M 402

Institute of Distance and Open Learning
Gauhati University

M.A./M.Sc. in Mathematics
Semester 4

Paper II
Numerical Analysis

Contents :

Math Paper II

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NUMERICAL ANALYSIS

INTRODUCTION :

With the advent of high speed digital computers, the numerical solution of Mathematical problem has come to be regarded as a viable alternative to the time honoured analytical solution. Numerical Analysis is concerned with the methods which give numerical solutions of problems like finding function values (interpolation), differentiation, integration, solutions of equations, solution of differential equations etc. . The method sometimes involve development of algorithms, a sequence of steps to solve a problem . In fact, the development of the subject has received an enormous impetus in the last four decades - not only from the Mathematicians but also from all users of Mathematics like technologist, economists etc..

Unit 1

FINITE DIFFERENCES AND INTERPOLATION

1.1 Finite Differences :

Let us assume that we have a table of values (x_i, y_i) , $i = 0,1,\ldots..n$ of any function $y = f(x)$, the values of x being equally spaced such that $x_1 - x_0 = h$, $x_2 - x_1 = h$, ... $x_n - x_{n-1} = h$. Suppose that we are required to evaluate the values of f(x) for some intermediate values of x or to evaluate the derivative of f(x) for some values of x in the interval $x_0 \le x \le x_n$ .. The various methods to obtain the solution of these problems are based on concept of the difference of a function .

1.2 Forward difference :

If $y_0, y_1, \ldots. y_n$ denote a set of values of any function $y = f(x)$, then $y_1 - y_0$, $y_2 - y_1$,.... $y_n - y_{n-1}$ are called the first differences of function y. Denoting the differences by Δy_0 , Δy_1 , ... Δy_n we have $\Delta y_0 = y_1 - y_0$, $\Delta y_1 = y_2 - y_1$, $\Delta y_2 = y_3 - y_2$, ... $\Delta y_{n-1} = y_n - y_{n-1}$

where Δ is called the forward difference operator . The differences of the first differences are called second differences and denoting them by $\Delta^2 y_0$, $\Delta^2 y_1$ etc. we have

$$\Delta^2 y_0 = \Delta y_1 - \Delta y_0 = y_2 - y_1 - (y_1 - y_0) = y_2 - 2y_1 + y_0$$

$$\Delta^2 y_1 = \Delta y_2 - \Delta y_1 = y_3 - y_2 - (y_2 - y_1) = y_3 - 2y_2 + y_1 \text{ etc.}$$

In like manner, the third , fourth differences etc. are

$$\Delta^3 y_0 = \Delta^2 y_1 - \Delta^2 y_0 = (y_3 - 2y_2 + y_1) - (y_2 - 2y_1 + y_0) = y_3 - 3y_2 + 3y_1 - y_0$$

$$\Delta^4 y_0 = y_4 - 4y_3 + 6y_2 - 4y_1 + y_0 \text{ etc.}$$

The following difference table shows how the difference of all orders are formed .

Forward Difference Table

X	Y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
x_0	y_0					
		Δy_0				
x_1	y_1		$\Delta^2 y_0$			
		Δy_1		$\Delta^3 y_0$		
x_2	y_2		$\Delta^2 y_1$		$\Delta^4 y_0$	
		Δy_2		$\Delta^3 y_1$		$\Delta^5 y_0$
x_3	y_3		$\Delta^2 y_2$		$\Delta^4 y_1$	
		Δy_3		$\Delta^3 y_2$		
x_4	y_4		$\Delta^2 y_3$			
		Δy_4				
x_5	y_5					

1.3 Backward Differences :

The differences $y_1 - y_0$, $y_2 - y_1$, ... $y_n - y_{n-1}$ when denoted by ∇y_1, ∇y_2, ... ∇y_n respectively, are called the first backward difference operator . In a similar manner, we can define backward differences of higher orders . Thus we have ,

$$\nabla^2 y_2 = \nabla y_2 - \nabla y_1 = y_2 - y_1 - (y_1 - y_0) = y_2 - 2y_1 + y_0$$

$$\nabla^3 y_3 = y_3 - 3y_2 + 3y_1 - y_0 \text{ etc.}$$

These differences are exhibited in the following

Backward Difference Table

X	Y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$	$\nabla^5 y$
x_0	y_0					
		∇y_1				
x_1	y_1		$\nabla^2 y_2$			
		∇y_2		$\nabla^3 y_3$		
x_2	y_2		$\nabla^2 y_3$		$\nabla^4 y_4$	
		∇y_3		$\nabla^3 y_4$		$\nabla^5 y_5$
x_3	y_3		$\nabla^2 y_4$		$\nabla^4 y_5$	
		∇y_4		$\nabla^3 y_5$		
x_4	y_4		$\nabla^2 y_5$			
		∇y_5				
x_5	y_5					

1.4 Shift Operator :

The shift operator E is defined by $E\, y(x) = y(x + h)$

A second operation with E would give $E^2 y(x) = y(x + 2h)$

and in general $E^n y(x) = y(x + nh)$

1.5 Relation between the operators :

We have, $\Delta y(x) = y(x+h) - y(x) = E\, y(x) - y(x) = (E - 1)\, y(x)$

$$\therefore \Delta = E - 1 \text{ or } E = 1 + \Delta$$

Further $y(x+h) - y(x) = \nabla\, y(x+h) = \nabla E\, y(x)$

$$\Rightarrow E\, y(x) - y(x) = \nabla E\, y(x) \Rightarrow E - 1 = \nabla E$$

$$\Rightarrow \nabla = 1 - E^{-1}$$

Interpolation

1.6 INTRIODUCTION

Interpolation is the technique of estimating the value of a function for any intermediate value of the independent variable from a set of discrete data available. Suppose we are given the values of $y = f(x)$ for a set of values of x :

x :	x_0	x_1	x_2	....	x_n
y :	y_0	y_1	y_2	......	y_n

Then the process of finding the values of y corresponding to any value of $x = x_i$ between x_0 and x_n is called the interpolation . If the function f(x) is not known explicitly, it is required to find a simple function $\phi(x)$, such that f(x) and $\phi(x)$ agree at the set of tabulated points. If $\phi(x)$ is a polynomial, then it is called the interpolating polynomial and the process is called the polynomial interpolation .

1.7 Newton's Forward Interpolation Formula :

Let $y = f(x)$ denote a function which takes the values $y_0, y_1, y_2, \ldots\ldots y_n$ for equidistant values $x_0, x_1, x_2, \ldots\ldots x_n$ of the independent variable x such that $x_1 - x_0 = h$, $x_2 - x_1 = h$ etc. Let $\phi(x)$ denote a polynomial in x of the nth degree. This polynomial may be written in the form

$$\phi(x) = a_0 + a_1(x-x_0) + a_2(x-x_0)(x-x_1) + a_3(x-x_0)(x-x_1)(x-x_2) + a_4(x-x_0)(x-x_1)(x-x_2)$$

$$(x-x_3) + \ldots + a_n(x-x_0)(x-x_1)(x-x_2)(x-x_3)\ldots(x-x_{n-1}) \qquad \ldots..(1)$$

We shall determine the coefficient $a_0, a_1, a_2, \ldots..a_n$ so as to make

$$\phi(x_0) = y_0, \quad \phi(x_1) = y_1, \phi(x_2) = y_2, \ \ldots \ \phi(x_n) = y_n.$$

Substituting the successive values $x_0, x_1, x_2, \ldots x_n$ for x in (1), at the same time putting $\phi(x_0) = y_0$, $\phi(x_1) = y_1$ etc. and remembering that $x_1 - x_0 = h$, $x_2 - x_0 = 2h$ etc., we have,

$$a_0 = y_0$$

$$y_1 = a_0 + a_1(x_1 - x_0) = y_0 + a_1 h \qquad \therefore a_1 = \frac{y_1 - y_0}{h} = \frac{\Delta y_0}{h}$$

$$y_2 = a_0 + a_1(x_2-x_0) + a_2(x_2-x_0)(x_2-x_1) = y_0 + \frac{y_1 - y_0}{h}(2h) + a_2(2h)(h)$$

$$\therefore a_2 = \frac{y_2 - 2y_1 + y_0}{2h^2} = \frac{\Delta^2 y_0}{2h^2}$$

$$y_3 = a_0 + a_1(x_3-x_0) + a_2(x_3-x_0)(x_3-x_1) + a_3(x_3-x_0)(x_3-x_1)(x_3-x_2)$$

$$= y_0 + \frac{y_1 - y_0}{h}(3h) + \frac{y_2 - 2y_1 + y_0}{2h^2}(3h)(2h) + a_3(3h)(2h)h$$

$$= y_0 + 3y_1 - 3y_0 + 3y_2 - 6y_1 + 3y_0 + 6h^3 a_3$$

$$\therefore a_3 = \frac{y_3 - 3y_2 + 3y_1 - y_0}{6h^3} = \frac{\Delta^3 y_0}{3!h^3}$$

Similarly, $a_4 = \dfrac{\Delta^4 y_0}{4!\,h^4}$, $\quad a_5 = \dfrac{\Delta^5 y_0}{5!\,h^5}$, $\quad \ldots\ldots\ldots \quad a_n = \dfrac{\Delta^n y_0}{n!\,h^n}$

Now since f(x) - ϕ(x) is the difference between the given function and the polynomial at any given point whose abscissa is x , it represents the error committed by replacing the given function by a polynomial . Hence , we have the error

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)(x - x_1)\cdots(x - x_n) \qquad \text{........(6)}$$

where ξ is some value of x between x_0 and x_n . This is the remainder term in formula (2) .

To obtain the remainder term in formula (4) we recall that

$$x-x_0 = hu, \qquad x-x_1 = h(u-1), \quad x-x_2 = h(u-2), \quad x-x_3 = h(u-3)$$

$$\text{............}, \qquad \text{...............}, \qquad x-x_n = h(u-n)$$

Substituting these values of $(x-x_0), (x-x_1) \ldots (x-x_n)$ in (6) , we have ,remainder term ,

$$R_n = \frac{h^{(n+1)} f^{(n+1)}(\xi)}{(n+1)!} u(u-1)(u-2)\cdots(u-n) \qquad \text{........(7)}$$

1.8 Newton's Backward Interpolation Formula :

Backward interpolation formula can be obtained in the same manner as done in the case of Forward interpolation formula . The formula is

$$\phi(x) = y_n + \frac{\nabla y_n}{h}(x - x_n) + \frac{\nabla^2 y_n}{2!h^2}(x - x_n)(x - x_{n-1}) + \cdots + \\ \frac{\nabla^n y_n}{n!h^n}(x - x_n)(x - x_{n-1})\cdots(x - x_1) \qquad (1)$$

Introducing $u = \frac{x - x_n}{h}$ i.e. $x = x_n + uh$, we get

$$\phi(x) = \phi(x_n + uh) = y_n + u\nabla y_n + \frac{u(u+1)}{2!}\nabla^2 y_n + \frac{u(u+1)(u+2)}{3!}\nabla^3 y_n \ldots\ldots \\ \ldots\ldots + \frac{u(u+1)(u+2)(u+n-1)}{n!}\nabla^n y_n \qquad (2)$$

This formula is used mainly for interpolating values of y near the end of a set of tabular values and also for extrapolating values of y a short distance ahead of y_n .

Note: This formula is used for interpolating the values of y near the beginning of a set of tabulated values and extrapolating values of y a little backward (i.e. to the left) of y_0 .

Remainder term of Newton's forward interpolation formula :

To find the remainder term of Newton's forward interpolation formula, we write down the arbitrary function

$$F(t)=f(t)-\phi(t)-[f(x)-\phi(x)]\frac{(t-x_0)(t-x_1)\cdots(t-x_n)}{(x-x_0)(x-x_1)\cdots(x-x_n)} \qquad \dots (5)$$

where f(x) denotes the given function, $\phi(x)$ a polynomial interpolation formula . We shall assume that f(x) is continuous and possesses continuous derivatives of all orders within the interval $[x_0, x_n]$.

Now F(t) vanishes for all (n+2) values $t = x, x_0, x_1, \ldots\ldots x_n$; and since f(x) is continuous and have continuous derivatives of all orders, the same is true for f(t) and hence for F(t) . F(t) therefore satisfies the condition of Rolle's theorem . Hence, the first derivative of f(t) vanishes at least once between every two consecutive zero values of F(t) . Therefore , in the interval from x_0 to x_n , F'(t) must vanish n+1 times ; F''(t) , n times ; F'''(t) (n-1) times etc. . Hence (n+1)th derivative of F(t) will vanish at least once at some point whose abscissa is ξ .

Since $\phi(t)$ is a polynomial of the nth degree, its (n+1)th derivative is zero . Further , since the expression $(t-x_0)$ $(t-x_1)$ .... $(t-x_n)$ is a polynomial of degree (n+1) . it follows that its (n+1)th derivative is the same as the (n+1)th derivative of t^{n+1} which is (n+1)! . Differentiating (5) (n+1) times with respect to t , we therefore have

$$F^{(n+1)}(t) = f^{(n+1)}(t) - 0 - [f(x) - \phi(x)]\frac{(n+1)!}{(x-x_0)(x-x_1)\cdots(x-x_n)}$$

But since $F^{(n+1)}(t) = 0$ at some point $t=\xi$ we have ,

$$0 = f^{(n+1)}(\xi) - [f(x) - \phi(x)]\frac{(n+1)!}{(x-x_0)(x-x_1)\cdots(x-x_n)}$$

Hence, $f(x) - \phi(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n)$

Here x = 1.2 and h = 0.5 . We take x_0=1.0 and hence

$$u = \frac{x - x_0}{h} = \frac{1.2 - 1.0}{0.5} = 0.4$$

Applying Newton's forward interpolation formula

$$f(1.2) = f_0 + u\Delta f_0 + \frac{u(u-1)}{2!}\Delta^2 f_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 f_0$$
$$= 9.0 + 0.4(23.75) + \frac{0.4(-0.6)}{2}(22.5) + \frac{0.4(-0.6)(-1.6)}{6}(7.5) = 9.0 + 9.5 - 2.7 + 0.48$$
$$= 16.28$$

Example 2 : Evaluate f(3.8) from the following data :

x:	0	1	2	3	4
f:	1	1.5	2.2	3.1	4.3

Solution : The finite backward difference table is

x	f	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$
0	1.0				
		0.5			
1	1.5		0.2		
		0.7		0	
2	2.2		0.2		0.1
		0.9		0.1	
3	3.1		0.3		
		1.2			
4	4.3				

Here x = 3.8, h = 1. We take x_n = 4.0 and hence $u = \frac{x - x_n}{h} = \frac{3.8-4}{1} = -0.2$

Applying Newton's backward interpolation formula , we have

$$f(x) = f(x_n) + u\nabla f(x_n) + \frac{u(u+1)}{2!}\nabla^2 f(x_n) + \frac{u(u+1)(u+2)}{3!}\nabla^3 f(x_n)$$

i.e. $f(3.8) = 4.3 - 0.2(1.2) + \frac{-0.2(-0.2+1)}{2} \times 0.3 + \frac{-0.2(-0.2+1)(-0.2+2)}{6} \times 0.1$

$$= 4.3 - 0.24 - 0.024 - 0.0048 = 4.0312$$

GU'90 **Example** : Given $\phi(-0.1) = 0.4602$, $\phi(-0.2) = 0.4207$, $\phi(-0.3) = 0.3021$, find $\phi(-0.15)$.

[Hints : Apply Newton's forward interpolation formula]

Remainder term :

To find the formula for the remainder term in Newton's backward interpolation formula we write down the arbitrary function

$$F(t) = f(t) - \phi(t) - [f(x) - \phi(x)]\frac{(t - x_n)(t - x_{n-1})\cdots(t - x_0)}{(x - x_n)(x - x_{n-1})\cdots(x - x_0)}$$

and differentiate it (n+1) times with respect to t and put $F^{(n+1)}(t) = 0$ for $t = \xi$. We thus find

$$f(x) - \phi(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_n)(x - x_{n-1})\cdots(x - x_0).$$

or, $$\text{Error} = R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_n)(x - x_{n-1})\cdots(x - x_0). \quad .....(3)$$

This is the remainder term of the formula (1) .

The remainder term in terms of $u\left(= \frac{x - x_n}{h}\right)$ is

$$R_n = \frac{h^{n+1}f^{(n+1)}(\xi)}{(n+1)!}u(u+1)(u+2)(u+3)\cdots(u+n) \quad ....(4)$$

Example 1. Compute f(1.2) from the data

x:	1.0	1.5	2.0	2.5	3.0
f:	9.0	32.75	79.0	155.25	269.0

Solution : Here since the required function value is near the beginning of the given table, we shall apply the Newton's forward interpolation formula to evaluate it .

The finite difference table is

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
1.0	9.0				
		23.75			
1.5	32.75		22.5		
		46.25		7.5	
2.0	79.0		30.0		0
		76.25		7.5	
2.5	115.25		37.5		
		113.75			
3.0	269.0				

From the relation (2), we have $f(x_0,x_1,x_2)=\frac{1}{x_0-x_2}[f(x_0,x_1)-f(x_1,x_2)]$

$$=\frac{1}{(x_0-x_2)}\left[\frac{f(x_0)}{x_0-x_1}+\frac{f(x_1)}{x_1-x_0}-\frac{f(x_1)}{x_1-x_2}-\frac{f(x_2)}{x_2-x_1}\right]$$

$$=\frac{f(x_0)}{(x_0-x_2)(x_0-x_1)}+\frac{f(x_1)}{(x_1-x_0)(x_1-x_2)}+\frac{f(x_2)}{(x_2-x_1)(x_2-x_0)} \qquad ....(5)$$

Thus the second divided difference $f(x_0,x_1,x_2)$ is symmetric in its arguments x_0, x_1, x_2. The results suggest that the nth order divided difference is also symmetric in its arguments. Thus,

$$f(x_0,x_1,\cdots x_n)=\frac{f(x_0)}{(x_0-x_1)(x_0-x_2)\cdots(x-x_n)}+\frac{f(x_1)}{(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)}+$$

$$\cdots\cdots+\frac{f(x_n)}{(x_n-x_0)(x_n-x_1)\cdots(x_n-x_{n-1})} \qquad ....(6)$$

It indicates that arguments of the divided difference can be written in any order. Thus,

$$f(x_0,x_1,x_2)=f(x_0,x_2,x_1)=f(x_2,x_1,x_0)$$

1.11 Divided difference when two or more arguments coincide :

If two or more arguments coincide, then the divided difference is defined as the limiting value when one of the coinciding arguments approaches the other. Thus ,

$$f(x_0,x_0)=\lim_{x_1\to x_0}\frac{f(x_1)-f(x_0)}{x_1-x_0}=f'(x_0) \qquad ....(1)$$

Similarly it can be shown that

$$f(x_0,x_0,x_0)=\frac{1}{2!}f''(x_0), \qquad f(x_0,x_0,\cdots x_0)=\frac{1}{r!}\frac{d^r}{dx^r}f(x_0)$$

$(r+1)$ arguments.

1.12 Newton's divided difference interpolation formula :

We have, from the definition of divided difference

$$f(x,x_0)=\frac{f(x)-f(x_0)}{x-x_0} \qquad \therefore f(x)=f(x_0)+(x-x_0)f(x,x_0) \qquad ....(1)$$

Example : Compute f(0.29) using

x:	0.20	1.22	0.24	0.26	0.28	0.30
f(x):	1.6596	1.6698	1.6804	1.6912	1.7024	1.7139

[Hints : Apply Newton's backward interpolation formula .]

1.9 Divided differences :

It is sometimes not possible to obtain values of a function at equidistant values of its arguments . In such cases, it is desirable to have interpolation formulas which are applicable when the functional values are given at unequal intervals of the argument, one of such formulas is known as Newton's divided difference formula .

1.10 Divided differences :

If (x_0,y_0) , (x_1,y_1) , (x_2,y_2), ... be given points , then the first divided difference for the arguments x_0,x_1 is defined by the relation

$$f(x_0, x_1) = \frac{f(x_0) - f(x_1)}{x_0 - x_1} \qquad \text{.......(1)}$$

The second divided difference for x_0, x_1, x_2 is

$$f(x_0, x_1, x_2) = \frac{f(x_0, x_1) - f(x_1, x_2)}{x_0 - x_2} \qquad \text{.........(2)}$$

And the nth divided difference for n+1 points is

$$\frac{f(x_0, x_1, \cdots x_{n-1}) - f(x_1, x_2, \cdots x_n)}{x_0 - x_n} \qquad \text{..........(3)}$$

Symmetry of divided difference :

We have ,

$$f(x_0,x_1) = \frac{f(x_0)}{x_0 - x_1} - \frac{f(x_1)}{x_0 - x_1} = \frac{f(x_0)}{x_0 - x_1} + \frac{f(x_1)}{x_1 - x_0} = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = f(x_1,x_0) \qquad \text{.......(4)}$$

$$\text{Thus } f(x_0,x_1) = f(x_1,x_0)$$

Solve : The divided difference table is :

x	$f(x)$	$\Delta' f(x)$	$\Delta'^2 f(x)$	$\Delta'^3 f(x)$	$\Delta'^4 f(x)$
4	48	$\frac{100-48}{5-4}=52$	$\frac{97-52}{7-4}=15$	$\frac{21-15}{10-14}=1$	
5	100	$\frac{294-100}{7-5}=97$	$\frac{202-97}{10-5}=21$	$\frac{27-21}{11-5}=1$	0
7	294	$\frac{900-294}{10-7}=202$	$\frac{310-202}{11-7}=27$	$\frac{33-27}{13-7}=1$	0
10	900	$\frac{1210-900}{11-10}=310$	$\frac{409-310}{13-10}=33$		
11	1210	$\frac{2028-1210}{13-11}=409$			
13	2028				

By Newton's divided formula are have

$$f(x)=48+52(x-4)+15(x-5)+1(x-4)(x-5)(x-7)=x^2(x-1)$$

$$\therefore f(8)=8^2(8-1) \quad =64.7=448$$

$$f(2)=2^2(2-1) \quad =4.1=4$$

$$f(15)=48+52(15-4)+15(15-4)(15-4)+1(15-4)(15-5)(15-7)=3150$$

Example 5 : - a) Find the third divided difference with arguments 2, 4, 9, 10 of the function $f(x)=x^3-2x$

b) Find a polynomial satis fied by $(-4,12,45)$, $(-1,33)$, $(0,5)$, $(2,9)$ and $(5,1335)$.

Example 6 : Using the following table find $f(x)$ as a polynomials in power of $(x-6)$

x	-1	0	2	3	7	10
f(x)	-11	1	1	1	141	561

1.13 Lagrange's interpolation formula :

Let f(x) denote a polynomial of the nth degree which takes the values $y_0, y_1, y_2, \ldots.. y_n$ when x has the values $x_0, x_1, x_2, \ldots.. x_n$ respectively. Then (n+1)th difference of this polynomial is zero. Hence $f(x, x_0, x_1, x_2, \ldots\ldots x_n)=0$ which gives

Again, $f(x,x_0,x_1)=\dfrac{f(x,x_0)-f(x_0,x_1)}{x-x_1}$ $\quad\therefore f(x,x_0)=f(x_0,x_1)+(x-x_1)f(x,x_0,x_1)$

Substituting this value in (1), we have

$$f(x)=f(x_0)+(x-x_0)f(x_0,x_1)+(x-x_0)(x-x_1)f(x,x_0,x_1) \qquad \text{....(2)}$$

Again, $$f(x,x_0,x_1,x_2)=\frac{f(x,x_0,x_1)-f(x_0,x_1,x_2)}{x-x_2}$$

$$\therefore f(x,x_0,x_1)=f(x_0,x_1,x_2)+(x-x_2)f(x,x_0,x_1,x_2)$$

Substituting this value in (2) we get

$$f(x)=f(x_0)+(x-x_0)f(x_0,x_1)+(x-x_0)(x-x_1)f(x_0,x_1,x_2) \\ +(x-x_0)(x-x_1)(x-x_2)f(x,x_0,x_1,x_2)$$

Continuing this process, we obtain

$$\begin{aligned} f(x) &= f(x_0)+(x-x_0)f(x_0,x_1)+(x-x_0)(x-x_1)f(x_0,x_1,x_2)+\cdots \\ &\qquad +(x-x_0)(x-x_1)\cdots(x-x_n)f(x,x_0,x_1,\cdots x_n) \\ &= f(x_0)+(x-x_0)f(x_0,x_1)+(x-x_0)(x-x_1)f(x_0,x_1,x_2) \\ &\qquad +(x-x_0)(x-x_1)(x-x_2)f(x_0,x_1,x_2,x_3)+(x-x_0)(x-x_1)\cdots(x-x_{n-1})f(x_0,x_1,\cdots,x_{n-1}) \\ &\qquad +\prod_{i=0}^{n}(x-x_i)f(x,x_0,x_1,\cdots,x_n) \end{aligned} \qquad \text{.........(3)}$$

This formula is called the Newton's divided difference interpolation formula where the last term is called the remainder term R.

$$i.e.\ R=\prod_{i=0}^{n}(x-x_i)f(x,x_0,x_1,\cdots x_n)=f(x,x_0,x_1,\cdots x_n)\prod_{i=0}^{n}(x-x_i) \qquad \text{.........(4)}$$

Examples :-4 By means of Newton's divided difference formula. Find the values of $f(2), f(8)$ and $f(15)$ from the folloing table

x :	4	5	7	10	11	13
f(x) :	48	100	294	900	1210	2028

1.14 Remainder term in Lagrange's formula :

Theorem : If $f^{(n+1)}(x)$ is continuous on an interval containing the distinct points $x_0, x_1, \ldots\ldots x_n$, then the remainder term

$$R_n = f(x) - \phi(x) = \frac{W(x)}{(n+1)!} f^{(n+1)}(\xi)$$

where $\phi(x)$ is the interpolating polynomial

$W(x) = (x - x_0)(x - x_1)\cdots(x - x_n) = \prod_{i=0}^{n}(x - x_i)$ and ξ is a point in the interval concerned.

