E-Materials II

Course Name: B.Sc. (H) Geology, B.Sc. (H) Electronics, B.A (H) Economics

(II Year, IV Semester)

Generic Elective: GE4: Numerical Methods

Faculty Name: Mahendra Ram

Richardson Extrapolation

Introduction

Richardson extrapolation is specifically a model for the errors in a numerical procedure. This method is used to improve the numerical method's solution estimation.

Let us consider

$$x_k = x^* + Mh^n \qquad \ldots(1)$$

$$x_k = k\text{th estimate of solution } x^*$$

$$Mh^n = \text{Error term}$$

If we replace h by rh, then we obtain another estimation for x^*

i.e. $$x_{k+1} = x^* + Mr^n h^n \qquad \ldots(2)$$

On multiplying equation (1) by r^n and solving x^*

we get,

$$x^* = x_R = \frac{x_{k+1} - r^n x_k}{1 - r^n}$$

This is known as **Richardson extrapolation** estimate.

Using Richardson extrapolation, we obtain higher order formula from lower order formula, which improves the estimation. This process is known as **extrapolation**.

On considering three-point central difference formula along with its error term we get,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(\theta)$$

$$= D(h) - \frac{h^2}{6} f'''(\theta) \qquad \ldots(1)$$

Here f(x) is exact solution approximated by D(h) and on removing error term, we obtain better approximation.

Now, replace h by rh in equation (1) to get better approximation for $f'(x)$

$$f'(x) = \frac{f(x+rh) - f(x-rh)}{2hr} - \frac{h^2 r^2}{6} f'''(\theta)$$

$$= D(rh) - \frac{h^2 r^2}{6} f'''(\theta) \qquad \ldots(2)$$

Error term can be eliminated by multiplying equation (1) by r^2 and then subtracting it from equation (2)

We get

$$f'(x) = \frac{D(rh) - r^2 D(h)}{1 - r^2} \qquad \ldots(3)$$

This is better estimation of $f'(x)$ as the error term h^2 has been eliminated.

For $r = 2$, equation (3) becomes

$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} \qquad \ldots(4)$$

Equation (4) is five point central difference formula which has error in order of h^4, this error can be further removed by eliminating error term containing h^4 and so on.

One of the commonly used choice for r is 0.5.

Putting $r = 0.5$ in equation (3) we get

$$f'(x) = \frac{f(x-h) - 8\left(x - \frac{h}{2}\right) + 8f\left(x + \frac{h}{2}\right) - f(x+h)}{6h} \qquad \ldots(5)$$

Note: The application of this formula depends on the availability of function values at x $\pm\frac{h}{2}$ points, this will act as restriction when Richardson extrapolation formula is applied to tabulated functions.

Example 1. Show that using the data given below, Richardson's extrapolation technique can provide better estimates for the following derivate:

x :	–0.5	–0.25	0	0.25	0.5	0.75	1.0	1.25	1.5
$f(x) = e^{2x}$	–3.6945	–1.8472	1	1.8472	3.6945	5.5417	7.3890	92363	11.0835

Solution: Let us estimate $f'(x)$ and assume $h = 0.5$ and $r = 1/2$ then, using three-point central formula, we have

$$D(h) = \frac{f(x+h) - f(x-h)}{2h}$$

$$D(0.5) = \frac{f(0.5+0.5) - f(0.5-0.5)}{2(0.5)} = \frac{f(1) - f(0)}{1}$$

$$= \frac{7.3890 - 1}{1} = 6.389 \qquad ...(1)$$

$$D(rh) = \frac{f(x+rh) - f(x-rh)}{2(rh)} = \frac{f(0.5+0.25) - f(0.5-0.25)}{2(0.25)}$$

$$= \frac{5.5417 - 1.8472}{0.5} = 7.389 \qquad ...(2)$$

$$f'(x) = \frac{D(rh) - r^2 D(h)}{1 - r^2}$$

Therefore $$f(0.5) = \frac{7.389 - (0.5)^2 (6.389)}{1 - (0.5)^2} = \frac{7.389 - 0.25(6.389)}{1 - 0.25}$$

$$= 7.7226 \qquad ...(3)$$

Note that the correct answer is 7.7226. The result is much better than the result obtained when $h = 0.5$ & $h = 0.25$ in three-point formula.

