{x_i - x_{i-1}} f''(x_{i-1}) + \frac{x - x_{i-1}}{x_i - x_{i-1}} f''(x_i) \quad \text{——— (12)}$$

Integrating (12) two times w.r.t. x, we get

$$f(x) = \frac{(x_i - x)^3}{6h_i} M_{i-1} + \frac{(x - x_{i-1})^3}{6h_i} M_i + c_1 x + c_2 \quad \text{——— (13)}$$

where $M_i = f''(x_i)$ and c_1 and c_2 are arbitrary constants to be determined by using the conditions

$$f(x_{i-1}) = f(x_{i-1}) \text{ and } f(x_i) = f(x_i)$$

From (13), we have

$$f_{i-1} = \frac{1}{6h_i}(x_i - x_{i-1})^3 M_{i-1} + c_1 x_{i-1} + c_2$$

or

$$f_{i-1} = \frac{1}{6} h_i^2 M_{i-1} + c_1 x_{i-1} + c_2 \quad \text{——— (14)}$$

and $$f_i = \frac{1}{6h_i}(x_i - x_{i-1})^3 M_i + c_1 x_i + c_2$$

or $$f_i = \frac{1}{6} h_i^2 M_i + c_1 x_i + c_2 \quad \text{——— (15)}$$

Subtracting (14) from (15), we get

$$c_1(x_i - x_{i-1}) = (f_i - f_{i-1}) - \frac{1}{6}(M_i - M_{i-1}) h_i^2$$

$$\Rightarrow \quad c_1 = \frac{1}{h_i}(f_i - f_{i-1}) - \frac{1}{6}(M_i - M_{i-1}) h_i \quad \text{——— (16)}$$

then, we have

$$c_2 = \frac{1}{h_i}(x_i f_{i-1} - x_{i-1} f_i) - \frac{1}{6}(x_i M_{i-1} - x_{i-1} M_i) h_i \quad \text{——— (17)}$$

Substituting the values of c_1 and c_2 in (13), we get

$$f(x) = \frac{1}{6h_i}(x_i - x)^3 M_{i-1} + \frac{1}{6h_i}(x - x_{i-1})^3 M_i + \frac{x}{h_i}(f_i - f_{i-1}) - \frac{x}{6}(M_i - M_{i-1}) h_i$$
$$+ \frac{1}{h_i}(x_i f_{i-1} - x_{i-1} f_i) - \frac{1}{6}(x_i M_{i-1} - x_{i-1} M_i) h_i$$

$$= \frac{1}{6h_i}\left[(x_i - x)\left\{(x_i - x)^2 - h_i^2\right\}\right] M_{i-1} + \frac{1}{6h_i}\left[(x - x_{i-1})\left\{(x - x_{i-1})^2 - h_i^2\right\}\right] M_i$$
$$+ \frac{1}{h_i}(x_i - x) f_{i-1} + \frac{1}{h_i}(x - x_{i-1}) f_i \quad \text{——— (18)}$$

Differentiating (18) w.r.t. x, we get

$$f'(x) = -\frac{(x_i - x)^2}{2h_i} M_{i-1} + \frac{(x - x_{i-1})^2}{2h_i} M_i - \frac{(M_i - M_{i-1}) h_i}{6} + \frac{f_i - f_{i-1}}{h_i} \quad \text{in } [x_{i-1}, x_i]$$
$$\text{——— (19)}$$

Setting $i = i+1$, we get

$$f'(x) = -\frac{(x_{i+1} - x)^2}{2h_{i+1}} M_i + \frac{(x - x_i)}{2h_{i+1}} M_{i+1} - \frac{(M_{i+1} - M_i) h_{i+1}}{6} + \frac{f_{i+1} - f_i}{h_{i+1}}$$
$$\text{in } [x_i, x_{i+1}]. \quad \text{——— (20)}$$

Now, we require that $f'(x)$ be continuous at $x = x_i \pm \epsilon$ as $\epsilon \to 0$. Letting $f'(x_i - \epsilon) = f'(x_i + \epsilon)$ as $\epsilon \to 0$, we get

$$\frac{h_i}{6} M_{i-1} + \frac{h_i}{3} M_i + \frac{1}{h_i}(f_i - f_{i-1}) = -\frac{h_{i+1}}{3} M_i - \frac{h_{i+1}}{6} M_{i+1} + \frac{1}{h_{i+1}}(f_{i+1} - f_i)$$

which may be written as

$$\frac{h_i}{6} M_{i-1} + \frac{h_i + h_{i+1}}{3} M_i + \frac{h_{i+1}}{6} M_{i+1} = \frac{1}{h_{i+1}}(f_{i+1} - f_i) - \frac{1}{h_i}(f_i - f_{i-1}), \quad i = 1, 2, \dots (n-1). \qquad (21)$$

This gives a system of $n-1$ linear equations in $n+1$ unknowns $M_0, M_1, \dots, M_n$. The two additional conditions may be taken in one of the following forms.

(i) $M_0 = M_n = 0$. (natural spline) $\qquad (22)$

(ii) $M_0 = M_n$, $M_1 = M_{n+1}$, $f_0 = f_n$, $f_1 = f_{n+1}$, $h_1 = h_{n+1}$. $\qquad (23)$

(periodic spline)

(iii) for a non-periodic spline, we use the conditions

$$f'(a) = f'(a) = f'_0 \text{ and } f'(b) = f'(b) = f'_n$$

Using (19), we get

$$\left.\begin{aligned} 2M_0 + M_1 &= \frac{6}{h_1}\left(\frac{f_1 - f_0}{h_1} - f'_0\right) \\ M_{n-1} + 2M_n &= \frac{6}{h_n}\left(f'_n - \frac{f_n - f_{n-1}}{h_n}\right) \end{aligned}\right\} \qquad (24)$$

For equispaced knots $h_i = h$ for all i, eqⁿ (18) and (21) becomes

$$f(x) = \frac{1}{6h}\left[(x_i - x)^3 M_{i-1} + (x - x_{i-1})^3 M_i\right] + \frac{1}{h}(x_i - x)\left(f_{i-1} - \frac{h^2}{6} M_{i-1}\right)$$
$$+ \frac{1}{h}(x - x_{i-1})\left(f_i - \frac{h^2}{6} M_i\right) \qquad (25)$$

and $M_{i-1} + 4M_i + M_{i+1} = \frac{6}{h^2}\left(f_{i-1} - 2f_i + f_{i+1}\right)$ —— (26)

This method gives the values of $M_i = f''(x_i)$, $i = 1, 2, \ldots, n-1$.
The solutions obtained for M_i, $i = 1, 2, \ldots, n-1$ are substituted in (18) or (25) to find the cubic spline interpolation. In this method, we need to solve only an $(n-1)\times(n-1)$ tridiagonal system of equations for finding M_i.

