M.Sc. (MATHEMATICS)

MAL-526

ADVANCED NUMERICAL METHODS

Directorate of Distance Education

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M.Sc. Mathematics (IInd Semester)
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MAL-526: M. Sc. Mathematics (Advanced Numerical Methods)

LESSON No. 1 **Written by- Dr. Joginder Singh**

INTERPOLATION

STRUCTURE

1.0 LEARNING OBJECTIVES

- This chapter will be devoted to explaining the main concepts of interpolation.
- Some theorems concerning the interpolation of the functions will be proved.
- Various interpolation relations/methods have been discussed.

1.1 INTRODUCTION

The calculus of finite differences deals with the changes that take place in the value of a function due to finite changes in the independent variable. On the other head, in infinitesimal calculus, we study those changes in a function that occurs when the independent variable changes continuously in a given interval.

Suppose that the function $y = f(x)$ is tabulated for equally spaced values (x_i, y_i), i = 1,2,3, $\cdots, n$ such that $x_i = x_0 + ih$. If we are required to recover the values of $f(x)$ or its derivatives for some intermediate values of x in the range $x_0 \leq x \leq x_n$, the following three types of differences are found useful.

FORWARD DIFFERENCES: The forward difference or simply difference operator is denoted by Δ and may be defined as

$$\Delta f(x) = f(x + h) - f(x)$$

or, writing in terms of y, at $x = x_i$, Eq.(i) becomes

$$\Delta f(x_i) = f(x_i + h) - f(x_i)$$

or $$\Delta y_i = y_{i+1} - y_i, \qquad i = 0, 1, 2, \ldots, n - 1$$

The differences between the first-order differences are called the second differences and they are denoted by

$$\Delta^2 y_0, \Delta^2 y_1, \ldots, \Delta^2 y_n.$$

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

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

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

$$\Delta^3 y_1 = y_4 - 3y_3 + 3y_2 - y_1, \text{ etc.}$$

Generalizing, we have

$$\Delta^{n+1}f(x) = \Delta[\Delta^n f(x)], \text{ i.e., } \Delta^{n+1}y_i = \Delta[\Delta^n y_i], \quad n = 0, 1, 2,$$

Also, $\Delta^{n+1}f(x) = \Delta^n[f(x + h) - f(x)] = \Delta^n f(x + h) - \Delta^n f(x)$

And $\Delta^{n+1}y_i = \Delta_n y_{i+1} - \Delta^n y_i$, $n = 0, 1, 2$

where $\Delta^0 \equiv$ identity operator i.e., $\Delta^0 f(x) = f(x)$ and $\Delta^1 = \Delta$.

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					

The forward differences for the arguments $x_0, x_1, \ldots, x_5$ are shown in the above Table.

Which is called a diagonal difference table or forward difference table. The first term in Table is y_0 and is called the leading term. The differences $\Delta y_0, \Delta^2 y_0, \Delta^3 y_0, \ldots$, are called the leading differences. Similarly, the differences with fixed subscripts are called forward differences.

BACKWARD DIFFERENCES: The backward difference operator is denoted by ∇ and it is defined as $\nabla f(x) = f(x) - f(x - h)$.

This can be written as $\nabla y_i = y_i - y_{i-1}$, $\quad i = n, n - 1, \ldots, 1$

or $\quad \nabla y_1 = y_1 - y_0, \quad \nabla y_2 = y_2 - y_1, \ldots, \nabla y_n = y_n - y_{n-1}$

These differences are called first differences. The second differences are denoted by $\nabla^2 y_2, \nabla^2 y_3, \ldots, \nabla^2 y_n$.

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

Similarly, $\nabla^2 y_3 = y_3 - 2y_2 + y_1$, $\nabla^2 y_4 = y_4 - 2y_3 + y_2$, and so on.

Generalising, we have $\nabla^k y_i = \nabla^{k-1} y_i - \nabla^{k-1} y_{i-1}$, $i = n, n-1, \ldots, k$

where $\nabla^0 y_i = y_i$, $\nabla^1 y_i = \nabla y_i$.

The backward differences written in a tabular form are shown in the following table as the differences $\nabla^n y$ with a fixed subscript 'i' lie along the diagonal upward sloping.

Backward difference or horizontal table:

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
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		$\nabla^3 y_4$	
x_3	y_3		$\nabla^2 y_4$		
		∇y_4			
x_4	y_4				

CENTRAL DIFFERENCES: The central difference operator is denoted by the symbol δ and is defined by

$$\delta f(x) = f(x + h/2) - f(x - h/2)$$

where h is the interval of differencing.

In terms of y, the first central difference is written as

$$\delta y_1 = y_{i+1/2} - y_{i-1/2}$$

where $y_{i+1/2} = f(x_i + h/2)$ and $y_{i-1/2} = f(x_i - h/2)$.

Hence $\delta y_{1/2} = y_1 - y_0$, $\delta y_{3/2} = y_2 - y_1$, …., $\delta y_{n-1/2} = y_n - y_{n-1}$.