Now, let us take $r = 2$ again,

$$D(rh) = D(2(0.5)) = D(1) = \frac{f(1.5) - f(-0.5)}{2(0.5)^2}$$

$$= \frac{11.0825 - (-3.6945)}{4(0.5)} = 7.3885$$

$$f'(0.5) = \frac{D(rh) - r^2 D(h)}{1 - r^2}$$

$$= \frac{7.3885 - 2^2 (6.389)}{1 - 4} \quad \text{[From (1), we have value of } D(h)\text{]}$$

$$= 6.0558 \qquad ...(4)$$

From (3) & (4), we observe that estimate of $r = 0.5$ is much better than estimate at $r = 2$.

Chapter 7

Numerical Integration

Introduction

Process of finding the approximate value of a definite integral from set of numerical values of integrand is called **numerical integration**. If the integrand is a function of single variable the process is called mechanical quadrature, but if the integrand is of two independent variables then this process is called mechanical quadrature.

General Procedure

Numerical integration is performed by changing the integrand into interpolation formula and then applying integration on the interpolation formula between the given limits i.e. we change '*f*' in $\int_a^b f(x)dx$ by an interpolation formula and then integrate the interpolating formula between the limits *a* and *b*.

General Quadrature Formula

Equidistant interpolation formula having relation between *x* and *p* is

$$x = x_0 + ph \qquad \ldots(1)$$

where h is distance between two given nodes then $dx = h*dp$

Let the limit of integration for x be x_0 and $x_0 + nh$, when we integrate the Newton's forward difference formula, we have n equidistant interval of width h.

The limits of p got changed to 0 and n in equation (1) by integrating Newton's forward difference formula:

$$f(x) = f_0 + p\Delta f_0 + \frac{p(p-1)}{2!}\Delta^2 f_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 f_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 f_0 + \ldots$$

On integration,

$$\int_{x_0}^{x_0+nh} f(x)dx = h\int_0^n \left[f_0 + p\Delta f_0 + \frac{p(p-1)}{2!}\Delta^2 f_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 f_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 f_0 + \ldots \right]dp$$

$$= h\left[nf_0 + \frac{n^2}{2}\Delta f_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 f_0}{2} + \left(\frac{n^4}{4} - n^3 + n^2\right)\frac{\Delta^3 f_0}{3!} + \ldots \right] \qquad \ldots(2)$$

Equation (2) represent the general formula.

Now, we can simply get the distinct quadrature formulae by putting *n* = 1, 2, 3 in equation (2).

TRAPEZOIDAL RULE

By putting $n = 1$ in equation (2) i.e., the general formula, we get the difference Δ^2, Δ^3, ..., to be zero and hence for interval $[x_0, x_1]$ we obtain

$$\int_{x_0}^{x_1} f(x)dx = h\left[f_0 + \frac{1}{2}\Delta f_0\right] = h\left[f_0 + \frac{1}{2}(f_1 - f_0)\right] = \frac{h}{2}(f_0 + f_1)$$

which is a **trapezoidal rule.**

Now for next interval $[x_1, x_2], [x_2, x_3], \ldots, [x_{n-1}, x_n]$ we have

$$\int_{x_1}^{x_2} f(x)dx = \frac{h}{2}f(f_1 + f_2)$$

$$\int_{x_2}^{x_3} f(x)dx = \frac{h}{2}(f_2 + f_3)$$

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

Sum up all these above expressions, we get

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}[f_0 + 2(f_1 + f_2 + \ldots + f_{n-1}) + f_n]$$

which is **composite trapezoidal rule.**

Here in this Figure 1 the curve through (x_0, y_0) & (x_1, y_1) is a straight line i.e. polynomial of first order so that difference of order higher than first becomes zero.