Proof : Let us consider the function defined by

$$F(t) = f(t) - \phi(t) - \frac{W(t)}{W(x)}[f(x) - \phi(x)] \qquad \ldots\ldots(1)$$

where x is distinct from all x_i.

We observe that $F(x)=0$ and $F(x_i)=0$ i.e. $F(t)$ vanishes at $(n+2)$ distinct points . Hence, by Rolle's theorem $F'(t)$ vanishes at least at $(n+1)$ points, $F''(t)$ vanishes at least at n points and so on . Finally $F^{(n+1)}(t)$ vanishes at least at one point, say ξ .

Hence, $$0 = F^{(n+1)}(\xi) = f^{(n+1)}(\xi) - \frac{(n+1)!}{W(x)}[f(x) - \phi(x)]$$

$\phi^{(n+1)}(t) = 0$ and $W^{(n+1)}(t) = (n+1)!$ *Thus,* $f(x) - \phi(x) = \frac{W(x)}{(n+1)!} f^{(n+1)}(\xi)$

If $f(x)$ is itself a polynomial of degree $\leq n$, then $f^{(n+1)}(x) = 0$ and $f(x) = \phi(x)$.

1.15 Advantage and disadvantage of Lagrange's interpolation :

In the Lagrange's interpolation formula one of the main advantage is that there is no restriction in spacing and order of the tabulating points $x_0, x_1, x_2, \ldots\ldots$ etc. However this has the advantage that if we want to increase the degree of the interpolating polynomial by one more interpolating point , the computation is to be made afresh . The previous computation is of little help. This disadvantage is not present in the Newton's divided interpolation formula .

$$\frac{y}{(x-x_0)(x-x_1)(x-x_2)\cdots(x-x_n)}+\frac{y_0}{(x_0-x)(x_0-x_1)(x_0-x_2)\cdots(x-x_n)}$$

$$+\frac{y_1}{(x_1-x)(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)}+\cdots$$

$$+\frac{y_n}{(x_n-x)(x_n-x_0)(x_n-x_1)\cdots(x_n-x_{n-1})}=0$$

$$\Rightarrow\frac{y}{(x-x_0)(x-x_1)(x-x_2)\cdots(x-x_n)}=\frac{y_0}{(x-x_0)(x-x_1)(x_0-x_2)\cdots(x_0-x_n)}+$$

$$\frac{y_1}{(x-x_1)(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)}+\cdots+$$

$$\frac{y_n}{(x-x_n)(x_n-x_0)(x_n-x_1)\cdots(x_n-x_{n-1})}$$

$$\therefore y=\frac{(x-x_1)(x-x_2)\cdots(x-x_n)}{(x_0-x_1)(x_0-x_2)\cdots(x_0-x_n)}y_0+\frac{(x-x_0)(x-x_2)\cdots(x-x_n)}{(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)}y_1+\cdots+$$

$$\frac{(x-x_0)(x-x_1)\cdots(x-x_{n-1})}{(x_n-x_0)(x_n-x_1)\cdots(x_n-x_{n-1})}y_n \qquad \text{.........(1)}$$

The formula can also be written as

$$f(x)=\frac{(x-x_1)(x-x_2)\cdots(x-x_n)}{(x_0-x_1)(x_0-x_2)\cdots(x_0-x_n)}f(x_1)+\frac{(x-x_0)(x-x_2)\cdots(x-x_n)}{(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)}f(x_2)+\cdots+$$

$$\frac{(x-x_0)(x-x_1)\cdots\cdots(x-x_{n-1})}{(x_n-x_0)(x_n-x_1)\cdots\cdots(x_n-x_{n-1})}f(x_n)$$

If we now set

$$\pi(x)=(x-x_0)(x-x_1)\cdots(x-x_{i-1})(x-x_i)(x-x_{i+1})\cdots(x-x_n) \qquad \text{.....(2)}$$

Then $\pi'(x_i)=\frac{d}{dx}[\pi(x)]_{x=x_i}$

$$=(x_i-x_0)(x_i-x_1)\cdots(x_i-x_{i-1})(x_i-x_{i+1})\cdots(x_i-x_n)$$

so that (1) becomes $y=f(x)=\sum_{i=0}^{n}\frac{\pi(x)}{(x-x_i)\pi'(x_i)}y_i$ ....(3)

1.16 Central Difference Interpolation Formulae :

Newton's forward and backward interpolation formulas derived in section 1.7 and section 1.8 are best suited for interpolation near the beginning and end respectively of tabulated values .For interpolation near the middle of tabulated values, central difference formulas are preferable . The most important central difference formulas are the two known as Stirling's and Bassel's formulas . We shall derive them by first deriving three different central difference formulas.

1.17 Gauss Forward Interpolation formula :

From Newton's divided difference interpolation formula , we have

$$f(x)=f(x_0)+(x-x_0)f(x_0,x_1)+(x-x_0)(x-x_1)f(x_0,x_1,x_2)$$
$$+(x-x_0)(x-x_1)(x-x_2)f(x_0,x_1,x_2,x_3)+\cdots\cdots \quad (1)$$

Putting $x_1=x_0+h$, $x_2=x_0-h$, $x_3=x_0+2h$, $x_4=x_0-2h$ etc. , we have

$$f(x)=f(x_0)+(x-x_0)f(x_0,x_0+h)+(x-x_0)(x-x_0-h)\times$$
$$f(x_0,x_0+h,x_0-h)+(x-x_0)(x-x_0-h)(x-x_0+h)\times$$
$$f(x_0,x_0+h,x_0-h,x_0+2h)+(x-x_0)\times(x-x_0-h)\times$$
$$(x-x_0+h)(x-x_0-2h)f(x_0,x_0+h,x_0-h,x_0+2h,x_0-2h)+\cdots$$
$$\text{........(2)}$$

Putting $u=\frac{x-x_0}{h}$ or $x-x_0=uh$ we get

$$f(x)=f(x_0)+hu\,f(x_0,x_0+h)+hu(hu-h)f(x_0-h,x_0,x_0+h)$$
$$+hu(hu-h)(hu+h)f(x_0-h,x_0,x_0+h,x_0+2h)$$
$$+hu(hu-h)(hu+h)(hu-2h)f(x_0-2h,x_0-h,x_0,x_0+h,x_0+2h)+\cdots$$
$$\text{........(3)}$$

Now $f(x_0,x_0+h)=\frac{\Delta y_0}{h}$

$$f(x_0-h,x_0,x_0+h)=\frac{\Delta^2 y_{-1}}{2h^2}$$

$$f(x_0-h,x_0,x_0+h,x_0+2h)=\frac{\Delta^3 y_{-1}}{3!\,h^3}$$

$$f(x_0-2h,x_0-h,x_0,x_0+h,x_0+2h)=\frac{\Delta^4 y_{-2}}{4!\,h^4}$$

Example 1: To what degree of accuracy the value of $\sqrt{70}$ you obtain using Lagrange formula for $f(x)=\sqrt{x}$ choosing the interpolation points $x_0=64$, $x_1=81$, $x_2=100$? [GU '94]

Solution : By Lagrange's interpolation formula we have ,

$$y=\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}y_0+\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}y_1+\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}y_2 \qquad ......(1)$$

Here $x_0=64$, $x_1=81$, $x_2=100$ and $y_0=8$, $y_1=9$, $y_2=10$. Hence, From (1)

$$y(70)=\sqrt{70}=\frac{(70-81)(70-100)}{(64-81)(64-100)}\times 8+\frac{(70-64)(70-100)}{(81-64)(81-100)}\times 9+\frac{(70-64)(70-81)}{(100-64)(100-81)}\times 10$$

$$=\frac{11\times 30}{17\times 36}\times 8+\frac{6(-30)}{17(-19)}\times 9+\frac{6(-11)}{36\times 19}\times 10=4.3137+5.0155-0.9649=8.3643$$

Actual value of $\sqrt{70}$ *is* 8.3667 approximately

Degree of accuracy is $8.3667-8.3643=0.24\times 10^{-2}$

Example 2: Calculate using Lagrange's interpolation formula from the following data :

x:	0.3	0.5	0.6
f(x):	0.6179	0.6915	0.7257

Ans 0.5462

Example 3 : calculate f(1.30), given

x:	0.0	1.2	2.4	3.7
f(x):	3.41	2.68	1.37	-1.18

[use Lagrange's interpolation formula] [Ans 2.60

Example 4 : Given the values

x:	5	7	11	13	17
f(x):	150	392	1452	2366	5202

Evaluate f(9) using Newton's divided difference formula Ans 810

Example 5 : Determine f(x) as a polynomial in x for the following data

x:	-4	-1	0	2	5
f(x):	1245	33	5	9	1335

[Use Newton's divided difference formula] [Ans $3x^4-5x^3+6x^2-14x+5$

$$f(x_0-2h,x_0-h,x_0,x_0+h)=\frac{\Delta^3 y_{-2}}{3!h^3}$$

$$f(x_0-2h,x_0-h,x_0,x_0+h,x_0+2h)=\frac{\Delta^4 y_{-2}}{4!h^4}$$

and so on. Substituting these values into (3), we get

$$f(x)=y_0+u\,\Delta y_{-1}+\frac{u(u+1)}{2!}\Delta^2 y_{-1}+\frac{u(u^2-1)}{3!}\Delta^3 y_{-2}$$
$$+\frac{u(u^2-1)(u+2)}{4!}\Delta^4 y_{-2}+\frac{u(u^2-1)(u^2-2^2)}{5!}\Delta^5 y_{-3}\cdots \quad (4)$$

which is the Gauss backward interpolation formula.

Note : It is used to interpolate the values of y for a negative value of u lying between -1 and 0 .

Example 7 : Use Gauss's forward formula to find the valve of y when y = 3.75 form the following table.

x :	2.5	3.0	3.5	4.0	4.5	5.0
y :	24.145	22.043	20.225	18.644	17.262	16.047

Solution : Taking 3.2 as the orgin and 0.5 and the unit the value of y required will be value

for $u=\frac{3.75-3.5}{0.5}=0.5$

Again Gauss's forward formula is

$$y_u=y_0+u\Delta y_0+\frac{u(u-1)}{2}\Delta^2 y_{-1}+\frac{(u+1)u(u-1)}{6}\Delta^3 y_{-1}$$
$$+\frac{(u+1)u(u-1)(u-2)}{24}\Delta^4 y_{-2}+\frac{(u+2)(u+1)(u-1)u(4-2)}{120}\Delta^5 y_{-2}\ \ldots\ldots\ldots\ldots$$

$$\therefore\ y_5=20.225+5(-1.581)+\frac{(.5)(.5-1)}{2}(.237)$$
$$+\frac{(.5+1)(.5)(.5-1)}{6}\times(-.038)+\frac{(.5+1)(.5)(.5-1)(.5-2)}{24}\times(.0009)$$
$$+\frac{(.5+2)(.5+1)(.5)(.5-1)(0.5-2)}{120}\times(.003)$$

$$=20.225-0.7905+0.029625+0.00238+0.0023750+0.002106=19.40(\text{approx})$$

Substituting these values in (3)

$$f(x)=f(x_0)+u\,\Delta\,y_0+u(u-1)\frac{\Delta^2 y_{-1}}{2!}+u(u^2-1)\frac{\Delta^3 y_{-1}}{3!}$$
$$+u(u^2-1)(u-2)\frac{\Delta^4 y_{-2}}{4!}+\frac{u(u^2-1)(u^2-2^2)}{5!}\Delta^5 y_{-2}+\cdots$$

$$\Rightarrow y=y_0+u\,\Delta\,y_0+u(u-1)\frac{\Delta^2 y_{-1}}{2!}+u(u^2-1)\frac{\Delta^3 y_{-1}}{3!}$$
$$+u(u^2-1)(u-2)\frac{\Delta^4 y_{-2}}{4!}+\frac{u(u^2-1)(u^2-2^2)}{5!}\Delta^5 y_{-2}+\cdots \quad .....(4)$$

which is Gauss forward interpolation formula .

Note: This formula is used to interpolate the values of y for u ($0 < u < 1$) measured forwardly from the origin .

1.17 Gauss Backward Interpolation formula :

We have , the Newton's divided difference interpolation formula

$$f(x)=f(x_0)+(x-x_0)f(x_0,x_1)+(x-x_0)(x-x_1)f(x_0,x_1,x_2)$$
$$+(x-x_0)(x-x_1)(x-x_2)f(x_0,x_1,x_2,x_3)+\cdots \quad ....(1)$$

Putting $x_1 = x_0-h$, $x_2= x_0+h$, $x_3 = x_0-2h$, $x_4= x_0+2h$ etc. , (1) becomes

$$f(x)=f(x_0)+(x-x_0)f(x_0,x_0-h)+(x-x_0)(x-x_0+h)\times$$
$$f(x_0,x_0-h,x_0+h)+(x-x_0)(x-x_0+h)(x-x_0-h)\times$$
$$f(x_0,x_0+h,x_0-h,x_0-2h)+\cdots \quad ....(2)$$

Substituting $u = \frac{x - x_0}{h}$ i.e. $hu = x - x_0$, we have from (2),

$$f(x)=f(x_0)+hu\,f(x_0-h,x_0)+h^2u\,f(x_0-h,x_0,x_0+h)$$
$$+h^3u(u+1)(u-1)f(x_0-2h,x_0-h,x_0,x_0+h)+$$
$$+h^4u(u+1)(u-1)(u+2)f(x_0-2h,x_0-h,x_0,x_0+h,x_0+2h)+\cdots \quad (3)$$

But

$$f(x_0-h,x_0)=\frac{\Delta y_{-1}}{h}$$
$$f(x_0-h,x_0,x_0+h)=\frac{\Delta^2 y_{-1}}{2h^2}$$

Again Gauss backward formula is $y_u = y_0 + {}^{u}c_1 \Delta y_{-1} + {}^{u-1}c_2 \Delta^2 y_{-1} + {}^{u+1}C_3 \Delta^3 y_{-2} + \ldots\ldots\ldots\ldots$

$$Or \quad y_u = y_0 + u\Delta y_{-1} \frac{(u+1)u}{2}\Delta^2 y_{-1} + \frac{(u+1)u(u-1)}{6}\Delta^3 y_{-2} + \frac{(u+2)(u+1)u(u-1)}{24}\Delta^4 y_{-2} + \ldots\ldots\ldots$$

$$Or \quad y_0 = 27 + 0.5\times 7 + \frac{1.5\times .5}{2}\times 5 + \frac{1.5\times .5\times(-0.5)}{6}\times 3$$

$$+ \frac{2.5\times 1.5\times 0.5\times(-0.5)}{24}\times(-7) + \frac{(2.5)\times 1.5\times(0.5)\times(-0.5)}{120}\times(-10)$$

$= 27 + 3.5 + 1.875 - 0.1875 + 0.2734 - 0.11718 = 32.6484 - 0.30468 = 32.3437$ (thousands)

1.18 A Third Gauss formula :

To derive this formula we advance the subscript of x and y by one unit in the Gauss backward formula and put $u - 1 = \frac{x - x_1}{h}$ i.e. $x - x_1 = hu - h$

These changes amount to advancing all subscripts in Gauss's backward formula by one unit and replacing u by (u-1). Thus we get

$$f(x) = y_1 + (u-1)\Delta y_0 + \frac{(u-1)u}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_{-1} + \frac{(u^2-1)u(u-2)}{4!}\Delta^4 y_{-1} + \cdots \qquad (1)$$

which is a Gauss third formula.

1.19 Stirling's formula :

We have, the Gauss forward and Gauss backward formulas,

$$y = y_0 + u\,\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_{-1} + \frac{u(u^2-1)}{3!}\Delta^3 y_{-1} + \frac{u(u^2-1)(u-2)}{4!}\Delta^4 y_{-2}$$
$$+ \frac{u(u^2-1)(u^2-2^2)}{5!}\Delta^5 y_{-2} + \cdots \qquad (1)$$

$$y = y_0 + u\,\Delta y_{-1} + \frac{u(u+1)}{2!}\Delta^2 y_{-1} + \frac{u(u^2-1)}{3!}\Delta^3 y_{-2}$$
$$+ \frac{u(u^2-1)(u+2)}{4!}\Delta^4 y_{-2} + \frac{u(u^2-1)(u^2-2^2)}{5!}\Delta^5 y_{-3} + \cdots \qquad (2)$$

u	y_u	Δy_u	$\Delta^2 y_u$	$\Delta^3 y_u$	$\Delta^4 y_u$	$\Delta^5 y_u$
-2	24.145					
		-2.102				
-1	22.043		0.284			
		-1.818		-0.047		
			.237		.009	
0	20.225			-.038		-.003
		-1.581			.006	
			.199	-.032		
1	18.644					
		-1.382				
			.167			
2	17.262					
		-1.215				
3	16.047					

Example 8:- Use Gauss's forward formula to find y_{30} given that

$y_{21} = 18.4708$, $y_{25} = 17.8144$, $y_{29} = 17.1070$, $y_{33} = 16.3432$, $y_{33} = 15.5154$.

Example :- Find by Gauss's backward formula the sales by a concern for the year 1936 given

Year	1901	1911	1921	1931	1941	1951
Sale	12	15	20	27	39	52

(In thousands)

Solution :- Taking 1931 as the argin and h=10 years as the unit, then sale of the concern is to be found for $u = \frac{1936-1931}{10} = .5$

The difference table is a under

x	$u = \frac{x-1931}{10}$	y_u	Δy_u	$\Delta^2 y_u$	$\Delta^3 y_u$	$\Delta^4 y_u$	$\Delta^5 y_u$
1901	-3	12					
			3				
1911	-2	15		2			
			5		0		
1921	-1	20		2		3	
			7		3		-10
1931	0	27		5		-7	
			12		-4		
1941	1	39		1			
			13				
1951	2	52					

The Striling's formula is

$$y_u = y_0 + u\frac{\Delta y_0 + \Delta y_{-1}}{2} + \frac{u^2}{2}\Delta^2 y_{-1} + \frac{u(u^2-1)}{6}\cdot\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} + \frac{u^2(u^2-1)}{24}\Delta^4 y_{-2}$$

Putting $u = -0.4$ and the values of various difference form the table, are get.

$$y_{-0.4} = 47236 + (-0.4)\frac{-1310-1080}{2} + \left(\frac{0.16}{2}\right)(-230) + \frac{(-0.4)(0.16-1)}{6}\cdot\left(\frac{-80-59}{2}\right) + \frac{(0.16)(0.16-1)}{24}(-21)$$

$$= 47236 + 478 - 18.4 - 3.8920 + .1176 \quad ie.y_{38} = 47692.$$

1.21 Bessel's formula :

We have, the Gauss forward formula and a third Gauss formula are respectively,

$$y = y_0 + u\,\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_{-1} + \frac{u(u^2-1)}{3!}\Delta^3 y_{-1} + \frac{u(u^2-1)(u-2)}{4!}\Delta^4 y_{-2} + \frac{u(u^2-1)(u^2-2^2)}{5!}\Delta^5 y_{-2} + \cdots \qquad \text{(i)}$$

$$y = y_1 + (u-1)\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_{-1} + \frac{u(u^2-1)(u-2)}{4!}\Delta^4 y_{-1} + \frac{u(u^2-1)(u-2)(u-3)}{5!}\Delta^5 y_{-2} + \cdots \qquad \text{(ii)}$$

Taking the mean of (i) and (ii), we have,

$$y = \frac{y_0 + y_1}{2} + \left(u - \frac{1}{2}\right)\Delta y_0 + \frac{u(u-1)}{2!}\cdot\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{u\left(u-\frac{1}{2}\right)(u-1)}{3!}\Delta^3 y_{-1} + \frac{u(u^2-1)(u-2)}{4!}\cdot\frac{\Delta^4 y_{-2} + \Delta^4 y_{-1}}{2} + \frac{u\left(u-\frac{1}{2}\right)(u^2-1)(u-2)}{5!}\Delta^5 y_{-2} + \cdots (I)$$

This is one form of Bessel's formula. (I) can be written in a slightly different form. Since $\Delta y_0 = y_1 - y_0$, the first two terms can be transformed to $y_0 + u\Delta y_0$. Thus (I) becomes, Taking mean of the two formulas (1) and (2) we obtain

$$y = y_0 + u\frac{\Delta y_{-1} + \Delta y_0}{2} + \frac{u^2}{2}\Delta^2 y_{-1} + \frac{u(u^2-1)}{3!}\cdot\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}$$
$$+ \frac{u^2(u^2-1)}{4!}\Delta^4 y_{-2} + \frac{u(u^2-1)(u^2-2^2)}{5!}\cdot\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2} + \cdots \qquad (3)$$

which is the Stirling's formula. It is should be noted that it goes horizontally through y_0.

The path of Stirling's formula across a diagonal difference table is shown below :

Y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$	$\Delta^6 y$
y_{-3}						
	Δy_{-3}					
y_{-2}		$\Delta^2 y_{-3}$				
	Δy_{-2}		$\Delta^3 y_{-3}$			
y_{-1}		$\Delta^2 y_{-2}$		$\Delta^4 y_{-3}$		
	Δy_{-1}		$\Delta^3 y_{-2}$		$\Delta^5 y_{-3}$	
y_0		$\Delta^2 y_{-1}$		$\Delta^4 y_{-2}$		$\Delta^6 y_{-3}$
	Δy_0		$\Delta^3 y_{-1}$		$\Delta^5 y_{-2}$	
y_1		$\Delta^2 y_0$		$\Delta^4 y_{-1}$		
	Δy_1		$\Delta^3 y_0$			
y_2		$\Delta^2 y_1$				
	Δy_2					
y_3						

Note : This formula involves mean of the odd differences just above and below the central line and even differences on this line.

Example -10 : Use stirling's formula to find y_{28}, given

$y_{20} = 49225,\ y_{25} = 48316,\ y_{30} = 47236,\ y_{35} = 45926,\ y_{40} = 44306$

Solution : Taking $x = 30$ as the origin and h=5 as the unit, all are to find the value of y for

$u = \frac{28-30}{5} = 0.4$

x	$u = \frac{x-30}{5}$	y_u	Δy_u	$\Delta^2 y_u$	$\Delta^3 y_u$	$\Delta^4 y_u$
20	-2	49225				
			-909			
25	-1	48316		-171		
			-1080		-59	
30	0	47236		-230		-21
			-1310		-80	
35	1	45926		-310		
			-1620			
40	2	44306				

Y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$	$\Delta^6 y$
y_{-3}						
	Δy_{-3}					
y_{-2}		$\Delta^2 y_{-3}$				
	Δy_{-2}		$\Delta^3 y_{-3}$			
y_{-1}		$\Delta^2 y_{-2}$		$\Delta^4 y_{-3}$		
	Δy_{-1}		$\Delta^3 y_{-2}$		$\Delta^5 y_{-3}$	
y_0		$\Delta^2 y_{-1}$		$\Delta^4 y_{-2}$		$\Delta^6 y_{-3}$
	Δy_0		$\Delta^3 y_{-1}$		$\Delta^5 y_{-2}$	
y_1		$\Delta^2 y_0$		$\Delta^4 y_{-1}$		$\Delta^6 y_{-2}$
	Δy_1		$\Delta^3 y_0$		$\Delta^5 y_{-1}$	
y_2		$\Delta^2 y_1$		$\Delta^4 y_0$		
	Δy_2		$\Delta^3 y_1$			
y_3		$\Delta^2 y_2$				
	Δy_3					
y_4						

1.22 Accuracy of Stirling and Bessel's formulas :

For a given table of differences, the rapidity of convergence depends upon the magnitude of u in Stirling's formula and upon magnitude of v in case of Bessel's formula (IV). The smaller the values of u and v, the more rapidly the series converge. We should therefore always choose the starting point x_0 so as to make u and v as small as possible. In most cases, it is possible to choose the starting point so as to make $-0.5 \le u \le 0.5$ and $-0.5 \le v \le 0.5$.