The second central difference is given by $\delta^2 y_i = y_{i+1/2} - y_{i-1/2}$

$$= (y_{i+1} - y_i) - (y_i - y_{i-1})$$

$$= y_{i+1} - 2y_i + y_{i-1}$$

Generalising, $\delta^n y_i = \delta^{n-1} y_{i+1/2} - \delta^{n-1} y_{i-1/2}$

The central difference table for the seven arguments $x_0, x_1, \ldots, x_4$ is shown in following table

Central difference table:

x	y	δy	$\delta^2 y$	$\delta^3 y$	$\delta^4 y$	$\delta^5 y$	$\delta^6 y$
x_0	y_0						
		$\delta y_{1/2}$					
x_1	y_1		$\delta^2 y_1$				
		$\delta y_{3/2}$		$\delta^3 y_{3/2}$			
x_2	y_2		$\delta^2 y_2$		$\delta^4 y_2$		
		$\delta y_{5/2}$		$\delta^3 y_{5/2}$		$\delta^5 y_{5/2}$	
x_3	y_3		$\delta^2 y_3$		$\delta^4 y_3$		$\delta^6 y_3$
		$\delta y_{7/2}$		$\delta^3 y_{7/2}$		$\delta^5 y_{7/2}$	
x_4	y_4		$\delta^2 y_4$		$\delta^4 y_4$		
		$\delta y_{9/2}$		$\delta^3 y_{9/2}$			
x_5	y_5		$\delta^2 y_5$				
		$\delta y_{11/2}$					
x_6	y_6						

It is noted in the above table all odd differences have fraction suffices and all the even differences are with integral suffices.

PROPERTIES OF THE OPERATOR (Δ):

1. If c is a constant then $\Delta c = 0$.

Proof: Let $f(x) = c$

Hence $f(x + h) = c$, where h is the interval of differencing.

Hence $\Delta f(x) = f(x + h) - f(x) = c - c = 0$

or $\Delta c = 0$

2. Δ is distributive, i.e., $\Delta[f(x) \pm g(x)] = \Delta f(x) \pm \Delta g(x)$.

Proof: $\Delta[f(x) + g(x)] = [f(x + h) + g(x + h)] - [f(x) + g(x)]$

$= f(x + h) - f(x) + g(x+ h) - g(x)$

$= \Delta f(x) + \Delta g(x)$.

Similarly, we have $\Delta[f(x) - g(x)] = \Delta f(x) - \Delta g(x)$

3. If c is a constant then $\Delta[cf(x)] = c\Delta f(x)$.

From properties 2 and 3 above, it is observed that Δ is a linear operator.

Proof: $\Delta[cf(x)] = cf(x + h) - cf(x) = c[f(x + h) - f(x)] = c\Delta f(x)$

Hence $\Delta[cf(x)] = c\Delta f(x)$.

4. If m and n are positive integers then $\Delta^m\Delta^n f(x) = \Delta^{m+n} f(x)$.

Proof: $\Delta^m\Delta^n f(x) = (\Delta\times\Delta\times\Delta \text{ ... m times}) (\Delta\times\Delta \text{ … n times}) f(x)$

$= (\Delta\Delta\Delta \text{ … (m + n) times}) f(x)$

$= \Delta^{m+n} f(x)$.

Similarly, we can prove the following properties:

5. $\Delta[f_1(x) + f_2(x) + \ldots + f_n(x)] = \Delta f_1(x) + \Delta f_2(x) + \ldots + \Delta f_n(x)$.

6. $\Delta[f(x)g(x)] = f(x)\,\Delta g(x) + g(x)\,\Delta f(x)$.

7. $\Delta\left[\dfrac{f(x)}{g(x)}\right] \dfrac{g(x)\Delta f(x) - f(x)\Delta g(x)}{g(x)g(x+h)}$

DIFFERENCE OPERATORS

(a) Shift operator E:

The shift operator is defined as

$E f(x) = f(x + h)$

or $Ey_i = y_{i+1}$

Hence, the shift operator shifts the function value y_i to the next higher value y_{i+1}. The second shift operator gives

$E^2 f(x) = E[Ef(x)] = E[f(x + h)] = f(x + 2h)$

E is linear and obeys the law of indices.

Generalizing, $E^n f(x) = f(x + nh)$ or $E^n y_i = y_{i+nh}$

The inverse shift operator E^{-1} is defined as

$E^{-1} f(x) = f(x - h)$

Similarly, second and higher inverse operators are given by

$E^{-2} f(x) = f(x - 2h)$ and $E^{-n} f(x) = f(x - nh)$

The more general form of E operator is given by

$E^r f(x) = f(x + rh)$

where r is positive as well as negative rationals.

(b) Average operator μ: The average operator μ is defined as

$$\mu\, f(x) = \frac{1}{2} f[(x+h/2)+f(x-h/2)]$$

i.e., $$\mu y_i = \frac{1}{2}[y_{i+1/2} + y_{i-1/2}]$$

(c) Differential operator D: The differential operator is usually denoted by D, where

$$Df(x) = \frac{d}{dx} f(x) = f'(x)$$

$$D^2 f(x) = \frac{d^2}{dx^2} f(x) = f''(x)$$

RELATION BETWEEN THE OPERATORS:

To develop approximations to differential equations, the following summary of operators is useful.

Operator	Definition
Forward difference operator Δ	$\Delta f(x) = f(x + h) – f(x)$
Backward difference operator ∇	$\nabla f(x)\ \nabla = f(x) – f(x – h)$
Central difference operator δ	$\delta f(x) = f(x + h/2) –f(x – h/2)$
Shift operator E	$E f(x) = f(x + h)$
Average operator μ	$\mu f(x) = 0.5[f(x+h/2) – f(x– h/2)]$
Differential operator D	$Df(x) = f'(x)$

Here h is the difference interval. For linking different operators with differential operator D we consider Taylor's formula:

In operator notation, we can write it as:

$$E\, f(x) = \left[1 + hD + \frac{1}{2!}(hD)^2 + \ldots..\right] f(x)$$

This series in brackets is the expression for the exponential and

$$f(x + h) = f(x) + hf\,'(x) + \frac{1}{2!}h^2 f''(x) + \ldots\ldots\ldots\ldots\ldots$$

hence we can write $E = e^{hD}$

This relation can be used by symbolic programs such as Maple or Mathematica to analyze the accuracy of finite difference schemes.