Ex. Obtain the cubic spline interpolation for the function defined by the data

x	x_0 0	x_1 1	x_2 2	x_3 3
$f(x)$	1 f_0	2 f_1	33 f_2	244 f_3

with $M(0) = 0$, $M(3) = 0$. Hence, find an estimate of $f(2.5)$.

Sol.ⁿ Direct Method

We have the cubic polynomial approximation as follows

$$\left.\begin{aligned} f(x) &= P_1(x) = a_1x^3 + b_1x^2 + c_1x + d_1, \quad 0 \le x \le 1 \\ f(x) &= P_2(x) = a_2x^3 + b_2x^2 + c_2x + d_2, \quad 1 \le x \le 2 \\ f(x) &= P_3(x) = a_3x^3 + b_3x^2 + c_3x + d_3, \quad 2 \le x \le 3 \end{aligned}\right\} \longrightarrow (*)$$

Continuity of $f(x)$ gives the following equations

$$P_1(x_1) = f_1 = a_1x_1^3 + b_1x_1^2 + c_1x_1 + d_1 = a_1 + b_1 + c_1 + d_1$$

$$P_2(x_1) = f_1 = a_2 + b_2 + c_2 + d_2$$

$$P_2(x_2) = f_2 = a_2x_2^3 + b_2x_2^2 + c_2x_2 + d_2 = 8a_2 + 4b_2 + 2c_2 + d_2$$

$$P_3(x_2) = f_2 = 8a_3 + 4b_3 + 2c_3 + d_3$$

Continuity of $f'(x)$ gives the following equations

$$3a_1x_1^2 + 2b_1x_1 + c_1 = 3a_2x_1^2 + 2b_2x_1 + c_2$$

or $$3a_1 + 2b_1 + c_1 = 3a_2 + 2b_2 + c_2$$

and $$3a_2x_2^2 + 2b_2x_2 + c_2 = 3a_3x_2^2 + 2b_3x_2 + c_3$$

or $$12a_2 + 4b_2 + c_2 = 12a_3 + 4b_3 + c_3$$

Continuity of $f''(x)$ gives the following equations

$$6a_1x_1 + 2b_1 = 6a_2x_1 + 2b_2$$

or $$6a_1 + 2b_1 = 6a_2 + 2b_2$$

and $$6a_2x_2 + 2b_2 = 6a_3x_2 + 2b_3$$

or $$12a_2 + 2b_2 = 12a_3 + 2b_3$$

At the end points, we have the interpolatory conditions

$$f_0 = a_1x_0^3 + b_1x_0^2 + c_1x_0 + d_1 = d_1$$

$$f_3 = a_3x_3^3 + b_3x_3^2 + c_3x_3 + d_3 = 27a_3 + 9b_3 + 3c_3 + d_3$$

From the given conditions $f''(x_0) = M_0 = M(x_0) = M(0) = 0$ and

$f''(x_3) = M_3 = M(x_3) = M(3) = 0$, we have

$$b_1 = 0 \quad \text{and} \quad 9a_3 + b_3 = 0$$

Substituting the values $b_1 = 0$, $b_3 = -9a_3$ and $d_1 = f_0 = 1$,

we get the system of equations

$$a_1 + c_1 = 1$$

$$a_2 + b_2 + c_2 + d_2 = 2, \quad 8a_2 + 4b_2 + 2c_2 + d_2 = 33,$$

$$-28a_3 + 2c_3 + d_3 = 33, \quad 3a_1 + c_1 - 3a_2 - 2b_2 - c_2 = 0,$$

$$12a_2 + 4b_2 + c_2 + 24a_3 - c_3 = 0, \quad 3a_1 - 3a_2 - b_2 = 0$$

$$6a_2 + b_2 + 3a_3 = 0, \quad -54a_3 + 3c_3 + d_3 = 244.$$

Solving this system of equations, we get

$a_1 = -4,\ c_1 = 5,\ a_2 = 50,\ b_2 = -162,\ c_2 = 167,$

$d_2 = -53,\ a_3 = -46,\ b_3 = 414,\ c_3 = -985,\ d_3 = 715$

Also, we have already $b_1 = 0$ and $d_1 = 0$.

Thus, the cubic polynomial approximation ⊛ becomes

$$P_1(x) = -4x^3 + 5x + 1, \quad 0 \le x \le 1$$

$$P_2(x) = 50x^3 - 162x^2 + 167x - 53, \quad 1 \le x \le 2$$

$$P_3(x) = -46x^3 + 414x^2 - 985x + 715, \quad 2 \le x \le 3$$

Hence, $f(2.5) = P_3(2.5) = 121.25$

By Alternate Method

Here, all the points are equispaced with $h = 1$.