As a general rule it may be stated that Bessel's formula will give a more accurate result when interpolating near the middle of an interval say from 0.25 to 0.75 ($v = -0.25$ to 0.25); whereas Stirling's formula will give the better result when interpolating near the beginning or end of an interval form $u = -0.25$ to 0.25, say.

1.23 Remainder term in Stirling's formula :

To find the remainder term in Stirling's formula, we write down the arbitrary function

$$F(t) = f(t) - \phi(t) - [f(x) - \phi(x)]\frac{(t-x_0)(t-x_1)(t-x_{-1})\cdots(t-x_n)(t-x_{-n})}{(x-x_0)(x-x_1)(x-x_{-1})\cdots(x-x_n)(x-x_{-n})} \quad \ldots\ldots\ldots\ldots(1)$$

This formula vanishes for the (n+2) values of $t = x, x_0, x_1, \ldots\ldots\ldots x_n, x_{-1}, x_{-2}, \ldots\ldots x_{-n}$. We assume that f(x) is continuous and has continuous derivative of all orders upto 2n+1 . Hence F(t) satisfies the conditions of Rolle's theorem . Also since $\phi(t)$is a polynomial of degree 2n , its (2n+1)th derivative is zero.Hence on differentiating (1) (2n+1) times and putting $F^{(2n+1)}(t) = 0$ for some value $t = \xi$, we get

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\cdot\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{u\left(u-\frac{1}{2}\right)(u-1)}{3!}\Delta^3 y_{-1}$$

$$+\frac{u(u^2-1)(u-2)}{4!}\cdot\frac{\Delta^4 y_{-2} + \Delta^4 y_{-1}}{2} + \frac{u\left(u-\frac{1}{2}\right)(u^2-1)(u-2)}{5!}\Delta^5 y_{-2} + \cdots \quad (II)$$

which is the general form of Bessel's formula. Putting $u = \frac{1}{2}$ in (II), we get

$$y = \frac{y_0 + y_1}{2} - \frac{1}{8}\cdot\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{3}{128}\cdot\frac{\Delta^4 y_{-2} + \Delta^4 y_{-1}}{2} - \frac{5}{1024}\cdot\frac{\Delta^6 y_{-3} + \Delta^6 y_{-2}}{2} + \cdots \quad (III)$$

Formula (III) is also called the 'formula for interpolating halves'. It is used for computing the values of the function midway between any two given values.

A more symmetrical and convenient form of Bessel's formula is obtained by putting $u - \frac{1}{2} = v$ or $u = v + \frac{1}{2}$.

Making the substitution in (II), we get

$$y = \frac{y_0 + y_1}{2} + v\Delta y_0 + \frac{\left(v^2 - \frac{1}{4}\right)}{2!}\cdot\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{v\left(v^2 - \frac{1}{4}\right)}{3!}\Delta^3 y_{-1}$$

$$+\frac{\left(v^2-\frac{1}{4}\right)\left(v^2-\frac{9}{4}\right)}{4!}\cdot\frac{\Delta^4 y_{-2} + \Delta^4 y_{-1}}{2} + \frac{v\left(v^2-\frac{1}{4}\right)\left(v^2-\frac{9}{4}\right)}{5!}\Delta^5 y_{-2}$$

$$+\frac{\left(v^2-\frac{1}{4}\right)\left(v^2-\frac{9}{4}\right)\left(v^2-\frac{25}{4}\right)}{6!}\cdot\frac{\Delta^6 y_{-3} + \Delta^6 y_{-2}}{2} + \cdots \quad (IV)$$

The following table shows the path of Bessel's formula across a diagonal difference table from which we get

$$[f(x)-\phi(x)] = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}(x-x_0)(x-x_1)(x-x_{-1})\cdots(x-x_n)(x-x_{-n})(x-x_{n+1})$$

or

$$\text{Error} = R_n = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}(x-x_0)(x-x_1)(x-x_{-1})\cdots(x-x_n)(x-x_{-n})(x-x_{n+1})$$

Putting

$$\frac{x-x_0}{h} = h \text{ i.e. } x-x_0 = hu \text{, we have}$$

$$x-x_1 = h(u-1),\ x-x_2 = h(u-2),\cdots,x-x_n = h(u-n)$$

and $x-x_{-1} = x-(x_0-h) = x-x_0+h = hu+h = h(u+1)$

$$x-x_{-2} = h(u+2),\ \cdots,x-x_{-n} = h(u+n)$$

as in the case of Stirling's formula, we get

$$R_n = \frac{h^{2n+2}f^{(2n+2)}(\xi)}{(2n+2)!}u(u-1)(u+1)(u-2)\cdots(u-n)(u+n)(u-n-1)$$

which is the remainder term in Bessel's formula..

Example 1 : Use an appropriate formula to find y when x=5.96 from the data given below

x :	5.85	5.90	5.95	6.00	6.05
y :	3.46	8.22	9.64	6.00	2.86

Explain the reason why you have selected the formula you have used . [GU'95

Solution : The difference table is

X	Y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
5.85	y_{-2}=3.46				
		4.76			
5.90	y_{-1}=8.22		-3.34		
		Δy_{-1}=1.42		$\Delta^3 y_{-2}$=-1.72	
x_0=5.95	y_0=9.64		$\Delta^2 y_{-1}$=-5.06		$\Delta^4 y_{-2}$=7.28
		Δy_0= -3.64		$\Delta^3 y_{-1}$=5.56	
6.00	y_1=6.00		0.50		
		-3.14			
6.05	y_2=2.86				

Here we take x_0= 5.95 and y_0= 9.64, h = 0.05 . Given x = 5.96

$$0 = f^{(2n+1)}(\xi) - 0 - [f(x) - \phi(x)]\frac{(2n+1)!}{(x-x_0)(x-x_1)(x-x_{-1})\cdots(x-x_n)(x-x_{-n})}$$

which gives

$$[f(x) - \phi(x)] = \frac{f^{(2n+1)}(\xi)}{(2n+1)!}(x-x_0)(x-x_1)(x-x_{-1})\cdots(x-x_n)(x-x_{-n})$$

$$\text{or, Error} = R_n = \frac{f^{(2n+1)}(\xi)}{(2n+1)!}(x-x_0)(x-x_1)(x-x_{-1})\cdots(x-x_n)(x-x_{-n}) \quad ....(2)$$

Putting $\frac{x-x_0}{h} = h$ i.e. $x - x_0 = hu$, we have

$x - x_1 = h(u-1)$, $x - x_2 = h\,(u-2), \cdots, x - x_n = h\,(u-n)$

and $x - x_{-1} = x - (x_0 - h) = x - x_0 + h = hu + h = h(u+1)$

$x - x_{-2} = h(u+2), \cdots, x - x_{-n} = h(u+n)$

$\therefore$ from (2) we get $\quad R_n = \frac{h^{2n+1} f^{(2n+1)}(\xi)}{(2n+1)!} u(u^2-1)(u^2-2^2)\cdots(u^2-n^2)$

where ξ is some value of x between x_{-n} and x_n .

1.24 Remainder term in Bessel's formula :

To find the remainder tern in Bessel's formula we write down the arbitrary function

$$F(t) = f(t) - \phi(t) - [f(x) - \phi(x)]\frac{(t-x_0)(t-x_1)(t-x_{-1})\cdots(t-x_n)}{(x-x_0)(x-x_1)(x-x_{-1})\cdots(x-x_n)} \times \frac{(t-x_{-n})(t-x_{n+1})}{(x-x_{-n})(x-x_{n+1})} \quad ....(1)$$

This formula vanishes at the 2n+3 points $t = x$, x_0 , x_1 , x_{-1} , ...x_n , x_{-n} , x_{n+1} . Since $\phi(t)$ is a polynomial of degree 2n+1 , its (2n+2)th derivative is zero . Hence on differentiating (1) 2n+2 times with respect to t and putting $F^{(2n+2)}(t) = 0$ for some value $t = \xi$, we get

$$0 = f^{(2n+2)}(\xi) - 0 - [f(x) - \phi(x)]\frac{(2n+2)!}{(x-x_0)(x-x_1)(x-x_{-1})\cdots(x-x_n)} \times \frac{1}{(x-x_{-n})(x-x_{n+1})}$$

i.e. $0.25 \le u \le 0.75$. Hence we apply Bessel's formula which is given by

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\cdot\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{u\left(u-\frac{1}{2}\right)(u-1)}{3!}\Delta^3 y_{-1}$$
$$+ \frac{u(u^2-1)(u-2)}{4!}\cdot\frac{\Delta^4 y_{-2} + \Delta^4 y_{-2}}{2} + \cdots \qquad (1)$$

Substituting the values of y_0 , Δy_0 , Δy_{-1} , Δy_{-2} etc. from the difference table in (1) we get

$$y(15) = 0 + 0.5\times 2 + \frac{0.5(0.5-1)}{2}\times\frac{3+1}{2} + \frac{0.5\left(0.5-\frac{1}{2}\right)(0.5-1)}{6}\times(-2)$$
$$+ \frac{0.5(0.5^2-1)(0.5-2)}{24}\times\left(\frac{-5}{2}\right)$$

$= 0.668$ approximately.

Example 3 : Use an appropriate central difference formula to compute f(5.6) from the given data below :

x :	3	4	5	6	7	8
f(x) :	6.28	8.92	16.50	12.62	7.35	5.37

[GU'96

Solution : The difference table is

X	Y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
3	$y_{-2}=6.28$					
		2.64				
4	$y_{-1}=8.92$		$\Delta^2 y_{-2}=4.94$			
		$\Delta y_{-1}=7.58$		$\Delta^3 y_{-2}=-16.4$		
$x_0=5$	$y_0=16.50$		$\Delta^2 y_{-1}=-11.46$		$\Delta^4 y_{-2}=26.47$	
		$\Delta y_0=-3.88$		10.07		$\Delta^5 y_{-2}=-31.86$
6	$y_1=12.62$		$\Delta^2 y_0=-1.39$		$\Delta^4 y_{-1}=-5.39$	
		−5.27		4.68		
7	$y_2=7.35$		3.29			
		−1.98				
8	$y_3=5.37$					

Here we take $x_0 = 5$, $y_0 = 16.50$. $h = 1$ and $x = 5.6$ (given).

$$\therefore u = \frac{x - x_0}{h} = \frac{5.6-5}{1} = 0.6$$

$$\therefore u = \frac{x - x_0}{h} = \frac{5.96 - 5.95}{0.05} = \frac{0.01}{0.05} = 0.2$$

Here, $-0.25 \le u \le 0.25$, hence we apply Stirling's formula which is given by

$$y = y_0 + u\frac{\Delta y_{-1} + \Delta y_0}{2} + \frac{u^2}{2}\Delta^2 y_{-1} + \frac{u(u^2-1)}{3!}\cdot\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} + \frac{u^2(u^2-1)}{4!}\Delta^4 y_{-2} + \cdots \quad (1)$$

Using (1) and the values of the differences Δy_0, Δy_{-1}, $\Delta^2 y_{-1}$, $\Delta^3 y_{-1}$ etc., we have

$$y(5.96) = 9.64 + 0.2 \times \frac{1.42 - 3.64}{2} + \frac{(0.2)^2}{2}(-5.06) + \frac{0.2\{(0.2)^2 - 1\}}{6} \times \frac{5.56 - 1.72}{2} + \frac{(0.2)^2\{(0.2)^2 - 1\}}{24} \times 7.28$$

$= 9.64 - 0.222 - 0.1092 - 0.06144 - 0.011648 \quad = 9.224$ approximately.

Example 2 : Given the data set

x :	10	12	14	16	18
y ;	2	1	0	2	5

Compute y for x=15. {GU'92

Solution : The difference table is

X	Y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
10	$y_{-2}=2$				
		-1			
12	$y_{-1}=1$		0		
		$\Delta y_{-1}=-1$		$\Delta^3 y_{-2}=3$	
$x_0=14$	$y_0=0$		$\Delta^2 y_{-1}=3$		$\Delta^4 y_{-2}=-5$
		$\Delta y_0=2$		$\Delta^3 y_{-1}=-2$	
16	$y_1=2$		$\Delta^2 y_0=1$		
		3			
18	$y_2=5$				

We take $x_0 = 14$ and $y_0 = 0$. Here $h = 2$ and $x = 15$ (given)

$$\therefore u = \frac{x - x_0}{h} = \frac{15 - 14}{2} = 0.5$$

Example : Apply Bessel's formula to obtain y_{25} given $y_{20} = 2854$, $y_{24} = 3162$,

$y_{28} = 3544$, $y_{32} = 3992$. [Ans 3256.78

1.25 Linear Interpolation :

Suppose a function f is linear in its argument x i.e. it is of the form

$f(x) = A_0 + A_1 x$, A_0 , A_1 are constants .

For $x = x_0$ and x_1 we have $f(x_0) = A_0 + A_1 x_0$, $f(x_1) = A_0 + A_1 x_1$

So that $f(x_1) - f(x_0) = A_1(x_1 - x_0)$ i.e. $\dfrac{f(x_1) - f(x_0)}{x_1 - x_0} = A_1$, which is a constant .

Thus the assumption that a function is approximately linear in a certain range is equivalent to the assumption that the ratio

$$\frac{f(x_1) - f(x_0)}{x_1 - x_0} \qquad \text{.................... (1)}$$

i.e. the first divided difference $f(x_0, x_1)$ of f relative to x_0 and x_1 is independent of x_0 and x_1 . So the linear approximation may be expressed in the form

$$f(x_0, x) \approx f(x_0, x_1) \qquad \text{................(2)}$$

This leads to the approximation formula $f(x) \approx f(x_0) + (x - x_0) f(x_0, x_1)$

$$\Rightarrow f(x) \approx f(x_0) + (x - x_0)\frac{f(x_1) - f(x_0)}{x_1 - x_0} \qquad (3)$$

$$= \frac{1}{x_1 - x_0}\left[(x_1 - x_0)f(x_0) + (x - x_0)\{f(x_1) - f(x_0)\}\right]$$

$$= \frac{1}{x_1 - x_0}\left[(x_1 - x)f(x_0) - (x_0 - x)f(x_1)\right] = \frac{1}{x_1 - x_0}\begin{vmatrix} f(x_0) & x_0 - x \\ f(x_1) & x_1 - x \end{vmatrix}$$

1.26 Error in Linear Interpolation :

A simple formula can be derived for the error involved in linear interpolation . The formula

Thus $0.25 \le u \le 0.75$

$\therefore$ We apply Bessel's formula which gives

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\cdot\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{u\left(u-\frac{1}{2}\right)(u-1)}{3!}\Delta^3 y_{-1}$$
$$+ \frac{u(u^2-1)(u-2)}{4!}\cdot\frac{\Delta^4 y_{-2} + \Delta^4 y_{-1}}{2} + \frac{u\left(u-\frac{1}{2}\right)(u^2-1)(u-2)}{5!}\Delta^5 y_{-2} + \cdots (1)$$

Substituting the values of y_0, Δy_0, Δy_{-1}, Δy_{-2} etc. from the difference table in (1) we get

$$f(5.6) = 16.5 + 0.6(-3.88) + \frac{0.6(0.6-1)}{2}\times\frac{-11.46-1.39}{2} +$$
$$\frac{0.6(0.6-0.5)(0.6-1)}{3!}(10.07) + \frac{0.6(0.36-1)(0.6-2)}{4!}\times$$
$$\frac{26.47-5.39}{2} + \frac{0.6(0.6-0.5)(0.36-1)(0.6-2)}{5!}(-31.86) + \cdots$$

$= 15.1245$ approximately.

Example : The following table gives the values of e^x for certain equidistant values of x. Find the value of e^x when x=0.644 using appropriate formula :

x	0.61	0.62	0.63	0.64	0.65	0.66	0.67
e^x	1.840	1.859	1.878	1.897	1.916	1.935	1.954

[Use Stirling's formula] [Ans 1.9045

Example : the function

$$k(\alpha) = \int_0^{\frac{\pi}{2}} \frac{dy}{\sqrt{1-\sin^2\alpha\sin^2\psi}}$$ is tabulated below

α	0	5	10	15	20
K(α)	1.5708	1.5738	1.5828	1.5981	1.6200

Compute k(9) by Stirling's formula [Ans 1.5805

Example: What is the maximum error of linear interpolation for logx with $0.4 < x < 0.5$?

[GU'93

Example : The function 1/N is tabulated in Barlow's tables at unit interval from 1 to 12500 . Find the possible error in the linear interpolation of this function when N=650 .

Solution : $f(N)=\frac{1}{N}$ $\therefore f''(N)=\frac{2}{N^3}$

Taking h = 1 , N = 650 , and substituting in

$E\le\frac{h^2M}{8}$, we have $E\le\frac{1}{4\times(650)^2}=\frac{1}{1098500000}$. *i.e.* $E\le10^{-9}$

❖❖❖

$$f(x) = f(x_0) + \frac{x - x_0}{x_1 - x_0}[f(x_1) - f(x_0)]$$

can be written as

$$f(x) = f(x_0) + \frac{x - x_0}{h}\Delta f(x_0) = y_0 + \frac{x - x_0}{h}\Delta y_0 \qquad \text{.............. (1)}$$

The formula (1) is the Newton's forward interpolation formula terminating after two terms i.e. with $n = 1$.

The error term in Newton's forward interpolation formula is

$$R_n = \frac{(x - x_0)(x - x_1)\cdots(x - x_n)}{(n+1)!} f^{(n+1)}(\xi) \qquad x_0 < \xi < x_n$$

Putting $n = 1$, the error in linear interpolation is

$$R_1 = \frac{(x - x_0)(x - x_1)}{2!} f''(\xi), \qquad x_0 < \xi < x_1$$

Taking $u = \frac{x - x_0}{h}$, we have

$$R_1 = \frac{h^2}{2} f''(\xi) u(u-1) \qquad \text{.................... (2)}$$

So, the maximum error involved will be

$$R_{1(max)} = \frac{h^2}{2} f''(\xi) u(u-1) = \frac{h^2}{2} M\, u(u-1) = \frac{h^2}{2} M(u^2 - u)$$

where M is the mean absolute value of $f''(x)$ in any interval h. For maximum error we have,

$$\frac{dR_1}{du} = \frac{h^2 M}{2}(2u - 1) = 0 \qquad \text{which gives } u = ½$$

$$|R_{max}| = \left|\frac{h^2 M}{2}\left(\frac{1}{4} - \frac{1}{2}\right)\right| = h^2 \frac{M}{8}$$

The formula for maximum error E is

$$E \le \frac{h^2 M}{8} \qquad \text{.............. (3)}$$

At $x = x_0$, $u = 0$. Hence putting $u = 0$ we have

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

Again differentiating (1) with respect to x, we get

$$\frac{d^2y}{dx^2} = \frac{d}{du}\left(\frac{dy}{dx}\right)\frac{du}{dx} = \frac{1}{h}\left[\frac{2}{2!}\Delta^2 y_0 + \frac{6u-6}{3!}\Delta^3 y_0 + \cdots\right]\frac{1}{h}$$

Putting $u = 0$, we obtain

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

***(II) Derivatives using Backward Difference formula and Central difference formula :**

Proceeding in the same manner as that in §2.2 (I), derivatives for backward and Central difference formula can be obtained as follows:

$$\left(\frac{dy}{dx}\right)_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \cdots\right] \qquad \ldots(4)$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \cdots\right] \qquad \ldots(5)$$

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left[\frac{\Delta y_0 + \Delta y_{-1}}{2} - \frac{1}{6}\frac{\Delta^3 y_{-1} + \Delta^4 y_{-2}}{2} + \cdots\right] \qquad \ldots(6)$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \frac{1}{90}\Delta^6 y_{-3} \cdots\right] \qquad \ldots(7)$$

[*For details, see any standard book on Numerical Analysis].

(4) and (5) are the derivatives using Backward difference interpolation formula and (6) and (7) are the derivatives using Stirling's formula.

Example 1 Compute $f'(0.1)$ from the following data :

x :	0	1	2	3	4
f :	1	0	1	10	33

Unit 2

Numerical Differentiation and Integration

2.1 Numerical Differentiation :

It is the process of calculating the value of the derivative, of a tabulated function at some assigned value of the independent variable x from the given set of values (x_i , y_i). To compute $\frac{dy}{dx}$, we first replace the exact relation $y = f(x)$ by the best interpolating polynomial $y = \varphi(x)$ and then differentiate the latter as many times as we desire. The choice of the interpolation formula to be used, will depend on the assigned value of x at which $\frac{dy}{dx}$ is desired.

If the values of x are equispaced and $\frac{dy}{dx}$ is required near the beginning of the table, we employ Newton's forward formula. For finding derivative near the end of the table we use Newton's Backward formula. For values near the middle of the table, $\frac{dy}{dx}$ is calculated by means of Stirling's or Bessel's formula.

2. 2 Formulae for derivatives :

Consider the function $y = f(x)$ which is tabulated for the values $x_i(=x_0 + ih)$, $i = 0, 1, 2, \ldots, n$.

(I) Derivatives using forward difference formula :

Newton's forward Interpolation formula is

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots \qquad \text{where } u = \frac{x - x_0}{h}$$

Differentiating both sides with respect to u, we have

$$\frac{dy}{du} = \Delta y_0 + \frac{2u-1}{2!}\Delta^2 y_0 + \frac{3u^2 - 6u + 2}{3!}\Delta^3 y_0 + \cdots$$

$$\text{Now, } \frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2u-1}{2!}\Delta^2 y_0 + \frac{3u^2 - 6u + 2}{3!}\Delta^3 y_0 + \cdots\right] \qquad (1)$$

$$\text{where} \qquad u = \frac{x - x_0}{h}$$

we have

$$\left(\frac{dy}{dx}\right)_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \frac{1}{5}\nabla^5 y_n + \frac{1}{6}\nabla^6 y_n + \cdots\right] \quad \text{(i)}$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \frac{137}{180}\nabla^6 y_n + \cdots\right] \quad \text{(ii)}$$

Here $h = 0.1$, $x_n = 1.6$, $\nabla y_n = 0.281$, $\nabla^2 y_n = -0.018$ etc.

Putting these values in (i) and (ii) we get

$$\left(\frac{dy}{dx}\right)_{x=1.6} = \frac{1}{0.1}\left[0.28 + \frac{1}{2}(-0.018) + \frac{1}{3}(0.005) + \frac{1}{4}(-0.001) + \frac{1}{5}(-0.001) + \frac{1}{6}(0.003)\right]$$

$$= 2.727$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=1.6} = \frac{1}{(0.1)^2}\left[-0.018 + 0.005 + \frac{11}{12}(-0.001) + \frac{5}{6}(-0.001) + \frac{137}{180}(-0.003)\right]$$

$$= -1.703$$

EXERCISES

1. Find $y'(0)$ and $y''(0)$ from the following table :

x :	0	1	2	3	4	5
y :	4	8	15	7	6	2

[Ans. –27.9, 117.67]

2. Find the first and second derivatives of the function tabulated below, at the point $x = 1.1$:

x :	1.0	1.2	1.4	1.6	1.8	2.0
f :	0	0.128	0.544	1.296	2.432	4.00

[Ans. 0.63, 6.6]

3. From the following table, find the values of $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at $x = 2.03$

x :	1.96	1.98	2.00	2.02	2.04
y:	0.7825	0.7739	0.7651	0.7563	0.7473

[Ans. –0.06, 0.5]

4. Compute $f'(6)$ and $f''(6.3)$ from the following table:

x :	6.0	6.1	6.2	6.3	6.4
f :	1.1750	0.8002	0.777	0.7578	0.7404

[Ans. –7.5492, -2.6633]

The difference table is

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
0	1				
		-1			
1	0		2		
		1		6	
2	1		8		0
		9		6	
3	10		14		
		23			
4	33				

Here h = 1, $u = \frac{x - x_0}{h} = \frac{0.1 - 0}{1} = 0.1$

$$\Delta f_0 = -1, \quad \Delta^2 f_0 = 2, \quad \Delta^3 f_0 = 6, \quad \Delta^4 f_0 = 0.$$

Hence from formula for derivative using forward difference formula is

$$f'(0.1) = -1 + \frac{(0.2 - 1)}{2} \times 2 + \frac{(0.03 - 0.6 + 2)}{6} \times 6 = -0.37 \text{(approximately)}$$

Example 2 Given that:

x :	1.0	1.1	1.2	1.3	1.4	1.5	1.6
f :	7.989	8.403	8.781	9.129	9.451	9.750	10.031

find $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at x = 1.6.