From the definition of Δ, we know that

$$\Delta f(x) = f(x + h) - f(x)$$

where h is the interval of differencing. Using the operator E we can write

$$\Delta f(x) = Ef(x) - f(x)$$

$$\Rightarrow \qquad \Delta\, f(x) = (E - 1)\, f(x)$$

The above relation can be expressed as an identity

$$\Delta = E - 1 \text{ i.e., } E = 1 + \Delta$$

1.2 INTERPOLATION

Let f(x) is a single-valued, continuous, and explicit function having the values of f(x) corresponding to certain values of x, as $x_0, x_1, x_2, \ldots\ldots\ldots x_n$ can be obtained easily and tabulated. The main problem is to converse the tabular values $(x_0, y_0), (x_1, y_1), (x_2, y_2)\ldots\ldots\ldots\ldots\ldots (x_n, y_n)$ satisfying the relation $y = f(x)$ where the explicit nature of f(x) is not known, it is required to find a simpler function [say, $\varphi(x)$], such that f(x) and $\varphi(x)$ satisfy the set of tabular points. This process of finding $\varphi(x)$'s known as ***Interpolation***.

There are different types of interpolation depending on whether $\varphi(x)$ is finite trigonometric series, a series of Bessel functions, etc. In other words "The study of interpolation is based on the assumption that there are no sudden jumps in the value of the dependent variable for the period under consideration. It is also assumed that the rate of change of figures from one period to another is uniform.

1.2.0 NEWTON'S FORWARD INTERPOLATION FORMULA

Let $(x_i, y_i), i = 0,1,2,\cdots n$ be the set of $(n+1)$ data values of the function $y = f(x)$, which are equispaced so that $x_i = x_0 + ih$, i $= 0,1,2,3,\cdots,n$. Suppose it is required to evaluate $f(x)$ for $x = x_0 + ph$, where p is any real number. Then

$$
\begin{aligned}
& y_p = f(x_0 + ph) = E^p f(x_0) = (1+\Delta)^p y_0, \left(\because E = 1 + \Delta, \mathrm{y}_0 = f(x_0)\right) \\
= \quad & \left[1 + p\Delta + \frac{p(p-1)}{2!}\Delta^2 + \frac{p(p-1)(p-2)}{3!}\Delta^3 + \cdots\right] y_0, \text{ by using the binomial theorem.} \\
= \quad & y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots
\end{aligned}
$$

If $y = f(x)$ is a polynomial of the nth degree, then $\Delta^{n+1} y_0$ and higher-order differences will be zero. Hence we have

$$
\begin{aligned}
y_p = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \\
+ \frac{p(p-1)\cdots(p - \overline{n-1})}{n!}\Delta^n y_0
\end{aligned}
$$

It is called Newton's forward interpolation formula. 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.

1.2.1 NEWTON'S BACKWARD INTERPOLATION FORMULA

Let $(x_i, y_i), i = 0,1,2,3\cdots n$ be the set of tabulated values of the function $y = f(x)$. Suppose it is required to evaluate $f(x)$ for $x = x_\mathrm{n} + ph$, where p is a real number. Then we have

$$
\begin{aligned}
y_p \quad & = f(x_n + ph) = E^p f(x_n) = (1-\nabla)^{-p} y_n, \left(\because E^{-1} = 1 - \nabla, \mathrm{y_n} = f(x_n)\right) \\
& = \left[1 + p\nabla + \frac{p(p+1)}{2!}\nabla^2 + \frac{p(p+1)(p+2)}{3!}\nabla^3 + \cdots\right] y_n, \text{ using the binomial theorem.} \\
& = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \frac{p(p+1)(p+2)}{3!}\nabla^3 y_n + \cdots
\end{aligned}
$$

If $y = f(x)$ is a polynomial of degree n then $\nabla^{n+1} y_n$ and higher-order differences vanish. Hence we have $y_p = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \cdots + \frac{p(p+1)(p+2)\cdots(p+n-1)}{n!}\nabla^n y_n$

It is called Newton's backward interpolation formula. This formula is used for interpolating the values of y near the end value of a set of tabulated values and also for extrapolating values of y a little ahead i.e. to the right of y_n.

1.2.2 CENTRAL DIFFERENCE INTERPOLATION

In this section, we shall discuss and develop central difference formulae which are best suited for interpolation near the middle of a tabulated set. The most important central difference formulae are due to Stirling, Bessel, and Everett. Gauss's formulae are also of interest from a theoretical standpoint only.

GAUSS'S FORWARD AND BACKWARD INTERPOLATION FORMULAE

Let us assume Gauss forward interpolation formula, which uses differences lie on the solid line in the forward difference table, of the form

$$y_p = y_0 + G_1\Delta y_0 + G_2\Delta^2 y_{-1} + G_3\Delta^3 y_{-1} + G_4\Delta^4 y_{-2} + \cdots \tag{1}$$

where $G_1, G_2, G_3, \cdots$ are to be determined. By Newton's forward difference formula, we have

$$\begin{aligned} y_p &= E^p y_0 = (1+\Delta)^p y_0 \\ &= y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \end{aligned} \tag{2}$$