So that we have from (26)

$$M_{i-1} + 4M_i + M_{i+1} = 6\left(f_{i-1} - 2f_i + f_{i+1}\right), \quad i = 1, 2$$

or
$$\left.\begin{aligned} M_0 + 4M_1 + M_2 &= 6\left(f_0 - 2f_1 + f_2\right) \\ M_1 + 4M_2 + M_3 &= 6\left(f_1 - 2f_2 + f_3\right) \end{aligned}\right\}$$
(and)

that gives with $M_0 = 0 = M_3$

$$\left.\begin{aligned} 4M_1 + M_2 &= 6(1 - 4 + 33) = 180 \\ M_1 + 4M_2 &= 6(2 - 66 + 244) = 1080 \end{aligned}\right\}$$
(and)

$$\Rightarrow M_1 = -24, \quad M_2 = 276.$$

Now from (25), the cubic splines in the corresponding intervals

on $[0,1]$: $F(x) = P_1(x) = \frac{1}{6}x^3(-24) + (1-x) + x\left[2 - \frac{1}{6}(-24)\right] = -4x^3 + 5x + 1$

On $[1,2]$: $f(x) = P_2(x) = \frac{1}{6}\left[(2-x)^3(-24) + (x-1)^3(276)\right] + (2-x)\left[2 - \frac{1}{6}(-24)\right]$
$+ (x-1)\left[33 - \frac{1}{6}(276)\right]$

$$= 50x^3 - 162x^2 + 167x - 53$$

On $[2,3]$: $f(x) = P_3(x) = \frac{1}{6}\left[(27 - 27x + 9x^2 - x^3)(276)\right] + (3-x)\left[33 - \frac{1}{6}(276)\right]$
$+ (x-2)(244)$

$$= -46x^3 + 414x^2 - 985x + 715$$

Hence, $f(2.5) = P_3(2.5) = 121.25$

Numerical Differentiation

Let $f(x)$ be a function that attains values $f(x_0), f(x_1), \ldots, f(x_n)$ at the points $x_0, x_1, \ldots, x_n$. The general approach for deriving the numerical differentiation of $f(x)$ is to first obtain the interpolating polynomial $P_n(x)$ and then differentiate this polynomial $P_n(x)$ r times $(r \leq n)$ to get $P_n^{(r)}(x)$. The value of $P_n^{(r)}(x_k)$ gives the approximate value of $f^{(r)}(x)$ at the nodal point x_k. The quantity

$$E^{(r)}(x) = f^{(r)}(x) - P_n^{(r)}(x) \quad \text{———} \circledast$$

is called the error of approximation in rth order derivative at any point x. Numerical differentiation methods are obtained using one of the following techniques

(i) Methods based on interpolation
(ii) Methods based on finite difference operators
(iii) Methods based on undetermined coefficients

Methods Based on Interpolation

Derivatives using Newton's forward difference formula

Newton's forward interpolation formula is

$$y(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \qquad (1)$$

where $p = (x-x_0)/h$ and $y_0 = f(x_0)$.

Diff. (1) w.r.t. p, we get

$$\frac{dy}{dp} = \Delta y_0 + \frac{(2p-1)}{2!}\Delta^2 y_0 + \frac{(3p^2-6p+2)}{3!}\Delta^3 y_0 + \frac{(4p^3-18p^2+22p-6)}{4!}\Delta^4 y_0 + \cdots \qquad (2)$$

From $p = (x-x_0)/h$, we have $\frac{dp}{dx} = \frac{1}{h}$.

Now, $\frac{dy}{dx} = \frac{dy}{dp}\cdot\frac{dp}{dx}$ and $\frac{d^2y}{dx^2} = \frac{d}{dp}\left(\frac{dy}{dx}\right)\cdot\frac{1}{h}$

$$\therefore \left(\frac{dy}{dx}\right)_{x=x_0+ph} = \frac{1}{h}\left[\Delta y_0 + \frac{(2p-1)}{2!}\Delta^2 y_0 + \frac{(3p^2-6p+2)}{3!}\Delta^3 y_0 + \frac{(4p^3-18p^2+22p-6)}{4!}\Delta^4 y_0 + \cdots\right] \qquad (3)$$

At $x = x_0$, $p = 0$

$$\therefore \left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^3 y_0 + \cdots\right]$$

and

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\Delta^2 y_0 + (p-1)\Delta^3 y_0 + \frac{(6p^2-18p+11)}{12}\Delta^4 y_0 + \cdots\right] \qquad (4)$$

At $x = x_0$, $p = 0$

$$\therefore \left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \cdots\right]$$

Derivatives using Newton's backward difference formula

Newton's backward interpolation formula is

$$y(x) = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \frac{p(p+1)(p+2)}{3!}\nabla^3 y_n + \cdots \quad \text{—— (5)}$$

where $p = (x - x_n)/h$ and $y_n = f(x_n)$.

In a similar manner as before, we have

$$\frac{dy}{dx} = \frac{1}{h}\left[\nabla y_n + \frac{(2p+1)}{2}\nabla^2 y_n + \frac{(3p^2+6p+2)}{6}\nabla^3 y_n + \frac{(2p^3+9p^2+11p+3)}{12}\nabla^4 y_n + \cdots\right] \quad \text{—— (6)}$$

At $x = x_n$, $p = 0$

$$\therefore \left(\frac{dy}{dx}\right)_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \cdots\right]$$

and

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\nabla^2 y_n + (p+1)\nabla^3 y_n + \frac{(6p^2+18p+11)}{12}\nabla^4 y_n + \cdots\right] \quad \text{—— (7)}$$

At $x = x_n$, $p = 0$

$$\therefore \left(\frac{d^2y}{dx^2}\right)_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \cdots\right]$$

Exp.1 Find $\frac{dy}{dx}$ for the following data

x	0	1	2	3	4
y	1	1	15	40	85

Hence find $y'(x)$ at $x = 0.5$.

Soln Here $h = 1$. Since $x = 0.5$ is near to $x_0 = 0$, we apply Newton's forward interpolation formula for derivative (3).

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$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{(2p-1)}{2!}\Delta^2 y_0 + \frac{(3p^2-6p+2)}{3!}\Delta^3 y_0 + \frac{(4p^3-18p^2+22p-6)}{4!}\Delta^4 y_0 + \cdots\right] \quad (3)$$

where $p = (x-x_0)/h$. Since $x_0 = 0$, $p = x$.