Solution : The difference table is

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$	$\nabla^5 y$	$\nabla^6 y$
1.0	7.989						
		0.414					
1.1	8.403		-0.036				
		0.378		0.006			
1.2	8.781		-0.030		-0.002		
		0.348		0.004		0.002	
1.3	9.129		-0.026		0.0		-0.003
		0.322		0.004		-0.001	
1.4	9.451		-0.023		-0.001		
		0.299		0.005			
1.5	9.750		-0.018				
		0.281					
1.6	10.031						

which is the general quadrature formula. We can obtain different integration formulae by putting n = 1, 2, 3, 4, 5, 6, ...etc.

2.4 Trapezoidal Rule :

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

$$\int_{x_0}^{x_0+h} y\,dx = h\left[y_0 + \frac{1}{2}\Delta y_0\right] = h\left[y_0 + \frac{1}{2}(y_1 - y_0)\right] = \frac{h}{2}[y_0 + y_1] \qquad \text{...(i)}$$

For the next interval $[x_1, x_2]$ we deduce similarly

$$\int_{x_1}^{x_2} y\,dx = \frac{h}{2}[y_1 + y_2] \qquad \text{...(ii)}$$

and so on. For the 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 these expressions, we obtain the rule,

$$\int_{x_0}^{x_n} y\,dx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + \cdots + y_{n-1}) + y_n]$$ which is the trapezoidal rule.

Error in Trapezoidal rule :

Let f be continuous and possess continuous derivatives in $[x_0, x_n]$. Expanding $y(=f(x))$ in Taylor's series around $x = x_0$, we get

$$\int_{x_0}^{x_1} y\,dx = \int_{x_0}^{x_0+h} [y_0 + (x - x_0)y'_0 + \frac{(x - x_0)^2}{2!}y''_0 + \cdots]\,dx$$

$$= hy_0 + \frac{h^2}{2}y'_0 + \frac{h^3}{6}y''_0 + \cdots \qquad (1)$$

Also, $$\frac{h}{2}[y_0 + y_1] = \frac{h}{2}\left[y_0 + (y_0 + hy'_0 + \frac{h^2}{2!}y''_0 + \cdots\right]$$

$$= hy_0 + \frac{h^2}{2}y'_0 + \frac{h^3}{4}y''_0 + \cdots \qquad \text{...(2)}$$

$\therefore$ Error in the interval $[x_0, x_1]$ $$\int_{x_0}^{x_1} y\,dx - \frac{h}{2}[y_0 + y_1] = -\frac{h^3}{12}y''_0$$

2.3 Numerical Integration

Numerical Integration is the process of computing the value of a definite integral from a set of tabulated values of the integrand f(x). The process when applied to a function of single variable, is known as quadrature.

The problem of numerical integration is solved by representing the integrand by an interpolation formula and then integrating this formula between the desired limits.

Thus to find the value of the definite integral $\int_b^a f(x)dx$, we replace the function f(x) by an interpolation formula and then integrate it between the limits a and b.

$$\text{Let } I = \int_b^a y dx = \int_b^a f(x)dx$$

Where y takes the values $y_0, y_1, \ldots, y_n$ for $x = x_0, x_1, \ldots, x_n$ respectively. Let the interval [a,b] be divided into n equal subintervals of width h so that $x_0 = a$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h \ldots, x_n = x_0 + nh$. Then

$$I = \int_{x_0}^{x_0+nh} f(x)dx$$

$$= h\int_0^n \left\{ y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots + \frac{u(u-1)\ldots(u-n+1)}{n!}\Delta^n y_0 \right\} du$$

$$\text{where } u = \frac{x - x_0}{h}$$

$$= h\left[ny_0 + \frac{n^2}{2}\Delta y_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 y_0}{2} + \left(\frac{n^4}{4} - n^3 + n^2\right)\frac{\Delta^3 y_0}{6} + \cdots \right]$$

$$= nh\left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \right.$$

$$\left(\frac{n^4}{5} - \frac{3n^3}{2} + \frac{11n^2}{3} - 3n\right)\frac{\Delta^4 y_0}{4!} + \left(\frac{n^5}{6} - 2n^4 + \frac{35n^3}{4} - \frac{50n^2}{3} + 12n\right)\frac{\Delta^5 y_0}{5!} +$$

$$\left.\left(\frac{n^6}{7} - \frac{15n^5}{6} + 17n^4 - \frac{225n^3}{4} + \frac{274n^2}{3} - 60n\right)\frac{\Delta^6 y_0}{6!}\right] \qquad (1)$$

Also A_1 = area over the first strip by Simpson's $\frac{1}{3}$ rule

$$= \frac{h}{3}[y_0 + 4y_1 + y_2] \qquad \ldots(2)$$

Also from (1) of §2.4

$$y_1 = y_0 + hy'_0 + \frac{h^2}{2!}y''_0 + \frac{h^3}{3!}y'''_0 + \cdots$$

Again putting $x = x_0 + 2h$ and $y = y_2$ in (1) of §2.4 we have

$$y_2 = y_0 + 2hy'_0 + \frac{4h^2}{2!}y''_0 + \frac{8h^3}{3!}y'''_0 + \cdots$$

Substituting these values of y_1 and y_2 in (2) we get

$$A_1 = \frac{h}{3}\left[y_0 + 4\left(y_0 + hy'_0 + \frac{h^2}{2!}y''_0 + \frac{h^3}{3!}y'''_0 + \cdots\right)\right.$$

$$\left. + \left(y_0 + 2hy'_0 + \frac{4h^2}{2!}y''_0 + \frac{8h^3}{3!}y'''_0 + \cdots\right)\right]$$

$$= 2hy_0 + 2h^2y'_0 + \frac{4h^3}{3}y''_0 + \frac{2h^2}{3}y'''_0 + \frac{5h^5}{18}y_0^{iv} + \cdots \qquad (3)$$

$\therefore$ Error in the interval $[x_0, x_2] = \int_{x_0}^{x_2} y\,dx - A_1$

$$= \left(\frac{4}{15} - \frac{5}{18}\right)h^5 y_0^{iv} + \cdots \qquad [(1)-(3)]$$

i.e. the principal part of the error in $[x_0, x_2]$

$$= \left(\frac{4}{15} - \frac{5}{18}\right)h^5 y_0^{iv} = -\frac{h^5}{90}y_0^{iv}$$

Similarly, the principal part of the error in $[x_2, x_4]$

$$= -\frac{h^5}{90}y_2^{iv} \text{ and so on.}$$

Hence the total error

$$E = -\frac{h^5}{90}\left[y_0^{iv} + y_2^{iv} + \cdots + y_{2(n-1)}^{iv}\right]$$

Assuming $y^{iv}(\bar{x})$ as the largest of

$$y_0^{iv}, y_2^{iv}, \cdots, y_{2(n-1)}^{iv} \text{ we get}$$

i.e. principal part of the error in $[x_0, x_1]$ is $-\frac{h^3}{12}y''_0$.

Similarly, principal part of the error in $[x_1, x_2]$ is $-\frac{h^3}{12}y''_1$ and so on.

$\therefore$ Total error $$E = -\frac{h^3}{12}[y''_0 + y''_1 + \cdots + y''_{n-1}] \qquad \ldots(3)$$

Assuming that $y''(\bar{x})$ is the largest of the n quantities $y''_0, y''_1, \ldots, y''_{n-1}$, we obtain

$$E < -\frac{nh^3}{12}y''(\bar{x}) = -\frac{(b-a)}{12}h^2 y''(\bar{x}) \qquad \ldots(4)$$

Hence the error in Trapezoidal rule is of the order h^2.

2.5 Simpson's one-third rule :

Simpson's $\frac{1}{3}$rule is obtained by putting n = 2 and neglecting the third and higher differences in the general quadrature formula (1). We have, then,

$$\int_{x_0}^{x_2} ydx = 2h[y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0] = \frac{h}{3}[y_0 + 4y_1 + y_2] \qquad \ldots(i)$$

For the next interval $[x_2, x_4]$

$$\int_{x_2}^{x_4} ydx = \frac{h}{3}[y_2 + 4y_3 + y_4] \qquad \ldots(ii)$$

and finally $\int_{x_{n-2}}^{x_n} ydx = \frac{h}{3}[y_{n-2} + 4y_{n-1} + y_n]$. Summing up we obtain

$$\int_{x_0}^{x_n} ydx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + \cdots + y_{n-1}) + 2(y_2 + y_4 + \cdots + y_{n-2}) + y_n] \qquad \ldots(1)$$

which is known as Simpson's $\frac{1}{3}$ rule or simply Simpson's rule. Here n is a multiple of 2.

Error in Simpson's rule :

Expanding $y = f(x)$ about $x = x_0$ by Taylor's series, we get

$$\int_{x_0}^{x_2} ydx = \int_{x_0}^{x_0+2h} [y_0 + (x - x_0)y'_0 + \frac{(x-x_0)^2}{2!}y''_0 + \cdots]dx$$

$$= 2hy_0 + \frac{4h^2}{2!}y'_0 + \frac{8h^3}{3!}y''_0 + \frac{16h^4}{4!}y'''_0 + \cdots \qquad \ldots(1)$$

Example 1. Compute $\int_{-1}^{1} e^x dx$ using (i) Trapezoidal rule and (ii) Simpson's rule. Verify that Simpson's rule give more accurate value.

Solution : We take number of sub-intervals 8 so that $h = \frac{1-(-1)}{8} = 0.25$. The values of $y = f(x) = e^x$ corresponding to x = -1, -0.75, -0.50, -0.25, 0, 0.25, 0.50, 0.75 and 1 are given below

x :	-1	-.75	-0.50	-0.25	0	.25	0.50	0.75	1
f(x)= y	0.3679	.4771	.6065	.7788	1	1.284	1.6487	2.1170	2.7183
	y_0	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

(i) **By Trapezoidal rule** .

$$\int_{-1}^{1} e^x dx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7) + y_8]$$

$$= \frac{0.25}{2}[0.3679 + 2(0.4771 + 0.6065 + .7788 + 1 + 1.2840 + 1.6487 + 2.1170) + 2.7183]$$

$$= 2.3638$$

(ii) **By Simpson's rule ,**

$$\int_{-1}^{1} e^x dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5 + y_7) + 2(y_2 + y_4 + y_6) + y_8]$$

$$= \frac{0.25}{2}[0.3679 + 4(0.4771 + .7788 + 1.2840 + 2.1170) + 2(0.6065 + 1.6487) + 2.7183]$$

$$= 2.3520$$

The actual value of $\int_{-1}^{1} e^x dx$ is 2.3504 which is nearer to 2.3520 obtained from Simpson's rule .

Hence Simpson's rule gives more accurate result.

EXERCISES

1. Evaluate $\int_{1}^{3} \frac{1}{x} dx$ by Simpson's rule taking 8 sub-intervals. [Ans. 1.099]

2. Evaluate $\int_{1}^{2} \sqrt{x}\, dx$ numerically. [G.U. 1995]

$$E < -\frac{nh^5}{90} y_0^{iv}(\bar{x}) = -\frac{(b-a)h^4}{180} y^{iv}(\bar{x}) \because 2nh = b-a$$

i.e. error in Simpson's $\frac{1}{3}$ rule is of order h^4.

2.6 Simpson's $\frac{3}{8}$ rule :

Simpson's $\frac{3}{8}$ rule is obtained by putting n = 3 in the general quadrature formula (1) and neglecting all differences higher than the third. Thus

$$\int_{x_0}^{x_3} ydx = 3h\left[y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0\right]$$

$$= 3h\left[y_0 + \frac{3}{2}(y_1 - y_0) + \frac{3}{4}(y_2 - 2y_1 + y_0) + \frac{1}{8}(y_3 - 3y_2 + 3y_1 + y_0)\right]$$

$$= \frac{3h}{8}[y_0 + 3y_1 + 3y_2 + y_3] \qquad \text{...(i)}$$

Similarly, $\int_{x_3}^{x_6} ydx = \frac{3h}{8}(y_3 + 3y_4 + 3y_5 + y_6)$ and so on. (ii)

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

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

which is known as Simpson's $\frac{3}{8}$ rule.

2.7 Weddle's rule :

Putting n = 6 in general quadrature formula (1) and neglecting all differences higher than the sixth, we get the Weddle's rule as

$$\int_{x_0}^{x_n} ydx = \frac{3h}{10}[y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + 2y_6 + 2y_7 + y_8 + \cdots]$$

Which is known as Weddle's rule.

In Weddle's rule we require the general quadrature formula, at least up to the 6th order differences. So it is suggested that the general quadrature formula is written in an extended way to include up to at least, the sixth differences. Otherwise, Weddle's rule may be derived in detail, in stead of simply giving the formula.

where $u_1, u_2, \ldots\ldots\ldots, u_n$ are the points of subdivision of the interval between u = -1 and u = 1 and $W_1, W_2, \ldots\ldots\ldots\ldots W_n$ are the weights which are symmetrical with respect to the middle point of the interval.

In equation (2) there are altogether 2n arbitrary parameters viz. W_i and u_i , i = 1, 2, 3, …n and therefore the weights and abscissa can be determined such that the formula is exact when F(u) is polynomial of degree not exceeding 2n – 1. Hence, we start with

$$F(u) = c_0 + c_1u + c_2u^2 + \ldots + c_{2n-1}u^{2n-1} \qquad \ldots(3)$$

We then obtain from (2),

$$\int_{-1}^{1} F(u)du = \int_{-1}^{1} (c_0 + c_1u + c_2u^2 + \cdots + c_{2n-1}u^{2n-1})du$$

$$= 2c_0 + \frac{2}{3}c_2 + \frac{2}{5}c_4 + \cdots \qquad \ldots(4)$$

By setting $u = u_i$ in (3), we obtain

$$F(u_i) = c_0 + c_1u_i + c_2u_i^2 + \ldots + c_{2n-1}u_i^{2n-1}$$

Substituting these values on the right hand side of (2), we obtain

$$\int_{-1}^{1} F(u)du = W_1[(c_0 + c_1u_1 + c_2u_1^2 + \cdots + c_{2n-1}u_1^{2n-1})] .$$

$$+ W_2[(c_0 + c_1u_2 + c_2u_2^2 + \cdots + c_{2n-1}u_2^{2n-1})] + \cdots +$$

$$+ W_n[(c_0 + c_1u_n + c_2u_n^2 + \cdots + c_{2n-1}u_n^{2n-1})]$$

which can be written as

$$\int_{-1}^{1} F(u)du = c_0[W_1 + W_2 + \cdots + W_n] + c_1[W_1u_1 + W_2u_2 + \cdots + W_nu_n]$$

$$+ c_2[W_1u_1^2 + W_2u_2^2 + \cdots + W_nu_n^2] + \cdots$$

$$+ c_{2n-1}[W_1u_1^{2n-1} + W_2u_2^{2n-1} + \cdots + W_nu_n^{2n-1}] \qquad \ldots(5)$$

Now, equations (4) and (5) are identical for all values of c_i and hence comparing the coefficients of c_0, c_1, c_2 etc. we obtain 2n equations.

3. Evaluate $\int_0^1 \frac{1}{1+x^2}dx$ using (i) Simpson's $\frac{1}{3}$ rule taking $h=\frac{1}{4}$

(ii) Simpson's $\frac{3}{8}$ rule taking $h=\frac{1}{6}$. [Ans. (i) 0.785 (ii) 0.785]

4. Use Simpson's $\frac{1}{3}$ rule with h = 0.5 to evaluate $\int_0^1 \frac{1}{1+x}dx$. Find the error bound and the actual error. [Ans. 0.694, -0.0083 < Error < 0.0003, -0.0013]

5. Calculate the value of $\int_0^{\frac{\pi}{2}} \sin x dx$ by Simpson's $\frac{1}{3}$ rule, using 11 ordinates. [Ans. 0.999]

2.8 Gauss's Quadrature Formula

Let us consider the integral

$$I=\int_a^b f(x)dx=\int_a^b ydx \qquad \text{...(1)}$$

In Simpson's and Weddle's formulae the ordinates are equally spaced. Gauss derived a formula which uses the same number of function values but with different spacing and gives better accuracy.

On changing the variable by the substitution $x=\frac{b-a}{2}u+\frac{a+b}{2}$

the limits of integration become u = -1 and u = 1.

$$\therefore I=\frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}u+\frac{a+b}{2}\right)du$$

$$=\int_{-1}^{1} F(u)du, \quad \text{where} \quad F(u)=\frac{b-a}{2}f\left(\frac{b-a}{2}u+\frac{a+b}{2}\right)$$

According to Gauss,

$$I=\int_{-1}^{1} F(u)du=W_1F(u_1)+W_2F(u_2)+\dots\dots+W_nF(u_n) \dots\dots\dots(2)$$

$$=\sum_{i=1}^{n} W_iF(u_i)$$

$$\therefore I = F\left(\frac{1}{\sqrt{3}}\right) + F\left(-\frac{1}{\sqrt{3}}\right)$$

Example 1 Use Simpson's rule with three points and Gauss quadrature with two points to evaluate $\int_2^5 \frac{dx}{x^2+1}$. Comment on the accuracy of the results. [G.U 1994]

Solution : According to Simpson's rule

$$I = \int_2^5 \frac{dx}{x^2+1} = \frac{h}{3}[y_0 + 4(y_1) + y_2] \quad \ldots(1) \quad \text{where } h = \frac{5-2}{2} = 1.5$$

$$y_0 = \frac{1}{2^2+1} = 0.2, \quad y_1 = \frac{1}{(3.5)^2+1} = 0.07547, \quad y_2 = \frac{1}{5^2+1} = 0.03846$$

$$\therefore I = \frac{1.5}{3}[0.2 + 4(0.07547) + 0.03846] = \frac{1.5}{3}[0.31393] = 0.270 \text{ up to three decimal places.}$$

By Gauss two point quadrature formula,

$$I = \int_2^5 \frac{dx}{x^2+1} = \int_2^5 f(x)dx, \quad f(x) = \frac{1}{x^2+1}$$

We take $x = \frac{5-2}{2}u + \frac{5+2}{2} = \frac{3}{2}u + \frac{7}{2}$ $\quad \therefore I = \frac{3}{2}\int_{-1}^{1} f\left(\frac{3}{2}u + \frac{7}{2}\right)du$

$$= \int_{-1}^{1} F(u)du, \quad F(u) = \frac{3}{2}f\left(\frac{3}{2}u + \frac{7}{2}\right)$$

$$\text{Also, } I = \int_{-1}^{1} F(u)du = F\left(\frac{1}{\sqrt{3}}\right) + F\left(-\frac{1}{\sqrt{3}}\right) \quad \ldots(2)$$

Now $F\left(\frac{1}{\sqrt{3}}\right) = \frac{3}{2}f\left(\frac{3}{2}u + \frac{7}{2}\right) = \frac{3}{2}f\left(\frac{3}{2}\frac{1}{\sqrt{3}} + \frac{7}{2}\right) = \frac{3}{2}f\left(\frac{\sqrt{3}}{2} + \frac{7}{2}\right) = \frac{3}{2}f(4.3660)$

$$F\left(-\frac{1}{\sqrt{3}}\right) = \frac{3}{2}f\left(-\frac{3}{2}\frac{1}{\sqrt{3}} + \frac{7}{2}\right) = \frac{3}{2}f\left(-\frac{\sqrt{3}}{2} + \frac{7}{2}\right) = \frac{3}{2}f(2.6340)$$

$$\therefore I = \frac{3}{2}[f(4.3660) + f(2.6340)] \quad \text{from (2)}$$

$$= \frac{3}{2}\left[\frac{1}{1+(4.3660)^2} + \frac{1}{1+(2.6340)^2}\right]$$

$$= 0.264 \quad \text{correct to three decimal places}$$

$$\left.\begin{aligned} &W_1 + W_2 + \cdots + W_n = 2 \\ &W_1u_1 + W_2u_2 + \cdots + W_nu_n = 0 \\ &W_1u_1^2 + W_2u_2^2 + \cdots + W_nu_n^2 = 0 \\ &W_1u_1^{2n-1} + W_2u_2^{2n-1} + \cdots + W_nu_n^{2n-1} = 0 \end{aligned}\right\} \qquad \ldots(6)$$

Solving these equations simultaneously it would be theoretically possible to find the 2n quantities $u_1, u_2, \ldots, u_n$ and $W_1, W_2, \ldots, W_n$.

We shall do this for n = 2 which is the Gauss quadrature formula for two points. We consider,

$$I = W_1F(u_1) + W_2F(u_2) \qquad \ldots(7)$$

In relation (7) there exists 4 unknowns. Therefore 4 relations between them are necessary which can be obtained such that the formula is exact for all polynomials of degree not exceeding 3.

$$\text{Let } F(u) = c_0 + c_1u + c_2u^2 + c_3u^3 \qquad \ldots(8)$$

$$\therefore \int_{-1}^{1} F(u)du = \int_{-1}^{1} (c_0 + c_1u + c_2u^2 + c_3u^3)du$$

$$= 2c_0 + \frac{2}{3}c_2 \qquad \ldots(9)$$

Also from (8)

$$F(u_1) = c_0 + c_1u_1 + c_2u_1^2 + c_3 u_1^3$$

$$F(u_2) = c_0 + c_1u_2 + c_2u_2^2 + c_3 u_2^3$$

$$\therefore I = W_1(c_0 + c_1u_1 + c_2u_1^2 + c_3u_1^3) + W_2(c_0 + c_1u_2 + c_2u_2^2 + c_3u_2^3)$$

$$= (W_1 + W_2)c_0 + c_1(u_1W_1 + u_2W_2) + c_2(u_1^2W_1 + u_2^2W_2) + c_3(u_1^3W_1 + u_2^3W_2) \qquad \ldots(10)$$

Comparing (9) and (10)

$$W_1 + W_2 = 2 \qquad \ldots(i)$$

$$u_1W_1 + u_2W_2 = 0 \qquad \ldots(ii)$$

$$u_1^2 W_1 + u_2^2W_2 = \frac{2}{3} \qquad \ldots(iii)$$

$$u_1^3 W_1 + u_2^3W_2 = 0 \qquad \ldots(iv)$$

Solving (i), (ii), (iii) and (iv) we get

$$u_1 = \frac{1}{\sqrt{3}} \qquad ,u_2 = -\frac{1}{\sqrt{3}}$$

and $W_1 = 1$, $\quad W_2 = 1$

Adding all these we get $F(x_n)-F(x_0)=\sum_{i=1}^{n-1} f(x_i)$........(1)

Now $\Delta F(x)=f(x)$

$$\Rightarrow F(x)=\Delta^{-1}f(x)=(E-1)^{-1}f(x)=\left(e^{hD}-1\right)^{-1}f(x)$$

$$=\left[\left(1+hD+\frac{h^2D^2}{2!}+\frac{h^3D^3}{3!}+.......\right)-1\right]^{-1}f(x)=(hD)^{-1}\left[1+\frac{hD}{2!}+\frac{h^2D^2}{3!}+...\right]^{-1}f(x)$$

$$=\frac{1}{h}D^{-1}\left[1+\frac{hD}{2!}+\frac{h^2D^2}{3!}+...\right]^{-1}f(x)$$

$$=\frac{1}{h}D^{-1}\left[1-\left(\frac{hD}{2!}+\frac{h^2D^2}{3!}+...\right)+\left(\frac{hD}{2!}+\frac{h^2D^2}{3!}+...\right)^2\right.$$

$$\left.-\left(\frac{hD}{2!}+\frac{h^2D^2}{3!}+...\right)^3+\left(\frac{hD}{2!}+\frac{h^2D^2}{3!}+...\right)^4+\cdots\right]f(x)$$

$$=\frac{1}{h}\int f(x)dx-\frac{1}{2}f(x)+\frac{h^2}{12}f'(x)-\frac{h^3}{720}f'''(x)+........ \qquad (2)$$

Putting x_n for x and x_0 for x and then subtracting we get

$$F(x_n)-F(x_0)=\frac{1}{h}\int_{x_0}^{x_n}f(x)dx-\frac{1}{2}[f(x_n-f(x_0)]$$

$$+\frac{h}{12}[f'(x)-f'(x_0)]-\frac{h^3}{720}[f'''(x_n)-f'''(x_0)]+........(3)$$

From (1) and (3)

$$\sum_{i=1}^{n-1}f(x_i)=\frac{1}{h}\int_{x_0}^{x_n}f(x)dx-\frac{1}{2}[f(x_n-f(x_0)]$$

$$+\frac{h}{12}[f'(x)-f'(x_0)]-\frac{h^3}{720}[f'''(x_n)-f'''(x_0)]+...$$

$$\sum_{i=1}^{n}f(x_i)=\frac{1}{h}\int_{x_0}^{x_n}f(x)dx+\frac{1}{2}[f(x_n-f(x_0)]+\frac{h}{12}[f'(x)-f'(x_0)]$$

$$-\frac{h^3}{720}[f'''(x_n)-f'''(x_0)]+... \qquad ...(4)$$

By actual integration,

$$I=\int_2^5 \frac{dx}{x^2+1} = \tan^{-1}5 - \tan^{-1}2 = 0.266$$

The value of the integral obtained by Gauss two point quadrature formula is nearer to the exact value. Hence Gauss two point quadrature formula gives better accuracy than that of Simpson's rule.