Now

$$\begin{aligned} \Delta^2 y_{-1} = \Delta^2 E^{-1} y_0 \quad &= \Delta^2(1+\Delta)^{-1} y_0 = \Delta^2(1-\Delta+\Delta^2-\Delta^3+\cdots)y_0 \\ &= \Delta^2 y_0 - \Delta^3 y_0 + \Delta^4 y_0 - \Delta^5 y_0 + \cdots \end{aligned}$$

$$\begin{gathered} \Delta^3 y_{-1} = \Delta^3 y_0 - \Delta^4 y_0 + \Delta^5 y_0 - \Delta^6 y_0 + \cdots \\ \Delta^4 y_{-2} = \Delta^4 E^{-2} y_0 = \Delta^4(1-\Delta)^{-2} y_0 = \Delta^4(1-2\Delta+3\Delta^2-4\Delta^3+\cdots)y_0 \\ = \Delta^4 y_0 - 2\Delta^5 y_0 + 3\Delta^6 y_0 - 4\Delta^7 y_0 + \cdots \end{gathered}$$

and so on. Thus, we have

$$\begin{aligned} y_p &= y_0 + G_1\Delta y_0 + G_2(\Delta^2 y_0 - \Delta^3 y_0 + \Delta^4 y_0 - \Delta^5 y_0 + \cdots) \\ &+G_3(\Delta^3 y_0 - \Delta^4 y_0 + \Delta^5 y_0 - \Delta^6 y_0 + \cdots) \\ &+G_4(\Delta^4 y_0 - 2\Delta^5 y_0 + 3\Delta^6 y_0 - 4\Delta^7 y_0 + \cdots) + \cdots \end{aligned}$$

Comparing (1) and (2), we obtain

$$G_1 = p,\ G_2 = \frac{p(p-1)}{2!}, G_3 = \frac{(p+1)p(p-1)}{3!}, G_4 = \frac{(p+1)p(p-1)(p-2)}{4!}. \text{ etc.}$$

Hence the Gauss forward interpolation formula is given by

$$y_p = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_{-1} + \frac{(p-1)p(p-1)}{3!}\Delta^3 y_{-1} + \frac{(p-1)p(p-1)(p-2)}{4!}\Delta^4 y_{-2} + \cdots$$

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

Gauss's Backward Interpolation formula uses the differences which lie on the dashed line in the forward difference Table and can therefore be assumed of the form

$$y_p = y_0 + G_1'\Delta y_{-1} + G_2'\Delta^2 y_{-1} + G_3'\Delta^3 y_{-2} + G_4'\Delta^4 y_{-2} + \cdots$$

where $G_1', \mathrm{G}_2', \mathrm{G}_3', \mathrm{G}_4' \cdots$ have to be determined. Following the above procedure and comparing it with Newton's backward difference formula, we obtain

$$G_1' = p, \mathrm{G}_2' = \frac{p(p+1)}{2!}, \mathrm{G}_3' = \frac{(p+1)p(p-1)}{3!}, \mathrm{G}_4' = \frac{(p+2)(p+1)p(p-1)}{4!} \text{ etc.}$$

Therefore, Gauss backward interpolation formula is given by

$$y_p = y_0 + p\Delta y_{-1} + \frac{p(p+1)}{2!}\Delta^2 y_{-1} + \frac{(p+1)p(p-1)}{3!}\Delta^3 y_{-2} + \frac{(p+2)(p+1)p(p-1)}{4!}\Delta^4 y_{-2} + \cdots$$

This formula is used to interpolate the values of y for a negative value of plying between -1 and 0. Gauss formulas are not of much practical use, however, these have theoretical significance.

STIRLING'S FORMULA

If we take the mean of the Gauss forward and backward formulas, we obtain

$$y_p = y_0 + p\frac{\Delta y_{-1} + \Delta y_0}{2} + \frac{p^2}{2}\Delta^2 y_{-1} + \frac{p(p^2-1)}{3!}\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} + \frac{p^2(p^2-1)}{4!}\Delta^4 y_{-2} + \cdots$$

This is known as Stirling's formula. In the central differences notation, the Stirling formula takes the form

$$y_p = y_0 + p\mu\delta y_0 + \frac{p^2}{2!}\delta^2 y_0 \frac{p(p^2-1^2)}{3!}\mu\delta^3 y_0 + \frac{p^2(p^2-1^2)}{4!}\delta^4 y_0 + \cdots$$

since

$$\frac{1}{2}(\Delta y_0 + \Delta y_{-1}) = \frac{1}{2}\left(\delta y_{1/2} + \delta y_{-1/2}\right) = \mu\delta y_0, \frac{1}{2}(\Delta^3 y_{-1} + \Delta^3 y_{-2}) = \frac{1}{2}\left(\delta^3 y_{\frac{1}{2}} + \delta^3 y_{-\frac{1}{2}}\right)$$
$$= \mu\delta^3 y_0 \text{ etc.}$$

BESSEL'S FORMULA

This is a very useful formula for practical interpolation, and it uses the differences as shown in the following table where brackets mean that the average has to be taken

$$\begin{array}{llllllllll} x_{-1} & y_{-1} & & & & & & & & \\ x_0 & \begin{pmatrix} y_0 \\ x_1 \end{pmatrix} & \Delta y_0 & \begin{pmatrix} \Delta^2 y_{-1} \\ \Delta^2 y_0 \end{pmatrix} & \Delta^3 y_{-1} & \begin{pmatrix} \Delta^4 y_{-2} \\ \Delta^4 y_{-1} \end{pmatrix} & \Delta^5 y_{-2} & \begin{pmatrix} \Delta^6 y_{-3} \\ \Delta^6 y_{-2} \end{pmatrix} \end{array}$$

Therefore, we have assumed Bessel's formula of the form

$$y_p = \frac{y_0 + y_1}{2} + B_1\Delta y_0 + B_2\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + B_3\Delta^3 y_{-1} + B_4\frac{\Delta^4 y_{-2} + \Delta^4 y_{-1}}{2} + \cdots$$
$$= y_0 + \left(B_1 + \frac{1}{2}\right)\Delta y_0 + B_2\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + B_3\Delta^3 y_{-1} + B_4\frac{\Delta^4 y_{-2} + \Delta^4 y_{-1}}{2} + \cdots$$