The forward difference table

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
0	1				
		0			
1	1		14		
		14		-3	
2	15		11		12
		25		9	
3	40		20		
		45			
4	85				

Therefore (3) becomes

$$\frac{dy}{dx} = \frac{1}{2}(2x-1)(14) + \frac{1}{6}(3x^2-6x+2)(-3) + \frac{1}{24}(4x^3-18x^2+22x-6)(12)$$

$$= 7(2x-1) - \frac{1}{3}(3x^2-6x+2) + (2x^3-9x^2+11x-3)$$

$$\Rightarrow y'(x) = 2x^3 - \frac{21}{2}x^2 + 28x - 11$$

Hence, $y'(0.5) = 0.625$.

Exp. 2 The population of a certain town is shown as

Year (x)	1931	1941	1951	1961	1971
Population (y)	40.62	60.80	79.95	103.56	132.65

Find the rate of growth of the population in 1961.

Soln. Here $h = 10$. Since $x = 1961$ is near to $x_n = 1971$, ($n=4$) we apply Newton's backward interpolation formula for derivative (6).

$$\frac{dy}{dx} = \frac{1}{h}\left[\nabla y_4 + \frac{(2p+1)}{2}\nabla^2 y_4 + \frac{(3p^2+6p+2)}{6}\nabla^3 y_4 + \frac{(2p^3+9p^2+11p+3)}{12}\nabla^4 y_4 + \cdots\right] \quad \text{(6)}$$

where $p = (x-x_4)/h = \dfrac{1961-1971}{10} = -1$.

<u>The backward difference table</u>

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
1931	40.62				
		20.18			
1941	60.80		−1.03		
		19.15		5.49	
1951	79.95		4.46		−4.47
		23.61		1.02	
1961	103.56		5.48		
		29.09			
1971	132.65				

Therefore (6) becomes

$$\left(\frac{dy}{dx}\right)_{p=-1} = \frac{1}{10}\Big[29.09 + \frac{1}{2}\{2(-1)+1\}(5.48) + \frac{1}{6}\{3(-1)^3+6(-1)+2\}(1.02)$$
$$+ \frac{1}{12}\{2(-1)^3+9(-1)^2+11(-1)+3\}(-4.47)\Big]$$

$$= \frac{1}{10}\left[29.09 - 2.74 - 0.17 + 0.3725\right]$$

$$= \frac{1}{10}\left[26.5525\right]$$

$$= 2.6553$$

Hence, $y'(1961) = 2.6553$.

Note: for non-equispaced points, we can use Lagrange's interpolation formula or Newton's divided differences formula to obtain the interpolating polynomial $P_n(x)$ for the function $f(x)$. Then $P_n^{(r)}(x)$, $r \le n$ will give the approximate value of $f^{(r)}(x)$.

Methods Based on Finite Differences

Consider the relation

$$e^{hD} = E$$

$$\Rightarrow \quad hD = \log E = \begin{cases} \log(1+\Delta) \\ \text{or} \\ -\log(1-\nabla) \end{cases}$$

$$\Rightarrow \quad hD = \begin{cases} \log(1+\Delta) = \Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \cdots\cdots \\ \text{or} \\ -\log(1-\nabla) = \nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \cdots\cdots \end{cases}$$

$$\Rightarrow \quad D = \begin{cases} \frac{1}{h}\left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \cdots\cdots\right) \\ \text{or} \\ \frac{1}{h}\left(\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \cdots\cdots\right) \end{cases} \qquad \text{—— (8)}$$

Now, we have

$$f'(x_k) = Df(x_k) = \begin{cases} \frac{1}{h}\left(\Delta f_k - \frac{1}{2}\Delta^2 f_k + \frac{1}{3}\Delta^3 f_k - \cdots\right) \\ \text{or} \\ \frac{1}{h}\left(\nabla f_k + \frac{1}{2}\nabla^2 f_k + \frac{1}{3}\nabla^3 f_k + \cdots\right) \end{cases} \qquad \text{—— (9)}$$

Also, we have $\quad \delta = \left(E^{1/2} - E^{-1/2}\right) = \left(e^{hD/2} - e^{-hD/2}\right) = 2\sinh(hD/2)$

$$\Rightarrow \quad D = \frac{2}{h}\sinh^{-1}\left(\frac{\delta}{2}\right) = \frac{1}{h}\left(\delta - \frac{1^2}{2^2 \cdot 3!}\delta^3 + \cdots\right) \qquad \text{—— (10)}$$

$$\Rightarrow \quad f'(x_k) = \frac{1}{h}\left(\delta f_k - \frac{1^2}{2^2 \cdot 3!}\delta^3 f_k + \cdots\right) \qquad \text{—— (11)}$$

Two-Point Difference formulae

forward difference derivative $f'(x) = \dfrac{f(x+h)-f(x)}{h}$ ——— (12)

$$\Rightarrow \quad f'(x_k) = \frac{f(x_k+h)-f(x_k)}{h} \quad \text{at } x = x_k.$$

Backward difference derivative $f'(x) = \dfrac{f(x)-f(x-h)}{h}$ ——— (13)

$$\Rightarrow \quad f'(x_k) = \frac{f(x_k)-f(x_k-h)}{h} \quad \text{at } x = x_k.$$

Here, $f'(x)$ is a two point difference approximation which is a good approximation for small h. The central difference derivative is also two-point difference approximation.

Central difference derivative $f'(x) = \dfrac{f(x+h)-f(x-h)}{2h}$ ——— (14)

$$\Rightarrow \quad f'(x_k) = \frac{f(x_k+h)-f(x_k-h)}{2h} \quad \text{at } x = x_k.$$

Exp. for the function $f(x) = x\ln(x)$, we have

x	1	2	3
$f(x)$	0	1.3863	3.2958

Approximate $f'(2)$ by each of the two-point difference formulae given above.