EXERCISES

1. Compute $\int_{0.4}^{0.5} e^x dx$ using two point Gauss formula and Simpson's rule with 3 equidistant points. Which one of the result is more accurate? [GU 1992]

2. Use Gauss quadrature formula to evaluate $\int_0^{\pi} \sin\ x dx$ [GU 1997]

3. Use Gauss quadrature formula to evaluate $\int_{-1}^{1} \cos\ x dx$ with two points. [Ans. 1.676]

4. Evaluate $\int_0^1 \frac{dt}{1+t}$ by two point Gaussian formula. [Ans. 0.692]

2.9 Euler's summation formula:

It is the approximate relation between integrals and sums which is stated as given below:

$$\sum_{i=0}^{n} f(x_i) = \frac{1}{h}\int_{x_0}^{x_n} f(x)dx + \frac{1}{2}[f(x_n)+f(x_0)] + \frac{h}{12}[f'(x_n)-f'(x_0)] - \frac{h^3}{720}[f'''(x_n - f'''(x_0)] + \cdots$$

where $f(x_0)$, $f(x_1)$,............,$f(x_n)$ are the values of f(x) corresponding to $x_0, x_1, \ldots, x_n$ which are equispaced with difference h.

Proof Let $\Delta F(x)=f(x)$

$$\therefore F(x_1)-F(x_0)=\Delta F(x_0)=f(x_0)$$

$$F(x_2)-F(x_1)=\Delta F(x_1)=f(x_1)$$

....

....

$$F(x_n)-F(x_{n-1})=\Delta F(x_{n-1})=f(x_{n-1})$$

Unit- 3

Solution of Algebraic and Transcendental equations.

3.1 Introduction

An expression of the form $f_n(x) = a_0x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n$ where $'a's$ are constants and n is a +ve integer, is said to be a polynomial in x of degree n provided $a_0 \neq 0$. The values of x which make $f_n(x)$ to zero are called as zeros or the roots of the polynomial $f_n(x)$ and every polynomial of n th degree has n zeroes.

The equation of the form $f_n(x)=0$ are called Algebric or Transcendental according as $f_n(x)$ is purely a polynomial in x or constains some other function such as logarithmic, exponential and trigonometric functions etc. eg. The equations $x^7 + 7x^4 + 5x^3 - 10 = 9$ and $8x^2 + \log(x+2) + e^{-2}\cos x = 0$ are called algebraic and transcendental respectively. By obtaining the solution of an equation $f_n(x) = 0$, we mean to find roots or zeroes of $f_n(x)$. Gerometrically, a root of equation is that value of x where graph of $y = f(x)$ crosses the x-axis and the process of finding the roots of an equation is known as the solution of the equation. If $f_n(x)$ is a quadratic, cubic or a biquadratic expression, algebraic solutions of equations are available. But the need arises to solve higher degree of transcendental equations for which no direct methods are available. Such equations can be solved by approximate methods.

3.2 Some properties of equation:

(a) If $f(x)$ is exactly divisible by $x-\alpha$, then α is a root of $f(x)=0$,

(b) Every equation of the nth degree has only n roots (real or complex) and conversely if $\alpha_1, \alpha_2, \ldots, \alpha_n$ are the roots of the nth degree equation $f_n(x) = 0$, then

$$f_n(x) = A(x-\alpha_1)\ldots(x-\alpha_n) \quad \text{where } A \text{ is a constant.}$$

Further, If a polynomial of degree n vanishes for more than n values of x, it must be identically zero.

which is the Euler's formula for summation.

Example Apply Euler's summation formula to evaluate

$$\frac{1}{51^2}+\frac{1}{53^2}+\frac{1}{55^2}+\ldots\ldots\ldots+\frac{1}{99^2}$$

Solution: Taking $f(x)=\frac{1}{x^2}$, $x_0=51$, $h=2$, $n=24$ we have

$$f'(x)=-\frac{2}{x^3}, f'''(x)=-\frac{24}{x^5}$$

Then Euler's summation formula gives

$$\frac{1}{51^2}+\frac{1}{53^2}+\frac{1}{55^2}+\ldots\ldots\ldots+\frac{1}{99^2}=\frac{1}{2}\int_{51}^{99}\frac{1}{x^2}dx+\frac{1}{2}\left(\frac{1}{99^2}+\frac{1}{55^2}\right)$$

$$+\frac{2}{12}\left[-\frac{2}{99^3}+\frac{2}{51^3}\right]-\frac{2^3}{720}\left[\frac{-24}{99^5}+\frac{24}{51^5}\right]+\ldots$$

$$=\frac{1}{2}\left[-\frac{1}{99}+\frac{1}{51}\right]+\frac{1}{2}\left[\frac{1}{99^2}+\frac{1}{51^2}\right]+\frac{1}{3}\left[\frac{-1}{99^3}+\frac{1}{51^3}\right]$$

$$-\frac{4}{15}\left[-\frac{1}{99^5}+\frac{1}{51^5}\right]+\ldots=0{\cdot}00499=0{\cdot}005 \text{ approximately.}$$

EXERCISES

1. Apply Euler summation formula, to evaluate

(i) $\frac{1}{400}+\frac{1}{402}+\frac{1}{404}+\ldots\ldots\ldots\ldots+\frac{1}{500}$ [Ans. 0.011]

(ii) $\frac{1}{(201)^2}+\frac{1}{(203)^2}+\frac{1}{(205)^2}+\ldots\ldots\ldots\ldots+\frac{1}{(299)^2}$ [Ans. 0.0008]

Then $13\left(\frac{y}{m}\right)^4+16\left(\frac{y}{m}\right)^3+4\left(\frac{y}{m}\right)^2-8\left(\frac{y}{m}\right)+11=0$

$$\Rightarrow 13y^4+m\left(16y^3\right)+m^2\left(4y^2\right)-m^3\left(y\right)+m^4\left(11\right)=0$$

which is same as multiplying the second term by m, third term by m^2 and so on in (i)

(i) To find an equation whose roots are with opposite signs to those of the given equation change the signs of every alternative term of the given equation beginning with the second.

(j) To find an equation whose roots are reciprocal of the roots of the given equation.

Change x to $\left(\frac{1}{x}\right)$

(k) Reciprocal equations : If an equation remains unaltered on change x to $\left(\frac{1}{x}\right)$. If is called a reciprocal equation.

i) A reciprocal equation of an odd degree having coefficients of terms equidistance from the beginning and end equal and has a roots = -1

ii) A reciprocal equation of an odd degree having coefficients of terms equidistance from the beginning and end equal but opposite in sign has a roots = 1

iii) A reciprocal equation of an even degree having coefficients of terms equidistant from the beginning and equal but opposite in sing and has two roots =1 and -1

The Substitution $x+\frac{1}{x}=y$ reduces the degree of the equation the half its former degree.

(l) Synthetic division of a polynomial by a linear expression.

The division of the polynomial.

$$f(x)=a_0x^n+a_1x^{n-1}+a_1x^{n-2}+\ldots\ldots\ldots\ldots+a_{n-1}x+a_n$$

By a binomial $x-\alpha$ is done by synthetic division as follows

α	a_0	a_1	$a_2\ldots\ldots\ldots a_{n-1}$	a_n
		αb_0	$\alpha b_1\ldots\ldots\ldots \alpha b_{n-2}$	αb_{n-1}
	a_0	$a_1+\alpha b_0$	$a_2+\alpha b_1\ldots\ldots\ a_{n-1}+\alpha b_{n-2}$	$a_n+\alpha b_{n-1}$
	$(=b_0)$	$(=b_1)$	$(=b_2)\ldots\ldots\ldots(=b_{n-1})$	$(=R)$

Hence quotient = $b_0x^n+b_1x^{n-1}+\ldots\ldots\ldots+b_{n-1}$, while remainder = R .

Rule i) Write the coefficients of the power of x supplying missing power of x by zero and write α an extreme left.

(c) Intermediate values property :- If f(x) is continuous in the interval [a, b] and $f(a)-f(b)$ have different signs. Then the equation $f(x)=0$ has at least one root between x=a and x=b.

(d) In an equation with real coefficients, imaginary roots occur in conjugate pairs, it if $\alpha+i\beta$ is a root of the equation $f(x)=0$, them $\alpha-i\beta$ must also be its second root.

Similarly if $\alpha+\sqrt{b}$ is an irrational root of an equation. Then $\alpha-\sqrt{b}$ must also be its second root.

Note :- Every equation of the odd degree has atleast are one real root.

(e) Descart's rule of signs : The equation $f(x)=0$ cannot have more positive roots than the changes of sign in $f(x)$, and more negative roots than the changes of signs in $f(-x)$. For example. Let us consider the equation $f(x)=12x^7-x^5+4x^3-15=0$.....(i) sign of $f(x)$ are + − + − Hence $f(x)$ has three changes of sign. Then (i) cannot have more than three positive roots.

Also, are have $f(-x)=12(-x)^7-(-x)^5+4(-x)^3-15 \quad =-12x^7+x^5-4x^3-15$ (ii)

i.e ∃ two changes of signs. Hence (ii) cannot have more than 2 negative roots,

(f) Existance of imaginary roots: If an equation of the nth degree has at the most 'p' positive roots and at the most 'q' negative roots, them the equation has at least n-(p+q) imaginary roots.

(g) Relations between roots and coefficients :- If $\alpha_1, \alpha_2\ \alpha_3$............ α_n be the roots of the equation $a_0x^n+a_1x^{n-1}+a_2x^{n+2}+$............$a_{n-1}x+a_n=0$

Then $\sum\alpha_1=-\frac{a_1}{a_n},\ \sum\alpha_1\alpha_2=\frac{a_2}{a_0},\ \sum\alpha_1\,\alpha_2\,\alpha_3=-\frac{a_3}{a_0},\ \alpha_1\,\alpha_2\,\alpha_3........\alpha_4=(-1)^n\frac{a_n}{a_0}$

(h) Tramsformation of equation :- To find an equation whose roots are m times the roots of the given equation:

Multiply the second term by m third term by m^2 and so on (all missing terms supplied with zero coefficients).

Let the given equation be $13x^4+16x^3+4x^2-8x+11=0$......................(i)

To multiply its roots by m, let us put y = mx $\left(\left(i.e\ x=\frac{y}{m}\right)in\ (i)\right.$

That $f(x_0)f(x_2)<0$ i.e. if it lies between x_0 and x_2 and $x_3 = \frac{x_1+x_2}{2}$ provided that $f(x_1)f(x_2)<0$. Further $x_4 = \frac{x_0+x_3}{2}$ provided that $f(x_0)f(x_3)<0$ and so on.

Thus – in each iteration we either find the root with desired accuracy or we narrow the range to half the previous. The length of the subinterval containing h is $\frac{(b-a)}{2}$. If the error is $<\varepsilon$ then $\frac{(b-a_1)}{2}<t \Rightarrow 2^n > \frac{b-a}{t}$ or $n > \frac{\log\frac{b-a}{2}}{\log 2}$

Example- 2 Solve $x^3-9x+1=0$ for the root between $x=2$ and $x=4$ by the method of interval having or Bolzano bisection procedure.

Solve:- Here $f(x)=x^3-9x+1$ so that $f(x)$ is continuous in $2 \le x \le 4$

Further- $f(2)=-9$, $f(4)=+29$ and $f(2)f(4)<0$. So that a root lies between 2 and 4

Now $x_2 = \frac{x_0+x_1}{2} = \frac{2+4}{2} = 3$ Also $f(3)=1$ so that $f(2)f(3)<0$ Thus the root lies between 2 and 3 Hence $x_3 = \frac{x_0+x_2}{2} = \frac{2+3}{2} = 2.5$ Further, $f(2.5)<0$ so that $f(3)f(2.5)<0$ $\therefore x_4 = \frac{3+2.5}{2} = 2.75$

Similarly $x_5 = 2.875$, $x_6 = 2.9375$ and so for higher iteration, so that the process can be continued as long as required.

3.4 Iteration method

Let f(x)=0 be an equation of which the roots are to be obtained. We rewrite the equation in the form $x = \varphi(x)$ ....(1)

Let $x = x_0$ be an initial approximation of the desired roots α. Then the first approximation x_1 is given by $x_1 = \varphi(x_0)$

Now treating x_1 as the initial value, the second approximation is $x_2 = \varphi(x_1)$

Proceeding in this manner the nth approximation is given by

$$x_n = \varphi(x_{n-1}) \qquad ....(2)$$

ii) Put $a_0(=b_0)$ as the first term of 3[rd] row and multiply it by α and write the product under a_1 and add giving $a_1 + 2b_0(=b_1)$

iii) Multiply b_1 by α and write the product under a_2 and add, giving $a_2 + \alpha b_1\ (=b_2)$ etc, and continue this process, till we get R

Example:- For the polynomial $f(x) = 2x^3 - 6x + 13$ find $f(2)$, $f'(2)$, $f''(2)$ and $f'''(2)$

Solution : using the method of synthetic division we have

	2	0	-6	13	
2		4	8	4	
	2	4	2	17	$= f(2)$
2		4	16		
	2	8	$18 = \frac{1}{11}f'(2)$		
2		4			
	2	$12 = \frac{1}{2!}f''(2)$			
	$2 = \frac{1}{3!}f'''(2)$				

$\therefore f''(2) = 12$

Hence $f(2) = 17$, $f'(2) = 18$, $f''(2) = 24$, $f'''(2) = 12$

3.3 Bolzano or Interval Halving or Bisection Method

This method of solving a transcendental equation consists in locating the roots of the equation $f(x) = 0$ between two numbers say x_0 and x_1 such that $f(x)$ is continuous for $x_0 \le x \le x_1$ and $f(x_0)$ and $f(x_1)$ are opposite sings so that the product $f(x_0)f(x_1) < 0$ i.e, the curve cross the x axis between x_0 and x_1.

Then the desired root is approximately

$$x_2 = \frac{x_0 + x_1}{2} \quad x_3 = \frac{x_0 + x_2}{2} \text{ provided}$$

Example 1 Find by method of iteration a real root of $2x - \log_{10}x = 7$

taking 3.8 as the initial approximation.

Solution: We rewrite the equation as

$$x = \frac{1}{2}\left(\log_{10}x + 7\right) = \varphi(x)\ (\text{say}) \qquad \ldots(1)$$

Here $$\left|\varphi'(x)\right|_{x=3.8} = \frac{1}{2}\left|\frac{1}{x}\log_{10}e\right|_{x=3.8} = \frac{1}{2}\left|\frac{1}{3.8} \times 0.4343\right| < 1$$

$\therefore$ Condition of convergence is satisfied

The 1st iteration is given by $x_1 = \frac{1}{2}\left(\log_{10}3.8 + 7\right)$ [Here $x_0 = 3.8$]

$$= \frac{1}{2}(0.57978 + 7) = 3.78985$$

Similarly the 2[nd] and 3[rd] iterations are,

$$x_2 = \frac{1}{2}(\log_{10}3.7899 + 7) = 3.7893$$

$$x_3 = \frac{1}{2}(\log_{10}3.7893 + 7) = 3.7893$$

$\therefore$ The root of the equation is $x = 3.789$

EXERCISES

1. Find the positive root of the equation $x^4 - x - 10 = 0$ by iteration method. [Ans. 1.856]
2. Find the root of the equation $x - \tan^{-1}x - 1 = 0$ [Ans. 2.132]
3. The equation $4x = e^x$ has two roots, one near 0.3 and the other near 2.1. Find them by iteration method. [Ans. 0.357, 2.153]

3.5 Graphical method :-

To solve the equation f(x)= o, we draw the graph of the function y =f(x) w.r.t.x and y-axis and then obtain x co-ordinate of those points for which y- co-ordinates are zero. This x-co-ordinate will then determine the real roots of the equation f(x)=0. In other words, the real roots may be interpreted as the x-coordinates of the points of intersection of the curve y=f(x) with x- axis. In case, f(x) involves difference of two functions etc, then we usually write f(x)=0

Note The initial approximation is obtained by locating the interval in which the roots of f(x)=0 lie. If f(x) is a continuous function in the interval [a ,b] and if f(a) and f(b) have opposite signs, then the equation f(x)=0 has at least one real root lying in the interval [a , b]. If f(a)<f(b) numerically , then a is taken as the initial approximation of the root otherwise b is taken as the initial approximation.

Condition for convergence of iterations:

Under certain conditions to be stated next, the sequence $x_0, x_1, x_2, \ldots$ converges to the desired root α.

Convergence theorem: If

(i) α be a root of the equation f(x)=0 which is equivalent to $x=\varphi(x)$,

(ii) I, be any interval containing the point $x=\alpha$,

(iii) $|\varphi'(x)|<1$ for all x in I,

then the sequence of approximations $x_0, x_1, x_2, \ldots\ldots x_n$ will converge to the root α provided the initial approximation x_0 is so chosen in I.

Proof: since α is a root of $x=\varphi(x)$, we have, $\alpha = \varphi(\alpha)$

If x_n and x_{n-1} be two successive approximations to α we have $x_n = \varphi(x_{n-1})$

$$\therefore x_n - \alpha = \varphi(x_{n-1}) - \varphi(\alpha) \qquad \ldots\ldots\ldots(1)$$

by Mean value theorem

$$\frac{\varphi(x_{n-1}) - \varphi(\alpha)}{x_{n-1} - \alpha} = \varphi'(\xi) \text{ where } x_{n-1} < \xi < \alpha$$

Hence (1) becomes $x_n - \alpha = (x_{n-1} - \alpha)\varphi'(\xi)$

If $|\varphi'(x_i)| \le K < I$ for all i, then $|x_n - \alpha| \le K|x_{n-1} - \alpha|$

Similarly $|x_{n-1} - \alpha| \le K|x_{n-2} - \alpha|$

i.e. $|x_n - \alpha| \le K^2|x_{n-2} - \alpha|$

Proceeding in this way

$$|x_n - \alpha| \le K^n|x_0 - \alpha|$$

As $n \to \alpha$, the right hand side tends to zero

$\therefore$ The sequence of approximations converges to the root α.

We can derive an equation to find successive approximations to the root from the above figure. From figure, we have

$$\frac{f(x_1)-f(x_0)}{x_1-x_0}=\tan\theta=\frac{f(x_1)}{x_1-x_2}$$

Or $$x_1-x_2=\frac{f(x_1)(x_1-x_0)}{f(x_1)-f(x_0)}$$

Or $$x_2=\frac{x_0 f(x_1)-x_1 f(x_0)}{f(x_1)-f(x_0)}$$

Or in general $$x_{n+1}=\frac{x_{n-1}f(x_n)-x_n f(x_{n-1})}{f(x_n)-f(x_{n-1})},\qquad n\geq 1$$

3.7 The Secant method :

The method is quite similar to that of Regula Falsi method except for the condition $f_1(x).f_2(x)<0$. Here, the graph of the function $y=f(x)$ in the neighbourhood of the root is approximated by a secant line (chord). Further, the interval at each iteration may not contain the root. Let initially the limits of interval be x_1 and x_2. Then the first approximation is given by

$$x_3=x_2+\frac{(x_2-x_1)f(x_2)}{f(x_1)-f(x_2)}$$

Again the formula for successive approximation is

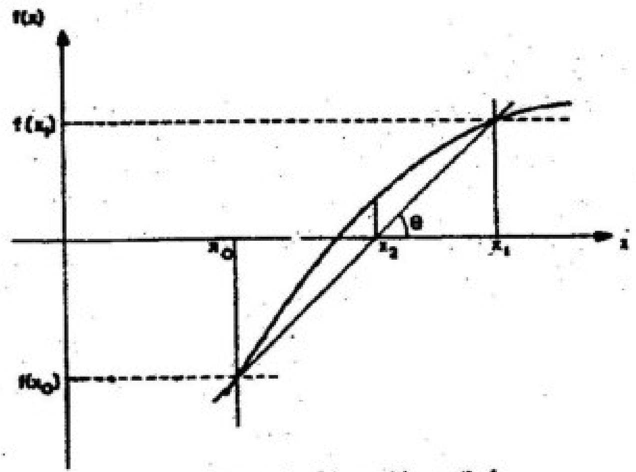
$$x_{n+1}=x_n+\frac{(x_n-x_{n-1})f(x_n)}{f(x_{n-1})-f(x_n)},\quad n\geq 1 \qquad (3.1)$$

In case at any stage $f(x_n)=f(x_{n-1})$ this method will fail. Thus, this method does not converge always whereas Regula Falsi method will always converge. Only advantage in this method lies with the fact that if it converges then it will converge more rapidly than the Regula Falsi method.

Geometrically in this method are replace the function f(x) by a straight line or a chord passing through the points (x_{n-1},f_{n-1}) and take the point of intersection of the straight line with x axis as the next approximation to the root- (fig. 1). It the approximations are such that ff_n, f_{n-1}< 0, Then method (3,1) is known as the Regular- Falsie method. The method is shown graphically in (fig. 2). Since $(x_{n-1},\ f_{n-1})$, $(x_n,\ f_n)$ are known before the start of the as $f_1(x)=f_2(x)$ where $f_1(x)$, $f_2(x)$ are both functions of x. To solve the above equation we draw the graphs of the two function $y= f_1(x)$ and $y=f_2(x)$ on the same axis. The real roots of the given equation are the abscissas of these two curves, at these points $y_1 = y_2$ and so $f_1(x)=f_2(x)$.

3.6 The method of False Position or Regula Falsi :

The bisection method guarantees that the iterative process will converge. It is, however slow. Thus, attempts have been made to speed up bisection method retaining its guaranteed convergence. A method of doing this is called the method of false position or regula falsi. This procedure is started by locating two points x_0 and x_1 where the function has opposite signs. Then the two points $f(x_0)$ and $f(x_1)$ are connected by a straight line to find where it cuts the x-axis. Let it cut x-axis say at x_2. Then again $f(x_2)$ is evaluated. If $f(x_2)$ and $f(x_0)$ are found to be of opposite signs then x_1 is replaced by x_2 and a straight line is drawn to connect the two points $f(x_0)$ and $f(x_2)$ to find the new intersection point at the x-axis. On the other hand If $f(x_2)$ and $f(x_0)$ are found to be of same signs then x_0 is replaced by x_2 and processed as before. In both cases the new interval of search is smaller than the initial interval and ultimately it is guaranteed to converge to the root.



Illustrating false position method.

Example- Use the scant and Regular-Falsi methods to determine the root of the equation $\cos x - xe^x = 0$

Solution -: Taking the initial approximation as $x_0 = 0,\ x_1 = 1,$ we obtain for the secant method.