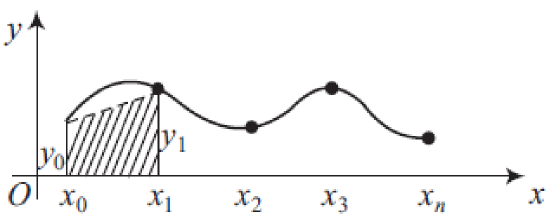

Fig. 1

SIMPSON'S ONE THIRD RULE

Put $n = 2$ in equation (2), then the differences Δ^3, Δ^4, ... are all zero then we have interval of integration from x_0 to $x_0 + 2h$ and the available functional values are f_0, f_1 and f_2 from equation (2), we have

$$\int_{x_0}^{x_0+2h} f(x)dx = 2\left[2f_0 + 2\Delta f_0 + \left(\frac{8}{3} - 2\right)\frac{\Delta^2 f_0}{2}\right]$$

$$= h\left[2f_0 + 2(f_1 - f_0) + \frac{1}{3}(f_2 - 2f_1 + f_0)\right]$$

$$\int_{x_0}^{x_0+2h} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2)$$

which is **Simpson's one third rule.**

Similarly,

$$\int_{x_2}^{x_4} f(x)dx = \frac{h}{3}[f_2 + 4f_3 + f_4]$$

$$\int_{x_4}^{x_6} f(x)dx = \frac{h}{3}[f_4 + 4f_5 + f_6]$$

$$\int_{x_{n-2}}^{x_2} f(x)dx = \frac{h}{3}[f_{n-2} + 4f_{n-1} + f_n]$$

Therefore for even value of *x*, the above expression given

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{h}{3}[(f_0 + f_n) + 4(f_1 + f_3 + \ldots + f_{n-1}) + 2(f_2 + f_4 + \ldots + f_{n-2})]$$

which is **composite Simpson's rule** (**Parabolic rule**)

Note: In this Figure 2 the curve through ($x0$, $y0$), ($x1$, $y1$) & ($x2$, $y2$) is a parabola i.e. polynomial of second order so that difference of higher order than second order vanishes.

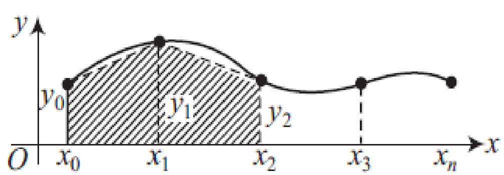

Fig. 2

Simpson's Three-Eight Rule

Put $n = 3$ in Equation (2), then the differences Δ^4, Δ^5, ..., are all zero, then we have available function values f_0, f_1, f_2, f_3, ... From equation (2), we shall obtain,

$$\int_{x_0}^{x_3} f(x)dx = \int_{x_0}^{x_0+3h} f(x)dx = \frac{3h}{8}[f_0 + 3f_1 + 3f_2 + f_3]$$

$$\int_{x_3}^{x_6} f(x)dx = \frac{3h}{8}[f_3 + 3f_4 + 3f_5 + f_6]$$

$$\int_{x_{n-3}}^{x_n} f(x)dx = \frac{3h}{8}[f_{n-3} + 3f_{n-2} + 3f_{n-1} + f_n]$$

Thus, if n is a multiple of 3, by sum up of all above expressions.

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{3h}{8}[(f_0 + f_n) + 3(f_1 + f_2 + f_4 + f_5 + \ldots + f_{n-1}) + 2(f_3 + f_6 + \ldots + f_{n-3})]$$

which is called **Simpson's three-eight rule.**

Note: In this Figure 3 the curve through (x_i, y_i)where i = 0, 1, 2, 3, is a polynomial of third order so that differences above the third order vanishes.

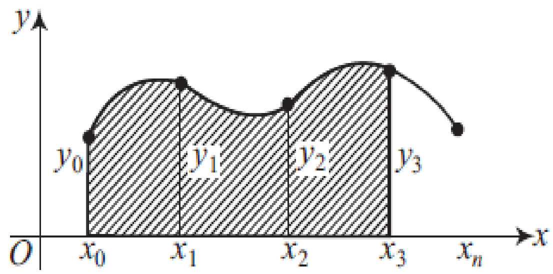

Fig. 3

Error term in Quadrature Formula

Since, we know that function f is approximated by a polynomial of degree n in Quadrature formula.