Solⁿ. We have $f(x) = x\ln(x) \Rightarrow f'(x) = 1+\ln(x)$

$$\Rightarrow \quad f'(2) = 1.6931 \quad \text{(Exact value)}$$

Here $h = 1$. By forward difference formula, we have

$$f'(x) = \frac{f(x+h) - f(x)}{h} \Rightarrow f'(2) = \frac{f(3) - f(2)}{1} = 1.9095$$

$$\text{Absolute error} = |(1 + \ln(2)) - 1.9095| = |1.6931 - 1.9095| = 0.2164$$

By backward difference formula, we have

$$f'(x) = \frac{f(x) - f(x-h)}{h} \Rightarrow f'(2) = \frac{f(2) - f(1)}{1} = 1.3863$$

$$\text{Absolute error} = |1.6931 - 1.3863| = 0.3068$$

By central difference formula, we have

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \Rightarrow f'(2) = \frac{f(3) - f(1)}{2} = 1.6479$$

$$\text{Absolute error} = |1.6931 - 1.6479| = 0.0452$$

This shows that the two-point central difference formula is more accurate.

Three-point difference formulae

Three-point forward difference formula $$f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} \qquad (15)$$

$$\underset{x}{*} - - - - - \underset{x+h}{*} - - - - - \underset{x+2h}{*}$$

Three-point backward difference formula $$f'(x) = \frac{f(x-2h) - 4f(x-h) + 3f(x)}{2h} \qquad (16)$$

$$\underset{x-2h}{*} - - - - - \underset{x-h}{*} - - - - - \underset{x}{*}$$

Order of a Numerical Differentiation Method

A numerical differentiation method is said to be of order p if

$$|E^{(r)}(x)| = |f^{(r)}(x) - P_n^{(r)}(x)| \leq ch^p \quad \text{——— (17)}$$

where c is a constant independent of h.

Note: (i) Methods (12) and (13) are first-order approximations i.e. both methods are of first-order i.e. are of $O(h)$.

(ii) Method (14) is of second-order i.e is of $O(h^2)$.

(iii) Methods (15) and (16) are of second-order i.e. are of $O(h^2)$.

Extrapolation:

It is an estimation of a value based on extending a known sequence of values or facts beyond the area that is certainly known. In a general sense, to extrapolate is to infer something that is not explicitly stated from existing information.

Richardson's Extrapolation:

In general, it is possible to obtain highly accurate results by combining the computed values obtained by using a certain method with different step sizes.

Let $g(h)$ and $g(2h)$ denote the approximate values of g, obtained by using a method of order p, with step lengths h and $2h$ respectively.

We have

$$g(h) = g + ch^p + O(h^{p+1})$$

and
$$g(2h) = g + c\,2^p h^p + O(h^{p+1})$$

Eliminating c from the above equations, we get

$$g = \frac{2^p g(h) - g(2h)}{2^p - 1} + O(h^{p+1})$$

Thus, we have

$$g^{(1)}(h) = \frac{2^p g(h) - g(2h)}{2^p - 1} = g + O(h^{p+1})$$

which is of order p+1 and $g^{(1)}(h)$ is newly defined approximation to g. This technique of combining two computed values obtained by using the same method with two different step sizes, to obtain a higher order method is called the Richardson's extrapolation.

<u>Note:</u> If a method has an error term $O(h^p)$, we say that the method is of order p. for example, if we use Taylor's expansion to approximate a function f(x) at $x = a+h$, we have

$$f(x) = f(a+h) = f(a) + hf'(a) + \frac{h^2}{2!}f''(a) + \frac{h^3}{3!}f'''(\xi), \quad a<\xi<a+h$$

then we say that the approximation is $O(h^3)$ or the method is of third order.

Let us consider the second-order central difference formula for $f'(x_i)$ which gives $O(h^2)$ approximation.

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

$$\Rightarrow \quad f'(x_i) = \frac{f(x_i + h) - f(x_i - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi) + O(h^4) \quad \text{——— (18)}$$

Let us denote

D = true value of the derivative i.e. $f'(x_i)$

D_h = approximate value of $f'(x_i)$ with step size h

$D_{h/2}$ = approximate value of $f'(x_i)$ with step size $h/2$

Then (18) can be written as

$$D = D_h - \frac{h^2}{6} f^{(3)}(\xi) + O(h^4) \quad \text{——— (19)}$$

Taking step size $h/2$, (18) gives

$$f(x_i) = \frac{f(x_i + h/2) - f(x_i - h/2)}{h} - \frac{h^2}{24} f^{(3)}(\xi) + O(h^4)$$

$$\Rightarrow \quad D = D_{h/2} - \frac{h^2}{24} f^{(3)}(\xi) + O(h^4)$$

$$\text{or} \quad 4D = 4D_{h/2} - \frac{h^2}{6} f^{(3)}(\xi) + O(h^4) \quad \text{——— (20)}$$

Subtracting (19) from (20), we get

$$3D = 4D_{h/2} - D_h + O(h^4)$$

$$\Rightarrow \quad \boxed{D = \frac{4D_{h/2} - D_h}{3}} \quad \text{——— (21)}$$

This gives an $O(h^4)$ approximation to $D = f'(x_i)$.

This process of extrapolating from D_h and $D_{h/2}$ to approximate D with higher order of accuracy is called Richardson's extrapolation.

Exp. Consider the following data points:

	x_0	x_1	x_2	x_3	x_4
x	1	2	3	4	5
$f(x)$	2	4	8	16	32
	f_0	f_1	f_2	f_3	f_4

Estimate $f'(3)$ using Richardson's extrapolation with $h=2$.

Solⁿ We have

$$D_h = \frac{f(x_i+h)-f(x_i-h)}{2h}$$

and

$$D_{h/2} = \frac{f(x_i+h/2)-f(x_i-h/2)}{h}$$

$$\Rightarrow \quad D_h = \frac{f(x_2+h)-f(x_2-h)}{2h} = \frac{f(3+2)-f(3-2)}{4}$$

$$= \frac{f(5)-f(1)}{4} = \frac{32-2}{4} = 7.5$$

and

$$D_{h/2} = \frac{f(x_2+h/2)-f(x_i-h/2)}{h} = \frac{f(3+1)-f(3-1)}{2}$$

$$= \frac{f(4)-f(2)}{2} = \frac{16-4}{2} = 6 \quad \text{(by central difference formula)}$$

Now, from (21) we have

$$D = \frac{4D_{h/2}-D_h}{3} = \frac{4(6)-7.5}{3}$$

$$= 5.5 \quad \text{(by Richardson's extrapolation)}$$

Note: Actual function is $f(x)=2^x$. Then $f'(x)=2^x \ln 2$. The exact value is $f'(3) \approx 5.5452$. This shows that Richardson's extrapolation gives more accuracy.