$f(x) = \cos x - xe^x$, If $x = 0,\ f(0) = 1$ and If $x = 1,\quad f(1) = \cos 1 - e = -2.177979523$

$$x_2 = x_1 - \left[\frac{x_1 - x_0}{f_1 - f_0}\right] f_1 = 0.3146653378 \qquad f_2 = f(x_2) = 0.519871175$$

$$x_3 = x_2 - \left[\frac{x_2 - x_1}{f_2 - f_1}\right] f_2 = 0.4467281466$$

$$f_3 = f(x_3) = 0.203544710, \quad x_4 = x_3 - \left[\frac{x_3 - x_2}{f_3 - f_2}\right] f_3 = 0.5317058606$$

Now, for the Regula Falsi Method, we get

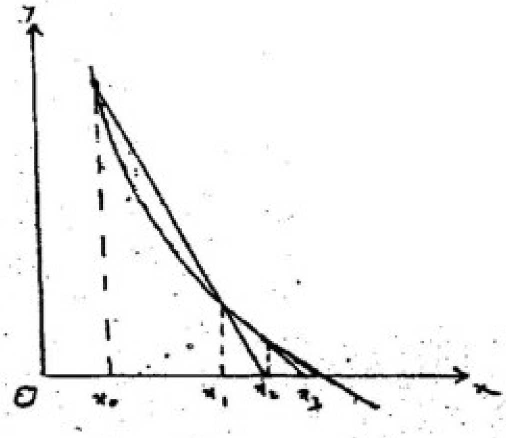
$$x_2 = x_1 - \left[\frac{x_1 - x_0}{f_1 - f_0}\right] f_1 = 0.4467281466 \qquad f_3 = f(x_3) = 0.203544710$$

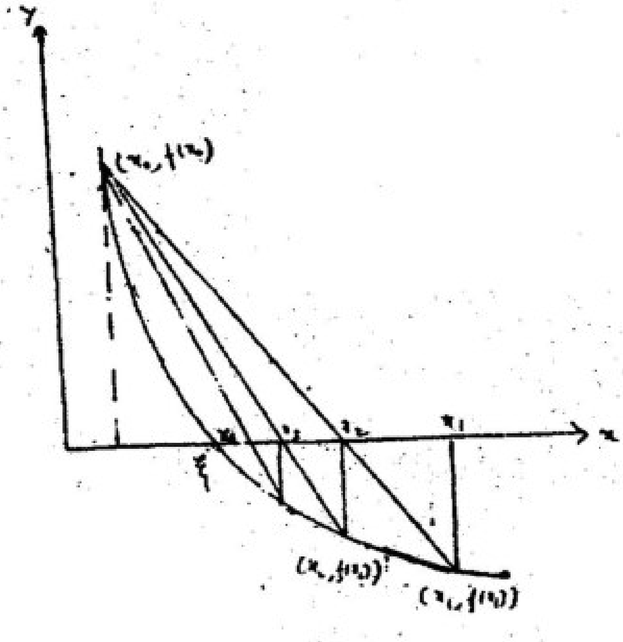
Since $f(x_1) + f(x_3) < 0 \xi \in (x_1,\ x_3)$ therefore $x_4 = x_3 - \left[\frac{x_3 - x_1}{f_3 - f_{1'}}\right] f_3 = 0.4940153366$

The computed results are tabulated in Table-1

K		Secants Method		Regula -Falsi Method
	x_{k+1}	$f(x_{k+1})$	x_{k+1}	$f(x_{k+1})$
1	0.3146653378	0.519871	0.3146653378	0.519871
2	0.44672814466	0.203545	0.4467281446	0.203545
3	0.5317058606	-0.429311(-01)	0.4940153366	0.708023(-01)
4	0.45169044676	0.259276(-02)	0.5099461404	0.236077(-01)
5	0.5177474653	0.301119(-04)	0.5152010099	0.776011(-02)
6	0.5177573708	-0.215132(-07)	0.5169222100	0.253886(-02)
7	0.5177573637	0.178663(-12)	0.5174846768	0.829358(-03)
8	0.5177573637	0.222045(-15)	0.5176683450	0.270786(-03)
10	–	–	0.5177478783	0.288554(-04)
20	–	–	0.5177573636	0.396288(-09)

iteration, the scant and the Regular –Falsi methods require one function evaluation per iteration.



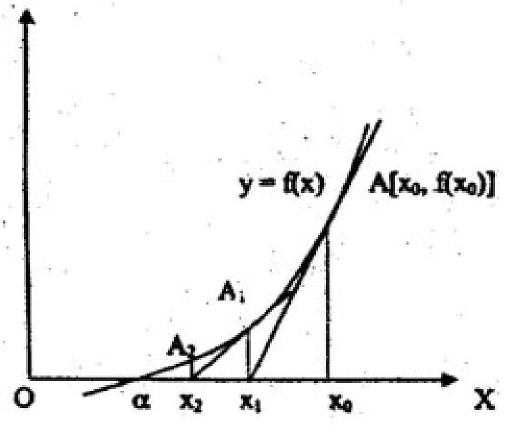


In the Figure, upper one is for Secant method and the lower one is for Regula Falsi method

This shows that the subsequent error at each step, is proportional to the square of the previous error and as such the rate of convergence is quadratic.

Geometircal Interpretation: Let x_0 be a point near the root α of the equation $f(x)=0$. Then the Equation of the tangent at A_0 $[x_0\ f(x_0)]$ as shown in the figure is

$$y - f(x_0) = f'(x_0)(x - x_0)$$



It intersects the x axis at $\quad x_1 = x_0 - \dfrac{f(x_0)}{f'(x_0)}$

Which is a first approximation to the root α. If A_1 is the point corresponding to x_1 on the curve, then the tangent at A_1 will intersect the x-axis at x_2 which is nearer to α and is therefore better approximation to the root. Repeating this process we approach the root α quite rapidly.

Example 1 Find by Newton's method the real rot of the equation $3x - \cos x - 1 = 0$

Solution Let $f(x) = 3x - \cos x - 1$ $\qquad \therefore f'(x) = 3 + \sin x$

we have $f(0) = -2 < 0$, $\qquad f(1) = 1.4597 > 0$

$\therefore$ The root of the equation lies between $x=0$ and $x=1$

Let us take initial approximation $x_0 = 0.6$

3.8 Newton Raphson method: Let x_0 be an approximate root of the equation $f(x)=0$. If $x_1=x_0+h$ is the exact, root, then $f(x_1)=0$ i.e. $f(x_0+h)=0$ where h is small.

Expanding $f(x_0+h)$ by Taylor series

$$f(x_0)+h\,f'(x_0)+\frac{h^2}{2!}f''(x_0)+\ldots\ldots=0$$

Since h is small, neglecting h^2 and other higher powers of h, we get

$$f(x_0)+hf'(x_0)=0 \qquad \Rightarrow h=-\frac{f(x_0)}{f'(x_0)}\ldots\ldots\ldots\ldots(1)$$

$\therefore$ A better approximation to the root is given by

$$x_1=x_0-\frac{f(x_0)}{f'(x_0)}$$

Similarly starting with x_1, still better approximation x_2 is given by $x_2=x_1-\dfrac{f(x_1)}{f'(x_1)}$

In general, $\qquad x_{n+1}=x_n-\dfrac{f(x_n)}{f'(x_n)}, \qquad n=0,1,2,3,\ldots\ldots\ldots$

Which is known as the Newton Raphson formula or Newton's iteration formula.

3.9 Rate of convergence of Newton –Raphson method:

Let us assume that x_n differ's from the root α by a small quantity ε_n so that $x_n=\alpha+\varepsilon_n$ and $x_{n+1}=\alpha+\varepsilon_{n+1}$

$$\therefore x_{n+1}=x_n-\frac{f(x_n)}{f'(x_n)} \text{ becomes } \alpha+\varepsilon_{n+1}=\varepsilon_n+\alpha-\frac{f(\alpha+\varepsilon_n)}{f'(\alpha+\varepsilon_n)}\Rightarrow \varepsilon_{n+1}=\varepsilon_n-\frac{f(\alpha+\varepsilon_n)}{f'(\alpha+\varepsilon_n)}$$

$$=\varepsilon_n-\frac{f(\alpha)+\varepsilon_n f'(\alpha)+\frac{1}{2!}\varepsilon_n^2 f''(\alpha)+\ldots\ldots\ldots}{f'(\alpha)+\varepsilon_n f''(\alpha)+\ldots\ldots\ldots} \text{ by Taylor's expansion}$$

$$=\varepsilon_n-\frac{\varepsilon_n f'(\alpha)+\frac{1}{2!}\varepsilon_n^2 f''(\alpha)+\ldots\ldots\ldots}{f'(\alpha)+\varepsilon_n f''(\alpha)+\ldots\ldots\ldots} \qquad [\because f(\alpha)=0]$$

$$=\frac{\varepsilon_n^2 f''(\alpha)}{2[f'(\alpha)+\varepsilon_n f''(\varepsilon)]} \qquad [\text{neglecting third and higher powers of } \varepsilon_n]$$

$$=\frac{\varepsilon_n^2 f''(\alpha)}{2f'(\alpha)}$$

Example: Find the double root of the equation $x^3-x^2-x+1=0$ taking initial approximation as $x_0 = 0.9$.

Solution : Let $f(x) = x^3-x^2-x+1$ So that $f'(x)=3x^2-2x-1$, $f''(x)=6x-2$

We have, $$x_1 = x_0 - 2\frac{f(x_0)}{f'(x_0)} = 0.9 - 2\times\frac{0.019}{-0.37} = 1.003$$

Also $$x_1 = x_0 - (2-1)\frac{f'(x_0)}{f''(x_0)} = 0.9 - \frac{-0.37}{3.4} = 1.009$$

The closeness of these values implies that there is a double root near x=1

∴ Choosing $x_1 = 1.01$ for the next approximation we get

$$x_2 = x_1 - 2\frac{f(x_1)}{f'(x_1)} = 1.01 - 2\frac{0.0002}{0.0403} = 1.0001$$

Also $$x_2 = x_1 - (2-1)\frac{f'(x_1)}{f''(x_1)} = 1.01 - \frac{0.0403}{4.06} = 1.0001$$

This shows that there is a double root at x=1.0001 which is quite near to the actual root x=1.

EXERCISES

1. Find by Newton-Raphson method, a root for the following equations correct to 3 decimal places:
   (i) $x^3-3x-5=0$ [Ans. 2.279]
   (ii) $x^3-5x+3=0$ [Ans. 1.834]
   (iii) $x^4-x-13=0$ [Ans. 1.967]
2. Find the smallest positive root of x tanx-1 =0 using three iterations.[GU'97]
3. Find a root of the equation $x^3-2x^2+x+5=0$ [GU90]
4. Use the iterative method to find a root of the equation $x^3+3x-1=0$ [GU 93]
5. Starting with the initial solution $x_0 = 1$, find the repeated double root of the equation, $x^3+3x^2+2.25x=0$ [GU96] [Ans-1.5]
6. Find the double root of the equation $x^3-2.236x^2-5x+11.18=0$ [GU 91]

Form Newton's formula

$$\therefore x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{3x_n - \cos x_n - 1}{3 + \sin x_n}$$

$$= \frac{x_n \sin x_n + \cos x_n + 1}{3 + \sin x_n} \quad \text{............(1)}$$

Putting $n = 0$, the 1st approximation is x_1 is given by

$$x_1 = \frac{x_0 \sin x_0 + \cos x_0 + 1}{3 + \sin x_0} = \frac{(0.6)\sin 0.6 + \cos(0.6) + 1}{3 + \sin(0.6)}$$

$$= \frac{0.6 \times 0.5729 + 0.8253 + 1}{3 + 0.5729} = 0.6071$$

Putting $n = 1$ in (1), the 2^{nd} approximation is

$$x_2 = \frac{0.6071 \times \sin(0.6071) + \cos(0.6071) + 1}{3 + \sin(0.6071)} = 0.6071$$

Hence the root of the equation is $x = 0.6071$

3.10 Generalized Newton's method for multiple roots:

If α is a root of the equation $f(x) = 0$ which is repeated m times, then

$$x_{n+1} = x_n - m\frac{f(x_n)}{f'(x_n)}$$

which is called the generalised Newton's formula. It reduces to Newton-Raphson formula when m=1.

Note: If α is a root of $f(x) = 0$ with multiplicity m, then it is also a root of $f'(x) = 0$ with multiplicity m-1, of $f''(x) = 0$ with multiplicity m-2 and so on

Thus $x_0 - m\dfrac{f(x_0)}{f'(x_0)}$, $x_0 - (m-1)\dfrac{f'(x_0)}{f''(x_0)}$, $x_0 - (m-2)\dfrac{f''(x_0)}{f'''(x_0)}$, ...

will have the same value .

$x_1 = x_2 = \ldots\ldots = x_n = 0$ if $\det(A) \neq 0$, therefore consider the system in which a parameter λ occurs and are determine values of λ, called eigen values, for which the system has a nontrivial solution. Such a solution is called on eigen vector and the entire system is called an eigen value problem or the characteristic value problem. The system (4.2), (b = 0) may then be written as

$$Ax = \lambda x \qquad (4.4)$$

$$\Rightarrow (A - \lambda I)x = 0 \qquad (4.5)$$

In order that equations (4.4) have a non trivial solution $x \neq 0$ the determinant of the matrix $(A - \lambda I)$ must be zero.

$$\text{Det } (A - \lambda I) = 0 \qquad (4.6)$$

The equation (4.6) is called the characteristic equation. The n roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ are called the eigen values of A and may be district or repeated real or complex. The largest eigen value in modulus is called the spectral radius of A. Corresponding to each eigen value λ_i, there exist an eigen vector x_i, which is nontrivial solution of $(A - \lambda_i I)x_i = 0$.

The method of solution of the linear algebraic equations (4.2) and the methods to determine the eigen values and eigen vectors of the system (4.3) may broadly be classified into two types.

(i) **Direct Method :** These method produce the exact solution after a finite number of steps.

(ii) **Introduction Method :** This methods give a sequence of approximate solutions, which converges when the number of steps tend to infinite.

4.3. Direct Methods :

The system of equation (4.2) $Ax = b$ can be directly solved in the following cases.

(i) A = D

The equations (4.2) becomes

$$\begin{aligned} a_{11}x_1 \qquad\qquad &= b_1 \\ a_{22}x_2 \qquad &= b_2 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & \\ a_{nn}x_n &= b_n \end{aligned}$$

Unit 4

Direct Method for solving system of linear equations.

4.1. Introduction :

A large number of methods of solving the system of linear equations and a variety of computers are available to solve such equations. We give below a few direct as well as indirect or iterative method for the solution of system of linear equation.

4.2. Linear system equation :

Consider a system of n linear algebraic equations in n unknowns

$$
\begin{aligned}
&a_{11}x_1 + a_{12}x_2 + \dots\dots\dots + a_{1n}x_n = b_1 \\
&a_{21}x_1 + a_{22}x_2 + \dots\dots\dots + a_{2n}x_n = b_2 \\
&\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\
&\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\
&a_{n1}x_1 + a_{n2}x_2 + \dots\dots\dots + a_{nn}x_n = b_n
\end{aligned}
\qquad (4.1)
$$

where a_{ij} $(i, j = 1, 2, ..., n)$ are known coefficients, b_{ij} $(i, j = 1, 2, ..., n)$ are the known values and x_i $(i = 1, 2, ..., n)$ are the unknown to be determined. We introduce the following notation definitions.

In the matrix notation the system (4.1) can be written as $Ax = b$ ---------- (4.2)

The matrix $[A|B]$ is called augmented matrix. It is formed by appending the column b to the $n \times n$ matrix A.

If all b_i are zero then the system of equation (4.1) is said to be homogenous and if at least one of b_i is not zero then it is said to be in-homogenous. The in homogenous system (4.1) has a unique solution if and only it the determinant of A is non zero.

$$
\text{i.e. } \det(A) = \begin{vmatrix} a_{11} & a_{12} & \dots\dots & a_{1n} \\ a_{21} & a_{22} & \dots\dots & a_{2n} \\ \dots\dots & \dots\dots & \dots\dots & \dots\dots \\ \dots\dots & \dots\dots & \dots\dots & \dots\dots \\ a_{n1} & a_{n2} & \dots\dots & a_{nn} \end{vmatrix} \neq 0
$$

The solution of the system (3.3) may be written as $X = A^{-1}b$ .... (4.3)

The homogenous system $(b_i = 0,\ i = 1, 2, ..., n)$ possesses only a trivial solution.

The unknowns are solved by back substitution and this method is called the back substitution method.

4.4. Gauss Elimination method:

Here, the unknowns are eliminated by combining equations such that the n equations in n unknowns are reduced to an equivalent upper triangular system which is then solved by back substitution method. Consider the 3×3 system

$$\left.\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3 \end{aligned}\right\} \text{---------- } (4.7)$$

In the first stage of elimination multiply the first row in (4.1) by $\frac{a_{21}}{a_{11}}$ and $\frac{a_{31}}{a_{11}}$ respectively and substract from the second and third rows

We get

$$\left.\begin{aligned} a_{22}^{(2)}x_2 + a_{23}^{(2)}x_3 = b_2^{(2)} \\ a_{32}^{(2)}x_2 + a_{33}^{(2)}x_3 = b_3^{(2)} \end{aligned}\right\} \text{-----}(4.8)$$

where $a_{22}^{(2)} = a_{22} - \frac{a_{21}}{a_{11}}a_{12}$, $\quad a_{23}^{(2)} = a_{23} - \frac{a_{21}}{a_{11}}a_{13}$

$a_{32}^{(2)} = a_{32} - \frac{a_{31}}{a_{11}}a_{12}$, $\quad a_{33}^{(2)} = a_{33} - \frac{a_{31}}{a_{11}}a_{13}$

$b_2^{(2)} = b_2 - \frac{a_{21}}{a_{11}}b_1$, $\quad b_3^{(2)} = b_3 - \frac{a_{31}}{a_{11}}b_1$

In the second stage of elimination, multiply the first row in (3.16) by $\left(\frac{a_{32}^{(2)}}{a_{22}^{(2)}}\right)$ and subtract from the second row in (4.2).

We get $\quad a_{33}^{(3)}x_3 = b_3^{(3)}$ ------- (4.9)

Where $\quad a_{33}^{(3)} = a_{33}^{(2)} - \frac{a_{32}^{(2)}}{a_{22}^{(2)}}a_{23}^{(2)}$, $\quad b_3^{(3)} = b_3^{(2)} - \frac{a_{32}^{(2)}}{a_{22}^{(2)}}b_2^{(2)}$

Collecting the first equation from each stage. i.e. from (4.1), (4.2) and (4.3) we obtain the system

The solution is given by $x_i = \frac{b_i}{a_{ii}}, \; i=1(1)_3$

$$a_{ii} \neq 0, i=1(1)_3$$

(ii) A = L

The equation (4.2) may be written as

$$\begin{aligned} a_{11}x_1 &= b_1 \\ a_{21}x_1 + a_{22}x_2 &= b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= b_3 \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots\cdots + a_{nn}x_n &= b_n \end{aligned}$$

Solving the first equation and then successively solving the second third and so on, are obtain

$$x_1 = \frac{b_1}{a_{11}}, \quad x_2 = \frac{(b_2 - a_{21}x_1)}{a_{22}}, \quad x_3 = \frac{(b_3 - a_{31}x_1 - a_{32}x_2)}{a_{33}}$$

$$\cdots\cdots\cdots, \quad x_n = \left(b_n - \sum_{j=1}^{n-1} \frac{a_{nj}x_j}{a_{nn}}\right)$$

where $a_{ii} \neq 0, \quad i = 1, 2, \ldots n$

Since the unknowns are solved by forward substitution, this method is called the forward substitution method.

(iii) A = U

The system of equations (4.3) becomes

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots\cdots\cdots\cdots + a_{1n}x_n &= b_1 \\ a_{22}x_2 + \cdots\cdots\cdots + a_{2n}x_n &= b_2 \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ a_{(n-1)(n-1)}x_{n-1} + a_{(n-1)n}x_n &= b_2 \\ a_{nn}x_n &= b_n \end{aligned}$$

Solving for the unknowns in the order $x_n, x_{n-1}, \ldots\ldots, x_1$, we get

$$x_n = \frac{b_n}{a_{nn}}, \quad x_{n-1} = \frac{(b_{n-1} - a_{n-1})}{a_{n-1,n-1}}, \cdots\cdots\cdots\cdots, x_1 = \left(b_1 - \frac{\sum_{j=2}^{n} a_{ij}x_j}{a_{11}}\right)$$

Solution : Eliminating x_1 from the last two equations, we get

$$x_1 + x_2 + x_3 = 6$$
$$\varepsilon x_2 + x_3 = 2$$
$$-x_2 + x_3 = 1$$

Here, the pivot in the second equation is ε which is a very small number.

If we do not use pivoting then are get

$$x_1 + x_2 + x_3 = 6$$
$$\varepsilon x_2 + x_3 = 2$$
$$\left(1+\frac{1}{\varepsilon}\right)x_3 = 1+\frac{2}{\varepsilon}$$

This solution is $x_3 = \dfrac{1+\left(\frac{2}{\varepsilon}\right)}{1+\left(\frac{1}{\varepsilon}\right)}$, $x_2 = \dfrac{1}{\varepsilon}\left[2-\dfrac{1+\left(\frac{2}{\varepsilon}\right)}{1+\left(\frac{1}{\varepsilon}\right)}\right]$ and $x_1 = 6 - x_2 - x_3$

However, this solution may be very inaccurate if ε is of the order of the round –off error. This situation can be avoided if pivoting is done at the second step. In this case we have.

$$x_1 + x_2 + x_3 = 6$$
$$-x_2 + x_3 = 1$$
$$(1+\varepsilon)x_3 = 2+\varepsilon$$

This solution is $x_3 = \dfrac{2+\varepsilon}{1+\varepsilon}$ $x_2 = -1+\dfrac{2+\varepsilon}{1+\varepsilon}$ and $x_1 = 6 - x_2 - x_3$

Example 2 : Solve the equations

$$10x_1 - x_2 + 2x_3 = 4, \quad x_1 + 10x_2 + x_3 = 3 \quad 2x_1 + 3x_2 + 20x_3 = 7$$

Using the Gauss elimination method.

4.5. Triangularization Method

This method is also known as the decomposition method or the factorization method. In this method the coefficient matrix A of the system of equations (4.2) is decomposed or factorized into the product of a lower triangular matrix L and an upper triangular matrix U. We write the matrix A as

$$A = LU \text{ ---------(4.13)}$$

$$\left.\begin{aligned} a_{11}^{(1)}x_1 + a_{12}^{(1)}x_2 + a_{13}^{(1)}x_3 &= b_1^{(1)} \\ a_{22}^{(2)}x_2 + a_{23}^{(2)}x_3 &= b_2^{(2)} \\ a_{33}^{(3)}x_3 &= b_3^{(3)} \end{aligned}\right\} ----(4.10)$$

Where $a_{ij}^{(1)} = a_{ij},\ b_i^{(1)} = b_i,\ i, j = 1, 2, 3$

The system (4.4) is an upper triangular system and can be solved using the back substitution method. Therefore, the Gauss elimination method gives

$$[A \mid b] \xrightarrow[\text{Eliminatio n}]{\text{Gauss}} [U \mid C]$$

Where [A | b] is an augmented matrix. The elements $a_{11}^{(1)}, a_{22}^{(2)}$ and $a_{33}^{(3)}$ which have been assumed to be non-zero are called pivot elements. The elimination procedure described above to determine the unknowns is called Gauss elimination method.

We now solve the system (4.1) in n unknowns by performing the Gauss elimination on the augmented matrix [A | b]. Denote

$$b_i^{(k)} = a_i^{(k)}{}_{n+1} \qquad i, k = 1, 2, \ldots, n \qquad (4.11)$$

The elements $a_{ij}^{(k)}$ with $i, j \geq k$ are given by

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} a_{kj}^{(k)} \quad ----- (4.12)$$

$$i = k+1, k+2, \ldots.. n, \text{ and } j = k+1, \ldots. n, n+1$$

Where $a_{ij}^{(1)} = a_{ij}$

The elimination is performed in (n-1) setps, k = 1, 2...... n-1. In the elimination process, if any one of the pivot elements $a_{11}^{(1)}, a_{22}^{(2)}, \ldots.. a_{nn}^{(3)}$ vanishes or becomes very small compared to other elements in that column, then are attempt to rearrange the remaining rows so as to obtain a non vanishing pivot or to avoid the multiplication by a large number .This strategy is called pivoting.

Example 1 : Solve the equations

$$x_1 + x_2 + x_3 = 6$$

$$3x_1 + (3 + \varepsilon)x_2 + 4x_3 = 20$$

$$2x_1 + x_2 + 3x_3 = 13$$

Using Gauss elimination method where ε is small such that $1 \neq \varepsilon^2 = 1$.

Next we find the third column of L followed by the third row of U.

Thus the relevant indices i and j, the elements are computed in the other

$$l_{i1},\ u_{1j},\ l_{i2},\ u_{2j},\ u_{3j},\ \ldots\ldots\ldots, l_{i,n-1},\ u_{n-1,j},\ l_{nn}$$

Having determined the matrices L and U, the system of equation (4.2) becomes

$$LU\,x = b \qquad (4.20)$$

We write (4.20) as the following two system of equations

$$Ux = z \qquad (4.21)$$

$$Lz = b \qquad (4.22)$$

This unknown $z_1, z_2, \ldots\ldots\ldots z_n$ in (3.33) are determined by forward substitution and the unknown $x_1, x_2, \ldots\ldots\ldots x_n$ in (4.21) are obtained by back substitution. Alternatively we find L^{-1} and U^{-1} to get $z = L^{-1}b$ and $x = U^{-1}z$

The inverse of A can also be determined from $A^{-1} = U^{-1}L^{-1}$

This method fails if any of the diagonals elements l_{ii} or u_{ii} is zero. This LU decomposition is guaranteed when the matrix A is positive definite. However, it is only a sufficient condition.