i.e. $$f(x) \approx P_n(x)$$

On integration, we have

$$\int_{x_0}^{x_n} f(x)dx \approx \int_{x_0}^{x_n} P_n(x)dx \qquad \ldots(1)$$

If $R_n(x)$ is taken as difference between $f(x)$ & $P_n(x)$

then $$f(x) = P_n(x) + R_n(x)$$

Therefore, $$\int_{x_0}^{x_n} f(x)dx = \int_{x_0}^{x_n} P_n(x)dx + \int_{x_0}^{x_n} R_n(x)dx$$

Hence, error between true value of integral and the value of equation (1) is

$$\int_{x_0}^{x_n} R_n(x)dx$$

For n degree polynomial, we have

$$R_n(x) = \frac{f^{(n+1)}(\xi)F(x)}{(n+1)!}, \text{ where } F(x) = \prod_{i=0}^{n}(x - x_i)$$

Now consider equi-spaced ordinates, then

$$x = x_0 + ph \; \& \; x_n = x_0 + nh$$

$$x - x_0 = ph$$

$$x - x_1 = (x_0 + ph) - (x_0 + h) = (p - 1)h$$

$$x - x_2 = (x_0 + ph) - (x_0 + 2h) = (p - 2)h$$

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

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

$$x - x_n = (x_0 + p_h) - (x_0 + nh) = (p - n)h$$

and so $\quad F(x) = h^{n+1}[p(p-1)\,(p-2), \ldots, (p-n)]$

Putting value of $F(x)$ in $R_n(x)$, we get

$$R_n(x) = h^{n+1} \frac{f^{(n+1)}(\xi)}{(n+1)!} p^{(n+1)}$$

where $\quad p^{n+1} = p(p-1)\,(p-2) \ldots (p-n)$

Therefore, error equation in quadrature formula is

$$E_n(x) = \int_{x_0}^{x_n} R_n(x)dx$$

$$= \frac{h}{(n+1)!} \int_0^n h^{n+1} f^{n+1}(\xi) p^{(n+1)} dp$$

$$E_n(x) = \frac{h^{n+2}}{(n+1)!} \int_0^n f^{n+1}(\xi) p^{(n+1)} dp$$

Here ξ is independent of p, integral (above) can be evaluated directly and $E_n(x)$ can be written in two forms

$$E_n(x) = \frac{h^{n+2}}{(n+1)!} f^{n+1}(\xi) \int_0^n p^{(n+1)} dp \; (n \text{ odd})$$

$$E_n(x) = \frac{h^{n+3}}{(n+1)!} f^{n+2}(\xi) \int_0^n \left(p - \frac{n}{2}\right) p^{n+1} \, dp \; (n \text{ even})$$

For example

(i) If $n = 1$, (odd), Trapezoidal rule is obtained.

i.e.,

$$E_1(x) = \frac{h^3}{2!} f''(\xi) \int_0^1 p(p-1)dp$$

$$= \frac{h^3 f''(\xi)}{2} \left[\frac{p^3}{3} - \frac{p^2}{2}\right]_0^1$$

$$= \frac{-h^3 f''(\xi)}{12}, \; x_0 < \xi < x_1$$

Summing up for n intervals,

$$E_n = -\frac{nh^3 f''(\xi)}{12}$$

$$= -\frac{h^2}{12}(x_n - x_0) f''(\xi)$$

Since, $nh = x_n - x_0$

Hence, error in trapezoidal is of order 2.

(ii) If $n = 2$ (even), Simpson's rule is obtained.

The error is given by

$$E_2(x) = \frac{h^5 f^{(iv)}(\xi)}{4!} \int_0^2 (p-1)p(p-1)(p-2)dp$$

$$= \frac{-h^5}{90} f^{(iv)}\,\xi, \quad x_0 < \xi < x_2$$

Summing up for $n/2$ intervals,

$$E_n = -\frac{n}{2}\frac{h^5}{90} f^{(iv)}(\xi) = \frac{-(x_n - x_0)h^4}{180} f^{(iv)}(\xi), \quad x_0 < \xi < x_n$$

Simpson's rule has error of order 4

Therefore, complete Simpson's formula is:

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{3}[f_0 + 4(f_1 + \ldots f_{n-1}) + 2(f_2 + f_4 + \ldots + f_{n-2}) + f_n]$$

$$-\frac{(x_n - x_0)}{180} h^4 f^{(iv)}(\xi)$$

Then the obtained value of E_n is zero if $f^{(iv)}$ is zero.