Exp. Consider the following data points:

x	-1	1	2	3	4	5	7
$f(x)$	1	1	16	81	256	625	2401

Estimate $f'(3)$ by Richardson's extrapolation with $h=4$, $h=2$ and $h=1$ using the following approximate formula

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

Sol: We are given three values h, $h/2$, $h/4$ of step size. Therefore, we can calculate approximations of $O(h^2)$, $O(h^4)$ and $O(h^6)$ following the table given below.

Step Size	$f'(3)$		
	$O(h^2)$	$O(h^4)$	$O(h^6)$
$h=4$	D_h		
		D_h^1	
$h/2 = 2$	$D_{h/2}$		D_h^2
		$D_{h/2}^1$	
$h/4 = 1$	$D_{h/4}$		

Therefore, we have

$$D_h = f'(3) = \frac{f(3+h)-f(3-h)}{2h} = \frac{f(7)-f(-1)}{8} = 300$$

$$D_{h/2} = f'(3) = \frac{f(5)-f(1)}{4} = 156$$

$$D_{h/4} = f'(3) = \frac{f(4)-f(2)}{2} = 120$$

Then, we have

$$D_h^1 = \frac{4D_{h/2} - D_h}{3} = \frac{4(156)-300}{3} = 108$$

$$D_{h/2}^1 = \frac{4D_{h/4} - D_{h/2}}{3} = \frac{4(120)-156}{3} = 108$$

and
$$D_h^2 = \frac{4^2 D_{h/2}^1 - D_h^1}{4^2-1} = \frac{16(108)-108}{15} = 108$$

Thus, we have
$$\boxed{D_h^m = \frac{4^m D_{h/2}^{m-1} - D_h^{m-1}}{4^m-1} \quad \text{General formula}}$$

$f'(3) = 108$ with $O(h^6)$ approximation.

Richardson's technique

$\boxed{\text{$O(h^p)$ formula with spacing h}} + \boxed{\text{$O(h^p)$ formula with spacing $h/2$}} \longrightarrow \boxed{\text{$O(h^{p+1})$ formula}}$

Numerical Integration

Let us assume two functions $f(x)$ and $F(x)$ s.t.
$$F'(x) = f(x)$$
then $f(x)$ is said to be derivative of $F(x)$ and
$F(x)$ is said to be anti-derivative of $f(x)$.

By the fundamental theorem of the integral calculus, we can evaluate the following integral
$$\int_a^b f(x)\,dx = \int_a^b \frac{d}{dx} F(x) = \left[F(x)\right]_a^b = F(b) - F(a).$$

then $f(x)$ is called integrand function. But some functions have no simple anti-derivatives i.e. difficult to find out then an approximation is needed and numerical integration is used. Numerical integration formulae is also called as quadrature formulae. "Numerical integration is an approximation to a definite integral derived from a set of tabulated values of integrand $f(x)$, which is not known explicitly."

Numerical Integration

Newton-cote's Formulae
(Nodes are equispaced)

Gaussian Quadrature
(Nodes are not chosen)

Newton-cote's Closed formulae

$\int_a^b f(x)dx$

(end points a & b are used as abscissas)

e.g. (i) Trapezoidal Rule

(ii) Simpson's Rules

Newton-cote's Open formulae

$\int_a^b f(x)dx$

(end points are not used.)

e.g. (i) Mid-point Rule

$\int_a^b f(x)dx \approx \sum_{i=0}^{n} c_i f(x_i)$

then x_i's are called abscissas or nodes.

Newton-cote's Closed formula

Let $I = \int_a^b f(x)dx$ where $f(x)$ takes the values $y_0, y_1, \dots, y_n$ at the points $x_0, x_1, \dots, x_n$. Divide the interval (a, b) into n subintervals of width h so that $x_0 = a$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h, \dots, x_n = x_0 + nh = b$. $\left(\because h = \frac{b-a}{n}\right)$

Therefore, we have

$$I = \int_a^b f(x)dx = h\int_0^n f(x_0 + ph)\,dp \quad \left(\text{Taking } p = \frac{x - x_0}{h}\right)$$

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

(by Newton's forward difference formula)

$$= h\left[p y_0 + \frac{p^2}{2}\Delta y_0 + \frac{1}{2}\left(\frac{p^3}{3} - \frac{p^2}{2}\right)\Delta^2 y_0 + \frac{1}{6}\left(\frac{p^4}{4} - p^3 + p^2\right)\Delta^3 y_0 + \cdots\right]_0^n$$

$$= h\left[n y_0 + \frac{n^2}{2}\Delta y_0 + \frac{1}{2}\left(\frac{n^3}{3} - \frac{n^2}{2}\right)\Delta^2 y_0 + \cdots\right]$$

$$\Rightarrow \boxed{\int_{x_0}^{x_0+nh} f(x)dx = h\left[ny_0 + \frac{n^2}{2}\Delta y_0 + \frac{1}{2}\left(\frac{n^3}{3} - \frac{n^2}{2}\right)\Delta^2 y_0 + \cdots\right]} \quad \text{—— (1)}$$

This is called Newton-Cote's formula. It is general quadrature formula from which we can derive various special formulae giving different values for n.

Trapezoidal Rule

Putting $n=1$ in the quadrature formula (1), we get

$$\int_{x_0}^{x_0+h} f(x)dx = h\left[y_0 + \frac{1}{2}\Delta y_0\right] \quad \left(\because \Delta^i y_0 = 0, \forall i>1\right)$$

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

$$\Rightarrow \int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(y_0 + y_1)$$

Similarly, we have

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

$$\cdots \quad \cdots \quad \cdots$$

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

Adding these n integrals, we get

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

$$\Rightarrow \boxed{\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}\left[(y_0+y_n) + 2(y_1+y_2+\cdots+y_{n-1})\right]} \quad \text{—— (2)}$$

This is known as Trapezoidal rule.