Newton's forward differences interpolation formula is given by

$$y_p = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 y_0 + \cdots$$

Comparing the above results after simplifying the differences, we obtain

$$B_1 + \frac{1}{2} = p,\ \mathrm{B}_2 = \frac{p(p-1)}{2!}, \mathrm{B}_3 = \frac{p(p-1)\left(p-\frac{1}{2}\right)}{3!}, \mathrm{B}_4 = \frac{(p+1)p(p-1)(p-2)}{4!} \text{ etc.}$$

Thus the Bessel formula becomes

$$y_p = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{p(p-1)\left(p-\frac{1}{2}\right)}{3!}\Delta^3 y_{-1}$$
$$+ \frac{(p+1)p(p-1)(p-2)}{4!}\frac{\Delta^4 y_{-2} + \Delta^4 y_7}{2} + \cdots$$

In central differences notation, this can be written as

$$y_p = y_0 + p\delta y_{\frac{1}{2}} \quad + \frac{p(p-1)}{2!}\mu\delta^2 y_{\frac{1}{2}} + \frac{\left(p-\frac{1}{2}\right)p(p-1)}{3!}\delta^3 y_{\frac{1}{2}}$$
$$+ \frac{(p+1)p(p-1)(p-2)}{4!}\mu\delta^4 y_{\frac{1}{2}} + \cdots$$

since

$$\frac{1}{2}(\Delta^2 y_{-1} + \Delta^2 y_0) = \mu\delta^2 y_{\frac{1}{2}}, \frac{1}{2}(\Delta^4 y_{-2} + \Delta^4 y_{-1}) = \mu\delta^4 y_{\frac{1}{2}} \text{ etc.}$$

EVERETT'S FORMULA

This formula is extensively used and involves only even differences on and below the central line as shown below.

$$\begin{array}{cccccc}
\mathrm{x}_0 & \mathrm{y}_0 & \Delta^2 y_{-1} & \Delta^4 y_{-2} & \Delta^6 y_{-3} \cdots & \text{Central line} \\
 & - & - & - & & - \\
x_1 & y_1 & \Delta^2 y_0 & \Delta^4 y_{-1} & & \Delta^6 y_{-2}
\end{array}$$

Hence this formula has the form

$$y_p = E_0 y_0 + E_2\Delta^2 y_{-1} + E_4^4 y_{-2} + \cdots + F_0 y_1 + F_2\Delta^2 y_0 + F_4\Delta^4 y_{-1} + \cdots$$

where coefficients E_0, $\mathrm{F}_0, \mathrm{E}_2$, $\mathrm{F}_2, \mathrm{E}_4$, $\mathrm{F}_4, \cdots$ can be determined by the earlier method as used in the proceeding cases, we obtain.

$$E_0 = 1 - p = q, \;\; \mathrm{F}_0 = p$$
$$E_2 = q(q^2 - 1^1) \;\; \mathrm{F}_2 = p(p^2 - 1^2)$$
$$E_4 = \frac{q(q2 - 1^2)(q^2 - 2^2)}{5!}, \; \mathrm{F}_4 = \frac{p(p^2 - 1^2)(p^2 - 2^2)}{5!} \text{ etc.}$$
$$y_p = qy_0 + \frac{q(q^2 - 1^2)}{3!}\Delta^2 y_{-1} + \frac{q(q^2 - 1^2)(q^2 - 2^2)}{5!}\Delta^4 y_{-2} + \cdot$$
$$+py_1 + p\frac{p^2 - 1^2}{3!}\Delta^2 y_0 + \frac{p(p^2 - 1^2)(p^2 - 2^2)}{5!}\Delta^4 y_{-1} + \cdots$$

where $q = 1 - p$. There is a close relationship between Bessel's formula and Everett's formula and one can be deduced from the other by suitable rearrangements. It is also interesting to observe that Bessel's formula truncated after third differences is Everett's formula truncated after second differences.

CHOICE OF AN INTERPOLATION FORMULA

As for as practical interpolation is concerned, we have to see which formula yields the most accurate results in a particular problem. The coefficients in the central difference formulae are smaller and converge faster than those in Newton's formulae. After a few terms, the coefficients in String's formula decrease more rapidly than those of Bessel's formula and the coefficients of Bessel's formula decrease more rapidly than those of Newton's formula. As such, whenever possible, the central difference formula should be used in preference to Newton's formulae. The right choice of an interpolation formula, however, depends on the position of the interpolated value in the given data.

(i) To find a tabulated value near the beginning of the table use Newton's forward formula.

(ii) To find a value near the end of the table, use Newton's backward formula.

(iii) To find an interpolated value near the center of the table, use either Stiring's or Bessel's, or Everett's formula.

If the interpolation is required for $\frac{-1}{2} \le p \le \frac{1}{4}$, prefer Stirling's s formula. If interpolation is required for $\frac{1}{4} \le p \le \frac{3}{4}$, then use Bessel's or Everette's formula. But in the case where a series of calculations have to be performed, it would be inconvenient to use both these formulae, and a choice must be made between them. The choice depends on the order of the highest difference that could be neglected so that contributions from it and further differences would be less than half a unit in the last decimal place. If this highest difference is of even order, Stirling's formula is recommended, if it is of even order, Bessel's formula might be preferred. Even the estimation of the maximum value of a difference of any order in an interpolation formula is also not difficult.