Hence, when $f(x)$ is a polynomial of either a first, second and a third degree, Simpson's rule yields exact value of $\int_{x_0}^{x_n} f(x)dx$.

Trapezoidal rule for solving integration is

$$\int_a^b f(x)dx \cong \frac{h}{2}[f(a) + f(b)] = \frac{h}{2}[f(x_0) + f(x_1)]$$

Example 1. Evaluate $\int_0^1 x \sin(\pi x)dx$ for $h = 1$.

Solution:

$$\int_0^1 x \sin(\pi x)dx = \frac{1}{2}[f(0) + f(1)] = \frac{1}{2}[0 + 1 \sin \pi]$$

$$= \frac{1}{2}\sin\pi = 0$$

Example 2. Evaluate $\int_0^4 2^x\,dx$ for $h = 4$.

Solution:

$$\int_0^4 2^x\,dx = \frac{4}{2}[f(0) + f(4)]$$
$$= 2[2^0 + 2^4]$$
$$= 2(1 + 2^4)$$
$$= 2 + 2^5 = 34.$$

Example 3. Evaluate $\int_0^2 \sqrt{x}\,dx$ for $h = 2$.

Solution:

$$\int_0^2 \sqrt{x}\,dx = \frac{2}{2}[f(0) + f(2)] = [\sqrt{0} + \sqrt{2}] = \sqrt{2}$$
$$= 1.414$$

Example 4. Evaluate $\int_{-1}^1 \frac{dx}{1+x^2}$

Solution: Here $h = b - a = 2$

$$\int_{-1}^1 \frac{dx}{1+x^2} = \frac{h}{2}\left[\frac{1}{1+1} + \frac{1}{1+1}\right]$$
$$= 1\left(\frac{1}{2} + \frac{1}{2}\right) = 1$$

Example 5. Evaluate $\int_0^2 \log(x^3 + 1)\,dx$

Solution: Here $h = b - a = 2 - 0 = 0$

$$\int_0^2 \log(x^3 + 1)\,dx = \frac{2}{2}[f(0) + f(2)]$$
$$= \log 1 + \log 9 = 0.954$$

Example 6. Dividing the range into 10 equal parts and then apply Simpson's rule to evaluate the integral $\int_0^5 \frac{1}{2x+5}dx$ correct to four decimal places. Hence, find the approximate value of $\log_e 3$.

Solution: The values of the integral for $h = 1/2$

x :	0	1/2	1	3/2	2	5/2	3	7/2	4	9/2	5
$f(x)$:	1/5	1/6	1/7	1/8	1/9	1/10	1/11	1/12	1/13	1/14	1/15

Therefore, by Simpson's one third rule:

$$\begin{aligned}
\int_0^5 \frac{dx}{2x+5} &= \frac{h}{3}[f_0 + 4(f_1 + f_3 + f_5 + f_7 + f_9) + 2(f_2 + f_4 + f_6 + f_8) + f_{10}] \\
&= \frac{1}{6}\left[\left(\frac{1}{5}+\frac{1}{15}\right)+4\left(\frac{1}{6}+\frac{1}{8}+\frac{1}{10}+\frac{1}{12}+\frac{1}{14}\right)+2\left(\frac{1}{7}+\frac{1}{9}+\frac{1}{11}+\frac{1}{13}\right)\right] \\
&= \frac{1}{6}(0.2666+2.1857+0.8436) \\
&= 0.5493
\end{aligned}$$

Also,

$$\begin{aligned}
\int_0^5 \frac{dx}{2x+5} &= \frac{1}{2}[\log(2x+5)]_0^5 \\
&= \frac{1}{2}[\log 15 - \log 5] = \frac{1}{2}\log_e 3 \\
\log_e 3 &= 2\int_0^5 \frac{dx}{2x+5} = 2(0.5493) = 1.0986
\end{aligned}$$