Note: The error in the Trapezoidal rule is of order h^2.

If $h = b-a$ i.e. the interval (a,b) is not divided into subintervals then the Trapezoidal rule is given by

$$\boxed{\int_a^b f(x)dx \approx \frac{(b-a)}{2}\left[f(a)+f(b)\right] = \frac{h}{2}\left[f(a)+f(b)\right]} \quad \text{--- (3)}$$

(Since $n=1$, x takes the values x_0 or x_1.)

Exp: Find $\int_0^2 f(x)dx$, where $f(x) = e^{-x^2}$.

Soln: By Trapezoidal rule, we have

$$\int_0^2 f(x)dx = \int_0^2 e^{-x^2}dx$$

$$= \frac{(2-0)}{2}\left[1+e^{-4}\right]$$

$$= 1+e^{-4}$$

$$= 1.0183$$

Exp: Evaluate $\int_0^1 \frac{1}{1+x^2}dx$ by Trapezoidal rule.

Soln: $\int_0^1 \frac{1}{1+x^2}dx = \left[\tan^{-1}x\right]_0^1 = \tan^{-1}(1) - \tan^{-1}(0) = \frac{\pi}{4} - 0 = 0.7854$

Exact Value

By Trapezoidal rule, we have

$$\int_0^1 \frac{1}{1+x^2}dx = \frac{(1-0)}{2}\left[f(0)+f(1)\right]$$

$$= \frac{1}{2}\left[1+\frac{1}{2}\right] = \frac{3}{4}$$

$$= 0.75$$

Error $(E) = |0.7854-0.75| = 0.0354$

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Exp Evaluate $\int_0^1 \frac{dx}{1+x}$ by Trapezoidal rule.

Solⁿ $\int_0^1 \frac{dx}{1+x} = \left[\ln(1+x)\right]_0^1 = \ln(2) - \ln(1) = 0.6931$

By Trapezoidal rule, we have

$$\int_0^1 \frac{dx}{1+x} = \frac{(1-0)}{2}\left[f(0)+f(1)\right] = \frac{1}{2}\left[1+\frac{1}{2}\right] = \frac{3}{4} = 0.75$$

$$\text{Error} = |0.6931 - 0.75| = 0.0569$$

Dividing the interval (0,1) into two subintervals, then

$h = \frac{(1-0)}{2} = 0.5$. We have

$x_0 = 0$, $x_1 = x_0 + h = 0 + 0.5 = 0.5$

$x_2 = x_0 + 2h = 0 + 2(0.5) = 1$

Therefore, by Trapezoidal rule ②, we have

$$\int_0^1 \frac{dx}{1+x} = \frac{h}{2}\left[f(x_0) + 2f(x_1) + f(x_2)\right]$$

$$= \frac{0.5}{2}\left[1 + 2\left(\frac{1}{1.5}\right) + 0.5\right]$$

$$= (0.25)\left[1.5 + 1.3333\right]$$

$$= 0.7083$$

$$\text{Error} = |0.6931 - 0.7083| = 0.0152$$

<u>Note:</u> For improving accuracy, we divide the interval into subintervals of equal length h i.e. more points are introduced between a and b s.t.
$x_0 = a$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h, \ldots, x_n = x_0 + nh = b$.

Simpson's One Third Rule

Putting $n=2$ in the quadrature formula (1), we get

$$\int_{x_0}^{x_0+2h} f(x)dx = h\left[2y_0+\frac{4}{2}\Delta y_0+\frac{1}{2}\left(\frac{8}{3}-\frac{4}{2}\right)\Delta^2 y_0\right] \quad (\because \Delta^i y_0 = 0, \forall i>2)$$

$$= h\left[2y_0+2(y_1-y_0)+\frac{1}{3}\Delta^2 y_0\right]$$

$$= h\left[2y_0+2(y_1-y_0)+\frac{1}{3}(E-1)^2 y_0\right]$$

$$= h\left[2y_0+2y_1-2y_0+\frac{1}{3}(E^2-2E+1)y_0\right]$$

$$= h\left[2y_1+\frac{1}{3}(y_2-2y_1+y_0)\right]$$

$$\Rightarrow \int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\left[y_0+4y_1+y_2\right]$$

Similarly, we have

$$\int_{x_2}^{x_4} f(x)dx = \frac{h}{3}\left[y_2+4y_3+y_4\right]$$

$$\cdots \quad \cdots \quad \cdots$$

$$\int_{x_{n-2}}^{x_n} f(x)dx = \frac{h}{3}\left[y_{n-2}+4y_{n-1}+y_n\right] \quad \text{(assuming } n \text{ to be even)}$$

Adding all these integrals, we get

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{h}{3}\left[(y_0+y_n)+2(y_2+y_4+\cdots)+4(y_1+y_3+\cdots)\right]$$

$$\Rightarrow \boxed{\int_{x_0}^{x_n} f(x)dx = \frac{h}{3}\left[(y_0+y_n)+2(y_2+y_4+\cdots)+4(y_1+y_3+\cdots)\right]} \quad (4)$$

This is called Simpson's one-third rule or Simpson's rule.

Note: The error in the simpson's one third rule is of $O(h^4)$.

Since $n=2$, x takes the values x_0, x_1 or x_2. Then we have

$h = (b-a)/2$, $x_0 = a$, $x_1 = x_0 + h = (a+b)/2$, $x_2 = x_0 + 2h = b$.

Then Simpson's one third rule is given by

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

$$\Rightarrow \quad \boxed{\int_a^b f(x)\,dx = \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]} \quad \text{——— (5)}$$

Exp. $\int_0^1 \frac{dx}{1+x^2}$. Solve by Simpson's one third rule

Sol^n $\int_0^1 \frac{dx}{1+x^2} = [\tan^{-1}x]_0^1 = \tan^{-1}(1) - \tan^{-1}(0) = \frac{\pi}{4} - 0 = 0.7854$

By Simpson's one third rule, we have

$$\int_0^1 \frac{dx}{1+x^2} = \frac{(1-0)}{6}\left[f(0) + 4f(0.5) + f(1)\right]$$

$$= \frac{1}{6}\left[1 + 4\left(\frac{1}{1+0.25}\right) + 0.5\right]$$

$$= \frac{1}{6}\left[\frac{47}{10}\right]$$

$$= 0.7833$$

Error $= |0.7854 - 0.7833| = 0.0021$

Exp. Evaluate $\int_0^2 e^{-x^2}dx$ by Simpson's one third rule.

taking $n=2$ and $n=4$ and compare both.