Example 1.1 Find $f(22)$ from the Gauss forward formula:

x:	20	25	30	35	40	45
$f(x)$:	354	332	291	260	231	204

Solution: Taking $x_0 = 25, h = 5$, we have to find the value of $f(x)$ for $x = 22$.

i.e., for $p = \frac{x-x_0}{h} = \frac{22-25}{5} = -0.6$ The difference table is as follows:

x	p	y_p	Δy_p	$\Delta^2 y_p$	$\Delta^3 y_p$	$\Delta^4 y_p$	$\Delta^5 y_p$
20	-1	$354(= y_{-1})$	-22				
25	0	$332(= y_0)$	-41	-19	29		
30	1	$291(= y_1)$	-31	10	-8	-37	45
35	2	$260(= y_2)$	-29	2	0	8	
40	3	$231(= y_3)$	-27	2			
45	4	$204(= y_4)$					

Gauss forward formula is

$$y_p = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_{-1} + \frac{(p+1)p(p-1)}{3!}\Delta^3 y_{-1}$$
$$+ \frac{(p+1)p(p-1)(p-2)}{4!}\Delta^4 y_{-2}$$
$$+ \frac{(p+1)(p-1)p(p-2)(p+2)}{5!}\Delta^5 y_{-2} + \cdots$$
$$\therefore f(22) = 332 + (0.6)(-41) + \frac{(-0.6)(-0.6-1)}{2!}(-19)$$
$$+ \frac{(-0.6+1)(-0.6)(-0.6-1)}{3!}(-8)$$
$$+ \frac{(-0.6+1)(-0.6)(-0.6-1)(-0.6-2)}{4!}(-37)$$
$$+ \frac{(-0.6+1)(-0.6)(-0.6-1)(-0.6-2)(-0.6+2)}{5!}(45)$$
$$= 332 + 24.6 - 9.12 - 0.512 + 1.5392 - 0.5241$$

Hence $f(22) = 347.983$.

Example 1.2 Use Gauss's forward formula to evaluate y_{30}, given that $y_{21} = 18.4708$, $y_{25} = 17.8144, y_{29} = 17.1070, y_{33} = 16.3432$ and $y_{37} = 15.5154$.

Solution: Taking $x_0 = 29, h = 4$, we require the value of y for $x = 30$

i.e., for $p = \frac{x-x_0}{h} = \frac{30-29}{4} = 0.25$ The difference table is given below:

x	p	y_p	Δy_p	$\Delta^2 y_p$	$\Delta^3 y_p$	$\Delta^4 y_p$
21	-2	18.4708				
			-0.6564			
25	-1	17.8144		-0.0510		
			-0.7074		-0.7074	
29	0	17.1070		-0.0564		-0.0022
			-0.7638		-0.0076	
33	1	16.3432		-0.0640		

			-0.8278			
37	2	15.5154				

Gauss's forward formula is

$$y_p = y_0 + p\Delta y_0 + \frac{p(p+1)}{1.2}\Delta^2 y_{-1} \quad + \frac{(p+1)p(p-1)}{1.2.3}\Delta^3 y_{-1} + \frac{(p+1)p(p-1)(p-2)}{1.2.3.4}\Delta^4 y_{-2} + \cdots$$

$$y_{30} = 17.1070 \quad +(0.25)(-0.7638) + \frac{(0.25)(-0.75)}{2}(-0.0564) + \frac{(1.25)(0.25)(-0.75)}{6}(-0.0076) + \frac{(1.25)(0.25)(-0.75)(-1.75)}{24} \times (-0.0022)$$

$$= 17.1070 \quad -0.19095 + 0.00529 + 0.0003 - 0.00004 = 16.9216 \text{ approx.}$$

Example 1.3 Using Gauss backward difference formula, find y(8) from the following table.

x	0	5	10	15	20	25
y	7	11	14	18	24	32

Solution: Taking $x_0 = 10, h = 5$, we have to find y for $x = 8$, i.e., for $p = \frac{x-x_0}{h} = \frac{8-10}{5} = -0.4$.

The difference table is as follows:

x	p	y_p	Δy_p	$\Delta^2 y_p$	$\Delta^3 y_p$	$\Delta^4 y_p$	$\Delta^5 y_p$
0	2	7					
			4				
5	1	11		-1			
			3		2		
10	0	14		1		-1	
			4		1		0
15	1	18		2		-1	

			6		0		
20	2	24		2			
			8				
25	3	32					

Gauss's backward formula is

$$y_p = y_0 + p\Delta y_{-1} + \frac{(p+1)p}{2!}\Delta^2 y_{-1} + \frac{(p+1)p(p-1)}{3!}\Delta^3 y_{-2}$$
$$+ \frac{(p+2)p(p+1)p(p-1)}{4!}\Delta^4 y_{-2} + \cdots$$
$$y(8) = 14 + (-0.4)(3) + \frac{(-0.4+1)(-0.4)}{2!}(1) + \frac{(-0.4+1)(-0.4)(-0.4-1)}{3!}(2)$$
$$+ \frac{(-0.4+2)(-0.4+1)(-0.4)(-0.4-1)}{4!}(-1)$$
$$= 14 - 1.2 - 0.12 + 0.112 + 0.034$$

Hence $y_{(8)} = 12.826$

Example 1.4 Interpolate using Gauss's backward formula, the population of a town for the year 1974, given that:

Year:	1939	1949	1959	1969	1979	1989
Population: (in thousands)	12	15	20	27	39	52

Solution: Taking $x_0 = 1969, h = 10$, the population of the town is to be found for

$$p = \frac{1974 - 1969}{10} = 0.5$$

The Central difference table is

x	p	y_p	Δy_p	$\Delta^2 y_p$	$\Delta^3 y_p$	$\Delta^4 y_p$	$\Delta^5 y_p$
1939	-3	12	3	2	0	3	-10