Example 1 : Find the inverse of the matrix

$$A = \begin{bmatrix} 3 & 2 & 1 \\ 2 & 3 & 2 \\ 1 & 2 & 2 \end{bmatrix}$$

Using LU decomposition method. Take $u_{11} = u_{22} = u_{33} = 1$

Solution :

We write

$$\begin{bmatrix} 3 & 2 & 1 \\ 2 & 3 & 2 \\ 1 & 2 & 2 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix}$$

And obtain as in the previous example

$$l_{11} = 3,\ l_{21} = 2,\ l_{31} = 1$$

$$u_{12} = \frac{2}{3} \qquad u_{13} = \frac{1}{3} \qquad l_{22} = \frac{5}{3} \qquad l_{32} = \frac{4}{3} \qquad u_{23} = \frac{4}{5} \qquad l_{33} = \frac{3}{5}$$

$$\text{where } L = \begin{bmatrix} l_{11} & 0 & 0\ldots\ldots0 \\ l_{21} & l_{22} & 0\ldots\ldots0 \\ l_{31} & l_{32} & l_{33}\ldots\ldots0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots \\ l_{n1} & l_{n2} & l_{n3}\ldots\ldots l_{nn} \end{bmatrix}, \qquad U = \begin{bmatrix} u_{11} & u_{12} & \ldots\ldots & u_{1n} \\ 0 & u_{22} & \ldots\ldots & u_{2n} \\ 0 & 0 & u_{33} \ldots & u_{3n} \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \\ 0 & 0 & 0\ldots\ldots & u_{nn} \end{bmatrix}$$

Using the matrix multiplication rule to multiplication the matrix Land U and comparing the elements of the resulting matrix with those of A are obtain

$$l_{i1}u_{1j} + l_{i2}u_{2j} + \ldots\ldots\ldots + l_{in}u_{nj} = a_{ij}, \quad j = 1(1)n \qquad (4.14)$$

where $l_{ij} = 0, j > i$ and $u_{ij} = 0, i > j$

The system of educations involves $n^2 + n$ unknowns. Thus, there are n parameter family of solutions. To produce a unique solution it is convenient to choose either $u_{ii} = 1$ or $l_{ii} = 1, i = 1(1)n$. When we choose.

(i) $l_{ii} = 1$, the method is called Doolittle's method

(ii) $u_{ii} = 1$, the method is called the Crout's method.

When are take $u_{ii} = 1$, i = 1 (1) n, the solution of the equations (3.26) may be written as

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik}u_{kj}, \; i \geq j$$

$$u_{ij} = \frac{\left(a_{ij} - \sum_{k=1}^{i-1} l_{ik}u_{kj}\right)}{l_{ii}}, \qquad i < j$$

$$u_{ii} = 1$$

We note that the first column of the matrix L is identical with the first column of the matrix

A. That is $l_{i1} = a_{i1}, \; i = 1(1)n$ (4.16)

We also note that $u_{1j} = \dfrac{a_{1j}}{l_{11}}, \qquad j = 2(1)n$ (4.17)

The first column of L and the first row of U have been determined. We can now proceed to determine the second column of L and the second row of U

$$l_{i2} = a_{i2} - l_{i1}u_{12}, \quad i = 2(1)n \qquad (4.18)$$

$$u_{2j} = \frac{\left(a_{2j} - l_{21}u_{1j}\right)}{l_{22}}, \qquad j = 3(1)n \qquad (4.19)$$

Now, let $u_{ii} = 1, 1 \le i \le 3$

$$A = LU$$

$$\Rightarrow \begin{pmatrix} 1 & 1 & -1 \\ 2 & 2 & 5 \\ 3 & 2 & -3 \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} l_{11} & l_{11}u_{12} & l_{11}u_{13} \\ l_{21} & l_{21}u_{12} + l_{22} & l_{21}u_{13} + l_{22}u_{23} \\ l_{31} & l_{31}u_{12} + l_{32} & l_{31}u_{13} + l_{32}u_{23} + l_{33} \end{pmatrix}.$$

1st column $l_{11} = 1, l_{21} = 2, l_{31} = 3$

1st row $l_{11}u_{12} = 1 \Rightarrow u_{12} = 1 \quad l_{11}u_{13} = -1 \Rightarrow u_{13} = -1$

2nd column $\quad l_{21}u_{12} + l_{22} = 2 \Rightarrow 2.1 + l_{22} = 2 \Rightarrow l_{22} = 0$

$\therefore$ **LU decomposition method fails in this case also.**

We note that the coefficient matrix is not a positive definite matrix and hence its LU decomposition is not guaranteed.

However, if we interchange the equations as

$$\begin{bmatrix} 3 & 2 & -3 \\ 2 & 2 & 5 \\ 1 & 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ -3 \\ 2 \end{bmatrix}$$

Now $A = LU$

$$\Rightarrow \begin{pmatrix} 3 & 2 & -3 \\ 2 & 2 & 5 \\ 1 & 1 & -1 \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} l_{11} & l_{11}u_{12} & l_{11}u_{13} \\ l_{21} & l_{21}u_{12} + l_{22} & l_{21}u_{13} + l_{22}u_{23} \\ l_{31} & l_{31}u_{12} + l_{32} & l_{31}u_{13} + l_{32}u_{23} + l_{33} \end{pmatrix}$$

1st column $\quad l_{11} = 3, \quad l_{21} = 2, \quad l_{31} = 1$

1st row $\quad l_{11}u_{12} = 2 \Rightarrow 3u_{12} = 2 \Rightarrow u_{12} = \frac{2}{3} \quad l_{11}u_{13} = -3 \Rightarrow 3u_{13} = -3 \Rightarrow u_{13} = -1$

2nd column $l_{21}u_{12} + l_{22} = 2 \Rightarrow 2.\frac{2}{3} + l_{22} = 2 \Rightarrow l_{22} = 2 - \frac{4}{3} = \frac{2}{3}$

Therefore We have

$$L=\begin{bmatrix}3 & 0 & 0\\ 2 & \frac{5}{3} & 0\\ 1 & \frac{4}{3} & \frac{8}{5}\end{bmatrix}, \qquad U=\begin{bmatrix}1 & \frac{2}{3} & \frac{1}{3}\\ 0 & 1 & \frac{4}{5}\\ 0 & 0 & 1\end{bmatrix}$$

We, now get

$$L^{-1}=\begin{bmatrix}\frac{1}{3} & 0 & 0\\ -\frac{2}{5} & \frac{3}{5} & 0\\ \frac{1}{8} & -\frac{1}{2} & \frac{5}{8}\end{bmatrix} \qquad U^{-1}=\begin{bmatrix}1 & -\frac{2}{3} & \frac{1}{5}\\ 0 & 1 & -\frac{4}{5}\\ 0 & 0 & 1\end{bmatrix}$$

Hence $A^{-1}=U^{-1}L^{-1}$

$$=\begin{bmatrix}1 & -\frac{2}{3} & \frac{1}{5}\\ 0 & 1 & -\frac{4}{5}\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}\frac{1}{3} & 0 & 0\\ -\frac{2}{5} & \frac{3}{5} & 0\\ \frac{1}{8} & -\frac{1}{2} & \frac{5}{8}\end{bmatrix}=\begin{bmatrix}\frac{5}{8} & -\frac{1}{2} & \frac{1}{8}\\ -\frac{1}{2} & \frac{8}{8} & -\frac{1}{2}\\ \frac{1}{8} & -\frac{1}{2} & \frac{5}{8}\end{bmatrix}$$

Example 2 : Show that the LU decomposition method fails to solve the system of equations

$$\begin{bmatrix}1 & 1 & -1\\ 2 & 2 & 5\\ 3 & 2 & -3\end{bmatrix}\begin{bmatrix}x_1\\ x_2\\ x_3\end{bmatrix}=\begin{bmatrix}2\\ -3\\ 6\end{bmatrix}$$

Solution : let $l_{ii}=1, 1\le i\le 3$

A = L U

$$\Rightarrow\begin{pmatrix}1 & 1 & -1\\ 2 & 2 & 5\\ 3 & 2 & -3\end{pmatrix}=\begin{pmatrix}l_{11}=1 & 0 & 0\\ l_{21} & l_{22}=1 & 0\\ l_{31} & l_{32} & l_{33}=1\end{pmatrix}\begin{pmatrix}u_{11} & u_{12} & u_{13}\\ 0 & u_{22} & u_{23}\\ 0 & 0 & u_{33}\end{pmatrix}.$$

$$=\begin{pmatrix}u_{11} & u_{12} & u_{13}\\ l_{21}u_{11} & l_{21}u_{12}+u_{22} & l_{21}u_{13}+u_{23}\\ l_{31}u_{11} & l_{31}u_{12}+l_{32}u_{22} & l_{31}u_{13}+l_{32}u_{23}+u_{33}\end{pmatrix}$$

1st column

$u_{11}=1 \qquad l_{21}u_{11}=2\Rightarrow l_{21}=2, \qquad l_{31}u_{11}=3\Rightarrow l_{31}=3$

1st row $u_{12}=1 \quad u_{13}=-1$

2nd column $\; l_{21}u_{12}+u_{22}=2 \;\Rightarrow u_{22}=2-2=0 \quad l_{31}u_{12}+l_{32}u_{22}=2$

$\therefore$ The LU decomposition method fails as the pivot $u_{22}=0$.

Example 3 : Solve the system of equations Ax = b

$$\text{Where } A=\begin{pmatrix}2 & 1 & 1 & -2\\ 4 & 0 & 2 & 1\\ 3 & 2 & 2 & 0\\ 1 & 3 & 2 & 1\end{pmatrix},\quad b=\begin{pmatrix}-10\\ 8\\ 7\\ -5\end{pmatrix}$$

Using the LU decomposition method. Take all the diagonal elements of L as 1. As find A^{-1}

4.6. Cholesky Method

This method is also known as the square root method. If the coefficient matrix A is symmetric and positive definite then the matrix A can be decomposed as

$$A = LL^T \text{ ------> } (4.23)$$

where $L = (l_{ij})$, $l_{ij} = 0$, $i < j$ is a lower triangular matrix.

Alternative, A may be decomposed as

$$A = UU^T \text{ -----> } (4.24)$$

Where U is a upper triangular matrix.

For, then the system Ax = b becomes

$$LL^T x = b \text{ -----> } (4.25)$$

We take $L^T x = z \text{ -----> } (4.26)$

$$Lz = b \text{ -----> } (4.27)$$

Alternatively $z = L^{-1}b$

$$x = (L^T)^{-1} z$$

$$= (L^{-1})^T z$$

Now $A = LL^T$

$$\Rightarrow \begin{pmatrix} l_{11} & 0 & 0.....0 \\ l_{21} & l_{22} & 0....0 \\ l_{31} & l_{32} & l_{33}....0 \\ ...... & ..... & .... \\ l_{n1} & l_{n2} & l_{n3}....l_{nn} \end{pmatrix} \begin{pmatrix} l_{11} & l_{21} & l_{31}....l_{n1} \\ 0 & l_{22} & l_{32}....l_{n2} \\ 0 & 0 & l_{33}....l_{n3} \\ ...... & ..... & .... \\ 0 & 0 & 0....l_{nn} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & .....a_{1n} \\ a_{21} & a_{22} & .....a_{2n} \\ .... & ..... & .... \\ .... & ..... & .... \\ a_{n1} & a_{n2} & .....a_{nn} \end{pmatrix}$$

2^{nd} row

$l_{21}u_{13} + l_{22}u_{23} = 5$

$\Rightarrow 2(-1) + \frac{2}{3}u_{23} = 5$

$\Rightarrow u_{23} = 7 \times \frac{3}{2} = \frac{21}{2}$

3^{rd} column

$l_{31}u_{13} + l_{32}u_{23} + l_{33} = -1$

$\Rightarrow 1(-1) + \frac{1}{3}.\frac{21}{2} + l_{33} = -1$

$\Rightarrow l_{33} = -\frac{7}{2}$

$$\therefore L = \begin{pmatrix} 3 & 0 & 0 \\ 2 & \frac{2}{3} & 0 \\ 1 & \frac{1}{3} & -\frac{7}{2} \end{pmatrix} \qquad U = \begin{pmatrix} 1 & \frac{2}{3} & -1 \\ 0 & 1 & \frac{21}{2} \\ 0 & 0 & 1 \end{pmatrix}$$

Now $Lz = b. \Rightarrow \begin{pmatrix} 3 & 0 & 0 \\ 2 & \frac{2}{3} & 0 \\ 1 & \frac{1}{3} & -\frac{7}{2} \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 6 \\ -3 \\ 2 \end{pmatrix} \Rightarrow \begin{pmatrix} 3z_1 \\ 2z_1 + \frac{2}{3}z_2 \\ z_1 + \frac{1}{3}z_2 + \left(-\frac{7}{2}\right)z_3 \end{pmatrix} = \begin{pmatrix} 6 \\ -3 \\ 2 \end{pmatrix}$

$$\Rightarrow 3z_1 = 6 \Rightarrow z_1 = 2 \Rightarrow \frac{2}{3}z_2 = -3-4 \Rightarrow z_2 = -7 \times \frac{3}{2} = -\frac{21}{2} \Rightarrow -z_3\frac{7}{2} = 2 - 2 + \frac{7}{2}$$

$\Rightarrow z_3 = -1 \qquad \therefore z = \begin{pmatrix} 2 \\ -\frac{21}{2} \\ -1 \end{pmatrix}$

Now $Ux = z$

$$\Rightarrow \begin{pmatrix} 1 & \frac{2}{3} & -1 \\ 0 & 1 & \frac{21}{2} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 2 \\ -\frac{21}{2} \\ -1 \end{pmatrix}$$

$\Rightarrow x_1 + \frac{2}{3}x_2 - x_3 = 2$

$x_2 + \frac{21}{2}x_3 = \frac{-21}{2}$

$x_3 = -1$

$\therefore x_2 = 0, x_1 = 2 - 1 = 1$

$\therefore x_1 = 1, x_2 = 0, x_3 = -1$

$$\Rightarrow u_{ij} = \frac{\left(a_{ij} - \sum_{k=j+1}^{n} u_{ik}\, u_{jk}\right)}{u_{jj}} \qquad j = i+1, i+2, \ldots\ldots, n-1$$

$$a_{ii} = u_{ii}^{\,2} + u_{i,i+1} + \ldots\ldots + u_{in}^{\,2}$$

$$\Rightarrow u_{ii} = \left(a_{ii} - \sum_{k=i+1}^{n} u_{ik}^{\,2}\right)^{\frac{1}{2}} \qquad \begin{array}{l} i = 1, 2, \ldots, n-1 \\ u_{ij} = 0, i > j \end{array}$$

Example 1 : Solve the system of equations

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 8 & 22 \\ 3 & 22 & 82 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 5 \\ 6 \\ -10 \end{pmatrix}$$

Using the cholesky method

Solution : We know

$$A = LL^T$$

$$\Rightarrow \begin{pmatrix} 1 & 2 & 3 \\ 2 & 8 & 22 \\ 3 & 22 & 82 \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix}\begin{pmatrix} l_{11} & l_{12} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} 1 & 2 & 3 \\ 2 & 8 & 22 \\ 3 & 22 & 82 \end{pmatrix} = \begin{pmatrix} l_{11} & l_{11}l_{12} & l_{11}l_{31} \\ l_{21}l_{11} & l_{21}l_{12} + l_{22}^{\,2} & l_{21}l_{31} + l_{22}l_{32} \\ l_{31}l_{11} & l_{31}l_{12} + l_{32}l_{22} & l_{31}^{\,2} + l_{32}^{\,2} + l_{33}^{\,2} \end{pmatrix}$$

1st column

$l_{11}^2 = 1 \qquad l_{21}l_{11} = 2 \qquad l_{31}l_{11} = 3$

$l_{11} = 1 \qquad l_{21} = 2 \qquad l_{31} = 3$

1st row

$l_{31} = 3$

2nd column

$l_{21}^{\,2} + l_{22}^{\,2} = 8 \Rightarrow 4 + l_{22}^{\,2} = 8 \Rightarrow l_{22} = 2 \;\;\&\; l_{31}l_{21} + l_{32}l_{22} = 22 \Rightarrow 3.2. + l_{32}.2 = 22 \Rightarrow l_{32} = 8$

2nd row

$l_{31}^{\,2} + l_{32}^{\,2} + l_{33}^{\,2} = 82 \Rightarrow 3^2 + 8^2 + l_{33}^{\,2} = 82 \Rightarrow l_{33}^{\,2} = 82 - 73 \Rightarrow l_{33}^{\,2} = 9 \Rightarrow l_{33} = 3$

Comparing the corresponding elements

$$l_{ii} = \left(a_{ii} - \sum_{j=1}^{i-1} l_{ij}^{2} \right)^{\frac{1}{2}}, i = 1, 2, ..., n$$

For i > j

$$\left(l_{i1}, l_{i2}, ...l_{ij} ....l_{ii} ...0...0\right)\left(l_{j1}, l_{j2}, ...l_{jj} ...0...0\right)$$

$$\Rightarrow l_{i1} l_{j1} + l_{i2} l_{j2} + ... + l_{ij} l_{jj} = a_{ij}$$

$$\Rightarrow \sum_{k=1}^{j-1} l_{ik} l_{jk} + l_{ij} l_{jj} = a_{ij} \Rightarrow l_{ij} = \frac{\left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} l_{jk} \right)}{l_{jj}}, i > j \quad \text{for } i < j, \quad l_{ij} = 0$$

Let A = UU ^{T} ⇒ UU ^{T} = A

$$\Rightarrow \begin{pmatrix} u_{11} & u_{12} & ..... & u_{1n} \\ 0 & u_{22} & ..... & u_{2n} \\ ..... & ..... & ..... & ..... \\ ..... & ..... & ..... & ..... \\ 0 & 0 & 0 & ...u_{nn} \end{pmatrix} \begin{pmatrix} u_{11} & 0 & 0 & .... & 0 \\ u_{12} & u_{22} & 0 & .... & 0 \\ ..... & ..... & ..... & ..... & ..... \\ ..... & ..... & ..... & ..... & ..... \\ u_{1n} & u_{2n} & ..... & ..... & u_{nn} \end{pmatrix} = \begin{pmatrix} a_{11}\ a_{12} \cdots a_{1n} \\ a_{21}\ a_{22} \cdots a_{2n} \\ .... \\ .... \\ a_{i1}\ a_{i2} .... a_{in} \\ a_{n1}\ a_{n2} ..... a_{nn} \end{pmatrix}$$

$$a_{nn} = u_{nn}^{2} \Rightarrow u_{nn} = a_{nn}^{\frac{1}{2}}$$

$$a_{in} = u_{in} u_{nn}$$

$$\Rightarrow u_{in} = \frac{a_{in}}{u_{nn}}, \qquad i = 1, 2, ... n-1$$

$$a_{ij} = \left(0, 0, ... u_{ii}, u_{ij}, u_{in}\right) \begin{pmatrix} 0 \\ 0 \\ u_{jj} \\ u_{j,j+1} \\ u_{j,n} \end{pmatrix}$$

$$\Rightarrow u_{ij} u_{jj} + u_{i,j+1} u_{j,j+1} + u_{i,j+2}\, u_{j,j+2+ \_\_\_\_,} u_{in} u_{jn} = a_{ij}$$

$$\Rightarrow \sum_{k=j+1}^{n} u_{ik} u_{jk} + u_{ij} u_{jj} = a_{ij}$$

1st column

$$l_{11}^2=1\Rightarrow l_{11}=1, l_{21}=1, l_{31}=2$$

2nd column

$$l_{21}^2+l_{22}^2=4\Rightarrow l_{22}^2=3\Rightarrow l_{22}=\sqrt{3} \qquad l_{31}l_{21}+l_{32}l_{22}=6\Rightarrow 2(-1)+l_{32}\sqrt{3}=6\Rightarrow l_{32}=\frac{8}{\sqrt{3}}$$

3rd column

$$l_{31}^2+l_{32}^2+l_{33}^2=29\Rightarrow 4+\frac{64}{3}+l_{33}^2=29\Rightarrow l_{33}^2=25-\frac{64}{3}=\frac{11}{3}\Rightarrow l_{33}=\frac{\sqrt{11}}{\sqrt{3}}$$

$$\therefore L=\begin{pmatrix}1 & 0 & 0\\ -1 & \sqrt{3} & 0\\ 2 & \frac{8}{\sqrt{3}} & \frac{\sqrt{11}}{\sqrt{3}}\end{pmatrix} \;\&\; L^T=\begin{pmatrix}1 & -1 & 2\\ 0 & \sqrt{3} & \frac{8}{\sqrt{3}}\\ 0 & 0 & \frac{\sqrt{11}}{\sqrt{3}}\end{pmatrix}$$

Let the inverse of L be a lower triangular matrix.

$$\therefore LX=I$$

$$\Rightarrow\begin{pmatrix}1 & 0 & 0\\ -1 & \sqrt{3} & 0\\ 2 & \frac{8}{\sqrt{3}} & \frac{\sqrt{11}}{\sqrt{3}}\end{pmatrix}\begin{pmatrix}x_{11} & 0 & 0\\ x_{21} & x_{22} & 0\\ x_{31} & x_{32} & x_{33}\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}$$

$$\Rightarrow\begin{pmatrix}x_{11} & 0 & 0\\ -x_{11}+\sqrt{3}x_{21} & \sqrt{3}x_{22} & 0\\ 2x_{11}+\frac{8}{\sqrt{3}}x_{21}+\frac{\sqrt{11}}{\sqrt{3}}x_{31} & \frac{8}{\sqrt{3}}x_{22}+\frac{\sqrt{11}}{\sqrt{3}}x_{32} & \frac{\sqrt{11}}{\sqrt{3}}x_{33}\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}$$

$$\Rightarrow x_{11}=1 \;\&\; \Rightarrow -1+\sqrt{3}x_{21}=0\Rightarrow x_{21}=\frac{1}{\sqrt{3}} \;\&\; \Rightarrow 2x_{11}+\frac{8}{\sqrt{3}}x_{21}+\frac{\sqrt{11}}{\sqrt{3}}x_{31}=0$$

$$\Rightarrow 2.1+\frac{8}{\sqrt{3}}.\frac{1}{\sqrt{3}}+\frac{\sqrt{11}}{\sqrt{3}}x_{31}=0\Rightarrow\frac{\sqrt{11}}{\sqrt{3}}x_{31}=-\frac{6+8}{3}\Rightarrow x_{31}=\frac{-14}{\sqrt{11}\sqrt{3}}=-\frac{14}{\sqrt{33}}$$

$$\&\;\sqrt{3}\,x_{22}=1\Rightarrow x_{22}=\frac{1}{\sqrt{3}}$$

and $\frac{8}{\sqrt{3}}x_{22}+\frac{\sqrt{11}}{\sqrt{3}}x_{32}=0\Rightarrow\frac{8}{\sqrt{3}}.\frac{1}{\sqrt{3}}=-\frac{\sqrt{11}}{\sqrt{3}}x_{32}\Rightarrow x_{32}=-\frac{8}{\sqrt{3}\sqrt{3}}\times\frac{\sqrt{3}}{\sqrt{11}}=-\frac{8}{\sqrt{33}}$

$$\therefore L = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 2 & 0 \\ 3 & 8 & 3 \end{pmatrix}$$

Now $\quad Lz = b \Rightarrow \begin{pmatrix} 1 & 0 & 0 \\ 2 & 2 & 0 \\ 3 & 8 & 3 \end{pmatrix}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 5 \\ 6 \\ -10 \end{pmatrix}$

$\Rightarrow z_1 = 5$

$\& \; 2z_1 + 2z_2 = 6 \Rightarrow z_2 = -2$

$\& \; 3z_1 + 8z_2 + 3z_3 = -10 \Rightarrow 3z_3 = -10 - 15 + 16 \Rightarrow 3z_3 = -9 \Rightarrow z_3 = -3$

$$\therefore z = \begin{pmatrix} 5 \\ -2 \\ -3 \end{pmatrix}$$

Now $\quad L^T x = z$

$$\Rightarrow \begin{pmatrix} 1 & 2 & 3 \\ 0 & 2 & 8 \\ 0 & 0 & 3 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 5 \\ -2 \\ -3 \end{pmatrix}$$

$\Rightarrow x_1 + 2x_2 + 3x_3 = 5$

$2x_2 + 8x_3 = -2$

$3x_3 = -3$

$\Rightarrow x_3 = -1, \quad \therefore x_2 = -2 + \frac{8}{2} = 3 \quad \& \; x_1 = 5 + 3 - 6 = 2 \quad \therefore x_1 = 2, x_2 = 3, x_3 = -1$

Example 2 : Find inverse of $\begin{pmatrix} 1 & -1 & 2 \\ -1 & 4 & 6 \\ 2 & 6 & 29 \end{pmatrix}$ Using cholesky method

Solution : We have $A = LL^T$

$$\Rightarrow \begin{pmatrix} 1 & -1 & 2 \\ -1 & 4 & 6 \\ 2 & 6 & 29 \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix}\begin{pmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{pmatrix}$$

$$= \begin{pmatrix} l_{11}^2 & l_{11}l_{21} & l_{11}l_{31} \\ l_{11}l_{21} & l_{21}^2 + l_{22}^2 & l_{21}l_{31} + l_{22}l_{32} \\ l_{11}l_{31} & l_{31}l_{21} + l_{32}l_{22} & l_{31}^2 + l_{32}^2 + l_{33}^2 \end{pmatrix}$$

Example 3 : Solve the equations $\begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & -1 \\ 0 & 0 & -1 & 4 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

Using the cholesky method. Also determine A^{-1}

4.7. Iterative Methods

A general linear iterative method for the solution of the system of equations (4.2) may be defined in the form $X^{(k+1)} = Hx^{(k)} + C, k = 0, 1, 2, \ldots\ldots$ ----(4.28)

where $x^{(k+1)}$ and $x^{(k)}$ are the approximations for x at the $(k+1)^{th}$ and k^{th} iterations, respectively. H is called the iteration matrix depending on A and C is a column vector. In the limiting case when $K \to \alpha$, $x^{(k)}$ converges to the exact solution.

$$X = A^{-1}b. \text{-------} > (4.29)$$

and the iteration equation (4.28) becomes, by substitution form (4.29)

$$A^{-1}b = HA^{-1}b + c \text{------} (4.30)$$

The column vector c is given by

$$C = (I - H)A^{-1}b \text{ ----} > (4.31)$$

We now determine the iteration matrix 'H' and the column vector c for a few well known iteration methods.