Sol^n Do yourself.

Simpson's Three Eight Rule

Putting $n=3$ in the quadrature formula ①, we get

$$\int_{x_0}^{x_0+3h} f(x)dx = \frac{3h}{8}\left[y_0 + 3y_1 + 3y_2 + y_3\right] \qquad (\because \Delta^i y_0 = 0, \forall i>3)$$

Similarly $\int_{x_3}^{x_6} f(x)dx = \frac{3h}{8}\left[y_3 + 3y_4 + 3y_5 + y_6\right]$ etc.

Assuming that n is a multiple of 3, we get

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{3h}{8}\Big[(y_0+y_n) + 3(y_1+y_2+y_4+y_5+\cdots+y_{n-1}) + 2(y_3+y_6+y_9+\cdots)\Big]$$

$$\Rightarrow \boxed{\int_{x_0}^{x_n} f(x)dx = \frac{3h}{8}\Big[(y_0+y_n) + 3(y_1+y_2+y_4+\cdots+y_{n-1}) + 2(y_3+y_6+y_9+\cdots)\Big]} \quad (6)$$

This is called simpson's three eight rule.

Note: The error in the Simpson's three eight rule is of $O(h^4)$.

Since $n=3$, x takes the values x_0, x_1, x_2 or x_3. Then we have $h = (b-a)/3$, $x_0 = a$, $x_1 = x_0 + h = (2a+b)/3$, $x_2 = x_0 + 2h = (a+2b)/3$ and $x_3 = x_0 + 3h = b$. Then Simpson's three eight rule is given by

$$\int_{x_0}^{x_3} f(x)dx \approx \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]$$

$$\Rightarrow \boxed{\int_a^b f(x)dx = \frac{(b-a)}{8}\left[f(a) + 3f\left(\frac{2a+b}{3}\right) + 3f\left(\frac{a+2b}{3}\right) + f(b)\right]} \quad (7)$$

Exp. Evaluate $\int_0^1 \frac{dx}{1+x}$ by Simpson's $\frac{3}{8}$ rule.

Sol^n: $\int_0^1 \frac{dx}{1+x} = \left[\ln(1+x)\right]_0^1 = \ln(\,) - \ln(1) = 0.6931$

By Simpson's 3/8 rule, we have

$$\int_0^1 \frac{dx}{1+x} = \frac{(1-0)}{8}\left[f(0) + 3f\left(\tfrac{1}{3}\right) + 3f\left(\tfrac{2}{3}\right) + f(1)\right]$$

$$= \frac{1}{8}\left[1 + 3\left(\frac{1}{1+1/3}\right) + 3\left(\frac{1}{1+2/3}\right) + \frac{1}{2}\right]$$

$$= \frac{1}{8}\left[\frac{3}{2} + \frac{9}{4} + \frac{9}{5}\right] = \frac{1}{8}\left[\frac{111}{20}\right]$$

$$= 0.6938$$

$$\text{Error} = |0.6931 - 0.6938| = 0.0007$$

Newton – Cote's Open Formulae

Here, we use only function evaluations at the points within the interval not at the end points.

Mid-point Rule

Here, $n=2$, $x_0 = a$, $x_1 = x_0 + h = (a+b)/2$, $x_2 = x_0 + 2h = b$, $h = \frac{b-a}{2}$.

$$\int_{x_0}^{x_2} f(x)dx = 2h\, f(x_0+h) = 2h f(x_1)$$

$$\Rightarrow \boxed{\int_a^b f(x)dx = (b-a) f\left(\frac{a+b}{2}\right)} \quad \text{—— (8)}$$

Two-point Rule

Here $n=3$, $h=(b-a)/3$, $x_0=a$, $x_1=(2a+b)/3$, $x_2=(a+2b)/3$, $x_3=b$.

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{2}\left[f(x_1) + f(x_2)\right]$$

$$\Rightarrow \boxed{\int_a^b f(x)dx = \frac{(b-a)}{2}\left[f\left(\frac{2a+b}{3}\right) + f\left(\frac{a+2b}{3}\right)\right]} \quad \text{—— (9)}$$

Exp. Find the approximate value of

$$I = \int_0^1 \frac{\sin x}{x} dx$$

using (i) mid-point rule (ii) two-point open type rule.

Solⁿ (i) Mid-point rule:

Here, we have $h = (b-a)/2 = 1/2$, $x_0 = 0, x_1 = 1/2, x_2 = 1$.

$$I = \int_0^1 f(x)dx = (b-a) f\left(\frac{a+b}{2}\right) = (1-0) f\left(\frac{1}{2}\right)$$

$$= \frac{\sin(1/2)}{1/2} = 2.\sin(1/2)$$

$$= 0.9589$$

(ii) Two-point rule:

Here, we have $h = (b-a)/3 = 1/3$, $x_0 = 0$,

$x_1 = x_0 + h = (2a+b)/3 = 1/3$ and $x_2 = x_0 + 2h = (a+2b)/3$, $x_3 = 1$.

$$I = \int_0^1 f(x)dx = \frac{(b-a)}{2}\left[f\left(\frac{2a+b}{3}\right) + f\left(\frac{a+2b}{3}\right)\right]$$

$$= \frac{(1-0)}{2}\left[f\left(\frac{1}{3}\right) + f\left(\frac{2}{3}\right)\right]$$

$$= \frac{1}{2}\left[3\sin\left(\frac{1}{3}\right) + \frac{3}{2}\sin\left(\frac{2}{3}\right)\right]$$

$$= 0.9546$$