1949	-2	15						
			5					
1959	-1	20		2				
			7		3			
1969	0	27		5		-7		
			12		-4			
1979	1	39		1				
			13					
1989	2	52						

Gauss's backward formula is

$$\begin{aligned}
y_p = y_0 \quad & +p\Delta y_{-1} + \frac{(p+1)p}{2!}\Delta^2 y_{-1} + \frac{(p+1)p(p-1)}{3!}\Delta^3 y_{-2} \\
+ \quad & \frac{(p+2)p(p+1)p(p-1)}{4!}\Delta^4 y_{-2} \\
& + \frac{(p+2)(p+1)p(p-1)(p-2)}{5!}\Delta^5 y_3 + \cdots \\
y_{0.5} = \quad & 27 + (0.5)(7) + \frac{(1.5)(0.5)}{2}(5) + \frac{(1.5)(0.5)(-0.5)}{6} \\
& + \frac{(2.5)(1.5)(-0.5)}{24}(-7) + \frac{(2.5)(1.5)(0.5)(-0.5)(1.5)}{120}(-10) \\
= \quad & 27 + 3.5 + 1.875 - 0.1875 + 0.2743 - 0.1172 \\
= \quad & 32.532 \text{ thousand approx.}
\end{aligned}$$

Example 1.5 Employ Stirling's formula to compute $y_{12.2}$ from the following table

$$(y_x = 1 + \log_{10} \sin x) :$$

$x°$:	10	11	12	13	14
$10^5 y_x$:	23,967	28,060	31,788	35,209	38,368

Solution: Taking the origin at $x_0 = 12°, h = 1$ and $p = x - 12$, we have the following central difference table:

p	y_x	Δy_x	$\Delta^2 y_x$	$\Delta^3 y_x$	$\Delta^4 y_x$
$-2 = x_{-2}$	$0.23967 = y_{-2}$				
		$0.04093 = \Delta y_{-2}$			
$-1 = x_{-1}$	$0.28060 = y_{-1}$		$-0.00365 = \Delta 2 y_{-2}$		
		$0.03728 = \Delta y_{-1}$		$0.00058 = \Delta^3 y_{-2}$	
$0 = x_0$	$0.31788 = y_0$		$-0.00307 = \Delta^2 y_{-1}$		$-0.00013 = \Delta^4 y_{-2}$
		$0.03421 = \Delta y_0$		$-0.00045 = \Delta^2 y_{-1}$	
$1 = x_1$	$0.35209 = y_1$		$-0.00062 = \Delta^2 y_0$		
		$0.03159 = \Delta y_1$			
$2 = x_2$	$0.38368 = y_2$				

At $x = 12.2, p = 0.2$. (As p lies between $-\frac{1}{4}$ and $\frac{1}{4}$, the use of String's formula will be Quite suitable.)

Stirling's formula is

$$y_p = y_0 \quad + \frac{p}{1} \frac{\Delta y_{-1} + \Delta y_{-0}}{2} + \frac{p^2}{2!} \Delta^2 y_{-1} + \frac{p(p^2-1)}{3!} \cdot \frac{\Delta^3 y_{-2} + \Delta^3 y_{-1}}{2} + \frac{p^2(p^2-1)}{4!} \Delta^4 y_{-2} + \cdots$$

When $p = 0.2$, we have

$$y_{0.2} = 0.3178 + 0.2 \left(\frac{0.03728 + 0.03421}{2} \right) + \frac{(0.2)^2}{2} (-0.00307)$$

$$+\frac{(0.2)^2[(0.2)^2-1]}{6}\left(\frac{0.00058+0.00054}{2}\right)+\frac{(0.2)^2[(0.2)^2-1]}{24}(-0.00013)$$

$$=0.31788+0.00715-0.00006-0.000002+0.0000002$$

$$=0.32497.$$

Example 1.6 Given

θ°:	0	5	10	15	20	25	30
$\tan\theta$:	0	0.0875	0.1763	0.2679	0.3640	0.4663	0.5774

Using Stirling's formula, estimate the value of $\tan 16^\circ$.

Solution: Taking the origin at $\theta^\circ = 15^\circ, h = 5^\circ$ and $p = \frac{\theta-15}{5}$, we have the following central difference table:

p	$y = \tan\theta$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
-3	0.0000					
		0.0875				
-2	0.0875		0.0013			
		0.0888		0.0015		
-1	0.1763		0.0028		0.0002	
		0.0916		0.0017		-0.0002
0	0.2679		0.0045		0.0000	
		0.0961		0.0017		0.0009
1	0.3640		0.0062		0.0009	
		0.1023		0.0026		
2	0.4663		0.0088			
		0.1111				
3	0.5774					

$$\text{At } \theta = 16°, p = \frac{16-15}{5} = 0.2$$

Stirling's formula is

$$y_p = y_o + \frac{p}{1} \cdot \frac{\Delta y_{-1} + \Delta y_0}{2} + \frac{p^2}{2!} \Delta^2 y_{-1} + \frac{p^2(p^2-1)}{3!} \cdot \frac{\Delta^2 y_{-2} + \Delta^3 y_{-1}}{2}$$
$$+ \frac{p^2(p^2-1)}{4!} \Delta^4 y_{-2} + \cdots$$
$$\therefore y_{0.2} = 0.2679 + 0.2\left(\frac{0.0916 + 0.0916}{2}\right) + \frac{(0.2)^2}{2}(0.0045) + \cdots$$
$$= 0.2679 + 0.01877 + 0.00009 + \cdots = 0.28676$$

Hence, $\tan 16° = 0.28676$.