4.8. Jacobi Iteration Method

We assume that the quantities a_{ii} in (4.1) are pivot elements. The equations (4.1) may be written as

$$\left.\begin{array}{l} a_{11}x_1 = -(a_{12}x_2 + a_{13}x_3 + \ldots\ldots\ldots + a_{1n}x_n) + b_1 \\ a_{22}x_2 = -(a_{21}x_1 + a_{23}x_3 + \ldots\ldots\ldots + a_{2n}x_n) + b_2 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ a_{33}x_3 = -(a_{31}x_1 + a_{32}x_2 + \ldots\ldots + a_{n,n-1}x_{n-1}) + b_n \end{array}\right\} \text{--}(4.32)$$

The Jacobi iteration method or Gauss-Jacobi iteration method may now be defined as

$$\& \ \frac{\sqrt{11}}{\sqrt{3}} x_{33} = 1 \Rightarrow x_{33} = \frac{\sqrt{3}}{\sqrt{11}}$$

$$\therefore x = L^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{14}{\sqrt{33}} & -\frac{8}{\sqrt{33}} & \frac{\sqrt{3}}{\sqrt{11}} \end{pmatrix}$$

$$\therefore \left(L^T\right)^{-1} = \left(L^{-1}\right)^T = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{14}{\sqrt{33}} & -\frac{8}{\sqrt{33}} & \frac{\sqrt{3}}{\sqrt{11}} \end{pmatrix} = \begin{pmatrix} 1 & \frac{1}{\sqrt{3}} & -\frac{14}{\sqrt{33}} \\ 0 & \frac{1}{\sqrt{3}} & -\frac{8}{\sqrt{33}} \\ 0 & 0 & \frac{\sqrt{3}}{\sqrt{11}} \end{pmatrix}$$

$$\therefore A = LL^T \Rightarrow A^{-1} = \left(LL^T\right)^{-1} = L^{-1}\left(L^T\right)^{-1} = \left(L^{-1}\right)\left(L^{-1}\right)^T$$

$$= \begin{pmatrix} 1 & \frac{1}{\sqrt{3}} & -\frac{11}{\sqrt{33}} \\ 0 & \frac{1}{\sqrt{3}} & -\frac{8}{\sqrt{33}} \\ 0 & 0 & \frac{\sqrt{3}}{\sqrt{11}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{14}{\sqrt{33}} & -\frac{8}{\sqrt{33}} & \frac{\sqrt{3}}{\sqrt{11}} \end{pmatrix}$$

$$= \begin{pmatrix} 1+\frac{1}{3}+\frac{196}{33} & \frac{1}{3}+\frac{112}{33} & -\frac{14}{11} \\ \frac{1}{3}+\frac{112}{33} & \frac{1}{3}+\frac{64}{33} & -\frac{8}{11} \\ -\frac{14}{11} & -\frac{8}{11} & \frac{3}{11} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{240}{33} & \frac{123}{33} & -\frac{14}{11} \\ \frac{123}{33} & \frac{75}{33} & -\frac{8}{11} \\ -\frac{14}{11} & -\frac{8}{11} & \frac{3}{4} \end{pmatrix}$$

$$= \frac{1}{11} \begin{pmatrix} 80 & 41 & -14 \\ 41 & 25 & -8 \\ -14 & -8 & 3 \end{pmatrix}$$

Perform their iteration

Solution : Here $A = \begin{pmatrix} 4 & 1 & 2 \\ 3 & 5 & 1 \\ 1 & 1 & 3 \end{pmatrix}$, $L = \begin{pmatrix} 0 & 0 & 0 \\ 3 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}$,

$U = \begin{pmatrix} 0 & 1 & 2 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$, $D = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 3 \end{pmatrix}$

Now, $H = -D^{-1}(L + U)$

$$= \begin{pmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{5} & 0 \\ 0 & 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 \\ 3 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} -\frac{1}{4} & 0 & 0 \\ 0 & -\frac{1}{5} & 0 \\ 0 & 0 & -\frac{1}{3} \end{pmatrix} \begin{pmatrix} 0 & 1 & 2 \\ 3 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & -\frac{1}{4} & -\frac{1}{2} \\ -\frac{3}{5} & 0 & -\frac{1}{5} \\ -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & -0.25 & -0.5 \\ -0.6 & 0 & -0.2 \\ -0.333 & -0.333 & 0 \end{pmatrix}$$

$$C = D^{-1}b = \begin{pmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{5} & 0 \\ 0 & 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 4 \\ 7 \\ 3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1.4 \\ 1 \end{pmatrix}$$

We know that

$$x^{(k+1)} = Hx^{(k)} + c, \qquad k = 0, 1, 2, 3.$$

$$x_1^{(k+1)} = -\frac{1}{a_{11}}\left(a_{12}x_2^{(k)} + a_{13}x_3^{(k)} + \ldots\ldots + a_{1n}x_n^{(k)} - b_1\right)$$

$$x_2^{(k+1)} = -\frac{1}{a_{22}}\left(a_{22}x_1^{(k)} + a_{23}x_3^{(k)} + \ldots\ldots + a_{2n}x_n^{(k)} - b_2\right)$$

....

$$x_n^{(k+1)} = -\frac{1}{a_{33}}\left(a_{31}x_1^{(k)} + a_{32}x_2^{(k)} + \ldots\ldots + a_{n,n-1}x_{n-1}^{(k)} - b_n\right)$$

$$K = 0, 1, 2, \ldots\ldots \qquad (4.33)$$

Since, we replace the complete vector $x^{(k)}$ in the right side of (3.69) at the end of each iteration, this method is also called the method of simultaneous displacement.

In matrix form the method can be written as

$$x^{(k+1)} = -D^{-1}(L+U)x^{(k)} + D^{-1}b \quad ------> (4.34)$$

$$= Hx^{(k)} + c, \quad k = 0, 1, 2, \ldots$$

where $H = -D^{-1}(L+U), C = D^{-1}b$ and L and U are respectively lower and upper triangular matrices with zero diagonal entries. D is the diagonal matrix such that

$$A = L + D + U.$$

Equation (4.34) can alternatively be written as

$$x^{(k+1)} = x^{(k)} - [I + D^{-1}(L+U)]x^{(k)} + D^{-1}b$$

$$= x^{(k)} - D^{-1}[D + L + U]x^{(k)} + D^{-1}b$$

$$= x^{(k)} + D^{-1}[b - Ax^{(k)}]$$

$$V^{(k)} = D^{-1}r^{(k)} \quad ---------> (4.35)$$

Where $v^{(k)} = x^{(k+1)} - x^{(k)}$ is the error in the approximation and $r^{(k)} = b - Ax^{(k)}$ is the residual vector.

We may rewrite the above equation as $DV^{(k)} = r^{(k)}$

We solve for $V^{(k)}$ and find $x^{(k+1)} = x^{(k)} + v^{(k)}$

These equations describe the Jacobi Iteration method in an error format.

Example 1 : Solve the following system using Jacobi iteration method

$$4x + y + 2z = 4$$

$$3x + 5y + z = 7, \qquad x^0 = 0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$x + y + 3z = 3$$

$$x_1^{(k+1)} = -\frac{1}{a_{11}}\left(a_{12}x_2^{(k)} + a_{13}x_3^{(k)} + ...+ a_{1n}x_n^{(k)}\right) + \frac{b_1}{a_{11}}$$

$$x_2^{(k+1)} = -\frac{1}{a_{22}}\left(a_{21}x_1^{(k)} + a_{23}x_3^{(k)} + ...+ a_{2n}x_n^{(k)}\right) + \frac{b_2}{a_{22}}$$

....

$$x_n^{(k+1)} = -\frac{1}{a_{nn}}\left(a_{n1}x_1^{(k+1)} + a_{n2}x_2^{(k+1)} + ...+ a_{n,n-1}x^{(k+1)}\right) + \frac{b_n}{a_{nn}}$$

which may be rearranged in the form

$$a_{11}x_1^{(k+1)} = -\sum_{i=3}^{n} a_{1i}x_i^{(k)} + b_1$$

$$a_{21}x_1^{(k+1)} + a_{22}x_2^{(k+1)} = -\sum_{i=3}^{n} a_{2i}x_i^{(k)} + b_2$$

....

$$a_{n1}x_1^{(k+1)} + ...+ a_{nn}x_n^{(k+1)} = b_n \longrightarrow (4.36)$$

Since we replace the vector $x^{(k)}$ in the right side of (4.33) element, this method is also called the method of successive displacement.

In matrix notation (4.36) becomes

$$(D+L)x^{(k+1)} = -Ux^{(k)} + b$$

Or $$x^{(k+1)} = -(D+L)^{-1}Ux^{(k)} + b(D+L)^{-1}$$

$$= Hx^{(k)} + C, \quad k = 0,1,2,.......... (4.37)$$

where $H = -(D+L)^{-1}U$ and $C = (D+L)^{-1}b$

Equation (4.34) can alternatively be written as

$$x^{(k+1)} = x^{(k)} - \left[I + (D+L)^{-1}U\right]x^{(k)} + (D+L)^{-1}b$$

$$= x^{(k)} - (D+L)^{-1}(D+L+U)x^{(k)} + (D+L)^{-1}b$$

$\therefore x^1 = Hx^0 = C$

$$=\begin{pmatrix} 0 & -0.25 & -0.5 \\ -0.6 & 0 & -0.2 \\ -0.333 & -0.333 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}+\begin{pmatrix} 1 \\ 1.4 \\ 1 \end{pmatrix}=\begin{pmatrix} 1 \\ 1.4 \\ 1 \end{pmatrix}$$

$x^2 = Hx^1 = C$

$$=\begin{pmatrix} 0 & -0.25 & -0.5 \\ -0.6 & 0 & -0.2 \\ -0.333 & -0.333 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1.4 \\ 1 \end{pmatrix}+\begin{pmatrix} 1 \\ 1.4 \\ 1 \end{pmatrix}$$

$$=\begin{pmatrix} -0.85 \\ -0.80 \\ -0.7999 \end{pmatrix}+\begin{pmatrix} 1 \\ 1.4 \\ 1 \end{pmatrix}=\begin{pmatrix} 0.15 \\ 0.6 \\ 0.2 \end{pmatrix}$$

$x^3 = Hx^2 + C$

$$=\begin{pmatrix} 0 & -0.25 & -0.5 \\ -0.6 & 0 & -0.2 \\ -0.333 & -0.333 & 0 \end{pmatrix}\begin{pmatrix} 0.15 \\ 0.6 \\ 0.2 \end{pmatrix}+\begin{pmatrix} 1 \\ 1.4 \\ 1 \end{pmatrix}$$

$$=\begin{pmatrix} -0.25 \\ -0.13 \\ -0.24975 \end{pmatrix}+\begin{pmatrix} 1 \\ 1.4 \\ 1 \end{pmatrix}=\begin{pmatrix} .75 \\ 1.27 \\ 0.75 \end{pmatrix}$$

Example 2 : Use Jacobi iteration method to solve

$10x + 4y - 27 = 12$

$x - 10y - z = -10, \qquad x^0 = 0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$

$5x + 2y - 10z = -3$

Perform 3 iterations

4.9. Gauss . Seidel Iteration Method

We now use on the right hand side of (4.33), all the available values from the present iteration. We write the Gauss- Seidel method as

$$\Rightarrow \begin{pmatrix} 5a & 0 & 0 \\ 3a+4b & 4c & 0 \\ 2a-3b+5d & -3c+5e & 5f \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\Rightarrow 5a = 1 \qquad \Rightarrow a = \frac{1}{5}$$

$\&\ 3a + 4b = 0$ $\qquad\qquad$ $\&\ 4c = 1$

$\Rightarrow 4b = -\frac{3}{5}$ $\qquad\qquad$ $\Rightarrow c = \frac{1}{4}$

$\Rightarrow b = -\frac{3}{20}$

$\&\quad 2a - 3b + 5d = 0$

$\Rightarrow 2\frac{1}{5} - 3\left(\frac{-3}{20}\right) + 5d = 0$

$\Rightarrow \frac{2}{5} + \frac{9}{20} + 5d = 0$

$\Rightarrow 5d = -\left(\frac{8+9}{20}\right)$

$\Rightarrow d = -\frac{17}{100}$

$\&\quad -3c + 5e = 0$

$\Rightarrow -\frac{3}{4} + 5e = 0$

$\Rightarrow e = \frac{3}{20}$

$\&\quad f = \frac{1}{5}$

$$\therefore (D+L)^{-1} = \begin{pmatrix} \frac{1}{5} & 0 & 0 \\ -\frac{3}{20} & \frac{1}{4} & 0 \\ -\frac{17}{100} & \frac{3}{20} & \frac{1}{5} \end{pmatrix}$$

$$=x^{(k)}-(D+L)^{-1}Ax^{(k)}+(D+L)^{-1}b$$

$$=x^{(k)}+(D+L)^{-1}(b-Ax^{(k)})$$

We write $V^{(k)}=(D+L)^{-1}r^{(k)}$

Where $V^{(k)}=x^{(k+1)}-x^{(k)}$ and $r^{(k)}=b-Ax^{(k)}$ is the residual vector.

We may rewrite the above equations as $(D+L)V^{(k)}=r^{(k)}$ ------> (4.38) and solve for $V^{(k)}$ by forward substitution.

The solution is then found from $x^{(k+1)}=x^{(k)}+v^{(k)}$

These equations describe the Gauss-Seidel method in an error format.

Example 1 : $\begin{bmatrix}5 & 1 & 2\\3 & 4 & -1\\2 & -3 & 5\end{bmatrix}\begin{bmatrix}x_1\\x_2\\x_3\end{bmatrix}=\begin{bmatrix}2\\-2\\10\end{bmatrix}$

Using Gauss Seidel Method-

Solution : Here $A=\begin{pmatrix}5 & 1 & 2\\3 & 4 & -1\\2 & -3 & 5\end{pmatrix}$, $L=\begin{pmatrix}0 & 0 & 0\\3 & 0 & 0\\2 & -3 & 0\end{pmatrix}$,

$D=\begin{pmatrix}5 & 0 & 0\\0 & 4 & 0\\0 & 0 & 5\end{pmatrix}$, $V=\begin{pmatrix}0 & 1 & -2\\0 & 0 & 1\\0 & 0 & 0\end{pmatrix}$

$$\therefore (L+D)=\begin{pmatrix}5 & 0 & 0\\3 & 4 & 0\\2 & -3 & 5\end{pmatrix}$$

Let $\begin{pmatrix}a & 0 & 0\\b & c & 0\\d & e & f\end{pmatrix}$ be the inverse of D + L

$$\therefore \begin{pmatrix}5 & 0 & 0\\3 & 4 & 0\\2 & -3 & 5\end{pmatrix}\begin{pmatrix}a & 0 & 0\\b & c & 0\\d & e & f\end{pmatrix}=I=\begin{pmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1\end{pmatrix}$$

$K = 2, x^3 = Hx^2 + C$

$$= \begin{pmatrix} 0 & -\frac{1}{5} & \frac{2}{5} \\ 0 & \frac{3}{20} & -\frac{1}{20} \\ 0 & \frac{17}{100} & -\frac{32}{100} \end{pmatrix} \begin{pmatrix} 1.104 \\ -0.988 \\ 0.9656 \end{pmatrix} + \begin{pmatrix} 0.4 \\ -0.8 \\ 1.36 \end{pmatrix}$$

$$= \begin{pmatrix} 0.58384 \\ -0.19648 \\ 0.351424 \end{pmatrix} + \begin{pmatrix} 0.4 \\ 0.8 \\ 1.36 \end{pmatrix} = \begin{pmatrix} 0.9838 \\ -0.9965 \\ 1.0086 \end{pmatrix}$$

Example 2 : Solve the system of equations

$2x_1 - x_2 + 0.x_3 = 7$

$-x_1 + 2x_2 - x_3 = 1$

$0.x_1 - x_2 + 2x_3 = 1$

Using the Gauss-Seidel method and its error format.

4.10. Successive Over Relaxation Method (SOR).

The method is a generalization of the Gauss-Seidel method. This method is often used when the coefficient matrix of the system of equations is symmetric and has property A. We define an auxiliary vector $\hat{x}$ as

$$\hat{x}^{(k+1)} = -D^{-1}Lx^{(k+1)} - D^{-1}Ux^{(k)} + D^{-1}b \quad ----> (4.39)$$

The final solution is now written as

$$x^{(k+1)} = x^{(k)} + W\left(\hat{x}^{(k+1)} - x^{(k)}\right)$$

$$\Rightarrow x^{(k+1)} = (1 - W)x^{(k)} + W\,\hat{x}^{(k+1)} \quad ----> (4.40)$$

Substituting (1) in (2)

$$x^{(k+1)} = (1 - W)x^{(k)} + W\left(D^{-1}Lx^{(k+1)} - D^{-1}Ux^{(k)} + D^{-1}b\right)$$

$$= -WD^{-1}Lx^{(k+1)} + \left(1 - W - WD^{-1}U\right)x^{k} + WD^{-1}b$$

$$\Rightarrow Dx^{(k+1)} = -WLx^{(k+1)} + [(1 - W)D - WU]x^{(k)} + Wb$$

$$\Rightarrow (D + WL)x^{(k+1)} = [(1 - W)D - WU]x^{(k)} + Wb$$

$$H=-(D+L)^{-1}U$$

$$=-\begin{pmatrix}\frac{1}{5} & 0 & 0\\ -\frac{3}{20} & \frac{1}{4} & 0\\ -\frac{17}{100} & \frac{3}{20} & \frac{1}{5}\end{pmatrix}\begin{pmatrix}0 & 1 & 2\\ 0 & 0 & -1\\ 0 & 0 & 0\end{pmatrix}$$

$$=-\begin{pmatrix}0 & \frac{1}{5} & -\frac{2}{5}\\ 0 & -\frac{3}{20} & \frac{1}{20}\\ 0 & -\frac{17}{100} & \frac{19}{100}\end{pmatrix}=\begin{pmatrix}0 & -\frac{1}{5} & \frac{2}{5}\\ 0 & \frac{3}{20} & -\frac{1}{20}\\ 0 & \frac{17}{100} & -\frac{19}{100}\end{pmatrix}$$

$$C=(D+L)^{-1}b$$

$$=\begin{pmatrix}\frac{1}{5} & 0 & 0\\ -\frac{3}{20} & \frac{1}{4} & 0\\ -\frac{17}{100} & \frac{3}{20} & \frac{1}{5}\end{pmatrix}\begin{pmatrix}2\\ -2\\ 10\end{pmatrix}=\begin{pmatrix}\frac{2}{5}\\ -\frac{14}{20}\\ \frac{136}{100}\end{pmatrix}=\begin{pmatrix}0.4\\ -0.8\\ 1.36\end{pmatrix}$$

Now $x^{k+1}=Hx^{k}+C$

$k=0,\ x^{1}=Hx^{0}+C$

$$=\begin{pmatrix}0 & -\frac{1}{5} & \frac{2}{5}\\ 0 & \frac{3}{20} & -\frac{1}{20}\\ 0 & \frac{17}{100} & -\frac{32}{100}\end{pmatrix}\begin{pmatrix}0\\ 0\\ 0\end{pmatrix}+\begin{pmatrix}0.4\\ -0.8\\ 1.36\end{pmatrix}=\begin{pmatrix}0.4\\ -0.8\\ 1.36\end{pmatrix}$$

$K=1,\ x^{2}=Hx^{1}+C$

$$=\begin{pmatrix}0 & -\frac{1}{5} & \frac{2}{5}\\ 0 & \frac{3}{20} & -\frac{1}{20}\\ 0 & \frac{17}{100} & -\frac{32}{100}\end{pmatrix}\begin{pmatrix}0.4\\ -0.8\\ 1.36\end{pmatrix}+\begin{pmatrix}0.4\\ -0.8\\ 1.36\end{pmatrix}$$

$$=\begin{pmatrix}.704\\ -0.188\\ -0.3944\end{pmatrix}+\begin{pmatrix}0.4\\ -0.8\\ 1.36\end{pmatrix}=\begin{pmatrix}1.104\\ -0.988\\ 0.9656\end{pmatrix}$$

2. Solve the following system of equations

$$\begin{bmatrix} 2 & 2 & 1 \\ 4 & 2 & 3 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

Using the Gauss elimination method with partial pivoting.

3. Determine the LU factorization of the matrix

$$\begin{bmatrix} 2 & -6 & 10 \\ 1 & 5 & 1 \\ -1 & 15 & -5 \end{bmatrix}$$

So that (i) $l_{ii} = 1$, (ii) $u_{ii} = 1$, (iii) $l_{ii} = 2$ (iv) $u_{ii} = 2$, $i = 1, 2, 3$

4. Solve the system of equations

$$\begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

By the cholesky method

5. Find the necessary and sufficient conditions on k, so that the (i) Jacobi method (ii) Gauss-Seidel method converges for solving of equations $Ax = b$, where

$$A = \begin{bmatrix} 1 & 0 & k \\ 2 & 1 & 3 \\ k & 0 & 1 \end{bmatrix}$$ and b is arbitrary.

6. Given $A = L + I + U$

$$A = \begin{bmatrix} 1 & 2 & -2 \\ 1 & 1 & 1 \\ 2 & 2 & 1 \end{bmatrix}$$

L and U are strictly lower and upper triangular matrices respectively, decided whether (a) Jacobi and (b) Gauss-Seidel methods converges to the solution of $A\,x = b$.

7. Show that both the (1) Jacobi method and (ii) Gauss-Seidel Methods diverge for solving the system of equations

$$\begin{bmatrix} 2 & 3 & 1 \\ 3 & 2 & 2 \\ 1 & 2 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 6 \end{bmatrix}$$

$$\Rightarrow x^{(k+1)} = (D+WL)^{-1}[(1-W)D-WU]x^{(k)} + W(D+WL)^{-1}b$$

$$= H x^{(k)} + C, \ k = 0, 1, 2, \ldots \quad ----> (4.41)$$

Where $H = (D+WL)^{-1}[(1-W)D-WU]$

$$C = W(D+WL)^{-1}b$$

$$(4.41) \Rightarrow x^{(k+1)} = x^{(k)} - (D+WL)^{-1}[(D+WL)-(1-W)D+WU]x^{(k)} + W(D+WL)^{-1}b$$

$$= x^{(k)} + W(D+WL)^{-1}r^{(k)}$$

Where $r^{(k)} = b - Ax^{(k)}$ is the residual are may write

$$v^{(k)} = W(D+WL)^{-1}r^{(k)}$$

Or $\quad (D+WL)v^{(k)} = Wr^{(k)} \quad ----> (4.42)$

The equation describes the SOR method in its error format. For computational purposes, it is convenient to use this equation.

When w =1, equation (4.42) reduces to the Gauss-Seidel method. The quantity w is called the relaxation parameter and $x^{(k+1)}$ is a weighted mean of $\hat{x}^{(k+1)}$ and $x^{(k)}$. From the equation (4.40).

We find that the weights are non-negative for $0 \le w \le 1$. If $w > 1$ then the method is called an over relaxation method and if $w < 1$, then it is called an under relaxation method.

EXERCISE

1. The matrix $A = \begin{pmatrix} 1+s & -s \\ s & 1-s \end{pmatrix}$ is given. Calculate p and q such that

   $A^3 = pA + qI$ and determine e^A

8. For the system of equations

(i) $$\begin{bmatrix} 3 & 2 & 0 \\ 2 & 3 & -1 \\ 0 & -1 & 2 \end{bmatrix} x = \begin{bmatrix} 5 \\ 4 \\ 1 \end{bmatrix}$$

(ii) $$\begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} x = \begin{bmatrix} 3 \\ 2 \\ 3 \end{bmatrix}$$

Find the optimal relaxation parameter W_{opt} for the SOR iteration scheme.

Determine the rate of convergence of this scheme.

■■■