Example 1.7 Apply Bessel's formula to obtain y_{25}, given $y_{20} = 2854, y_{24} = 3162$, $y_{28} = 3544, y_{32} = 3992$.

Solution: Taking the origin at $x_0 = 24, h = 4$, we have $p = (x - 24)$.

$\therefore$ The central difference table is

p	y	Δy	$\Delta^2 y$	$\Delta^3 y$
-1	2854			
		308		
0	$\underline{3162}$		$\underline{74}$	
		$\underline{382}$		$\underline{-8}$
1	3544		$\underline{66}$	
		448		
2	3992			

At $x = 25, p = \frac{(25-24)}{4} = \frac{1}{4}$. (As p lies between $\frac{1}{4}$ and $\frac{3}{4}$, the use of Bessel's formula will yield accurate results)

Bessel's formula is

$$y_p = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{\left(p-\frac{1}{2}\right)p(p-1)}{2!}\Delta^3 y_{-1} + \cdots$$

When $p = 0.25$, we have

$$\begin{aligned} y_p &= 3162 + 0.25 \times 382 + \frac{0.25(-0.75)}{2!}\left(\frac{74+66}{2}\right) + \frac{(0.25)0.25(-0.75)}{2!} - 8 \\ &= 3162 + 95.5 - 6.5625 - 0.0625 \\ &= 3250.875 \text{ approx.} \end{aligned}$$

Example 1.8 Apply Bessel's formula to find the value of $f(27.5)$ from the table:

x:	25	26	27	28	29	30
$f(x)$:	4.000	3.846	3.704	3.571	3.448	3.333

Solution: Taking the origin at $x_0 = 27, h = 1$, we have $p = x - 27$ The central difference table is

x	p	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
25	-2	4.000				
			-0.154			
26	-1	3.846		0.012		
			-0.142		-0.003	
27	0	3.704		0.009		0.004
			-0.133		-0.001	
28	1	3.571		0.010		-0.001
			-0.123		-0.002	
29	2	3.448		0.008		
			-0.115			
30	3	3.333				

At $x = 27.5, p = 0.5$ (As p lies between $1/4$ and 3/4, the use of Bessel's formula will yield an accurate result),

Bessel's formula is

$$
\begin{aligned}
y_p = y_0 \quad & +p\Delta y_0 + \frac{p(p-1)}{2!}\frac{\Delta^2 y_{-1} + \Delta^2 y_0}{2} + \frac{\left(p-\frac{1}{2}\right)p(p-1)}{3!}\Delta^3 y_{-1} \\
& + \frac{(p+1)p(p-1)(p-2)}{4!}\left(\frac{\Delta^4 y_{-2} + \Delta^4 y_{-1}}{2}\right) + \cdots
\end{aligned}
$$

When $p = 0.5$, we have

$$
\begin{aligned}
y_p = \quad & 3.704 - \frac{(0.5)(0.5-1)}{2}\left(\frac{0.009 + 0.010}{2}\right) + 0 \\
& + \frac{(0.5+1)(0.5)(0.5-1)(0.5-2)}{2}\frac{(-0.001 - 0.004)}{2} \\
= \quad & 3.704 - 0.11875 - 0.00006 = 3.585
\end{aligned}
$$

Hence $f(27.5) = 3.585$.

Example 1.9 Using Everett's formula, evaluate $f(30)$ if $f(20) = 2854, f(28) = 3162$, $f(36) = 7088, f(44) = 7984$

Solution: Taking the origin at $x_0 = 28, h = 8$, we have $p = \frac{x-28}{8}$. The central table

x	p	y	Δy	$\Delta^2 y$	$\Delta^3 y$
20	-1	2854			
			308		
28	0	3162		3618	
			3926		-6648
36	1	7088		-3030	
			896		
44	2	7984			

At $x = 30, p = \frac{30-28}{8} = 0.25$ and $q = 1 - p = 0.75$

Everett's formula is

$$\begin{aligned}
y_p &= qy_0 + \frac{q(q^2-1^2)}{3!}\Delta^2 y_{-1} + \frac{q(q^2-1^2)(q^2-2^2)}{5!}\Delta^4 y_{-2} + \cdots \\
&+py_1 + \frac{p(p^2-1^2)}{3!}\Delta^2 y_0 + \frac{p(p^2-1^2)(p^2-2^2)}{5!}\Delta^4 y_{-2} + \cdots \\
&= (0.75) + (3162) + \frac{0.75(0.75^2-1)}{6}(3618) + \cdots \\
&+0.25 + (7080) + \frac{0.25(0.25^2-1)}{6}(-3030) + \cdots \\
&= 2371.5 - 351.75 + 1770 + 94.69 = 3884.4
\end{aligned}$$

Hence $f(30) = 3884.4$

Example 1.10 Given the table

x:	310	320	330	340	350	360
$\log x$:	2.49136	2.50515	2.51851	2.53148	2.54407	2.55630

find the value of $\log 337.5$ by Everett's formula.

Solution: Taking the origin at $x_0 = 330$ and $h = 10$, we have $p = \frac{x-330}{10}$. The central difference table is

p	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
-2	2.49136					
		0.01379				
-1	2.50515		-0.00043			
		0.01336		0.00004		
0	2.51881		-0.00039		-0.00003	
		0.01297		0.00001		0.00004
1	2.53148		-0.00038		0.00001	

		0.01259		0.00002		
2	2.54407		−0.00036			
		0.01223				
3	2.55630					

To evaluate log 337.5, i.e., for $x = 337.5, p = \frac{337.5-330}{10} = 0.75$

(As $p > 0.5$ and $= 0.75$, Everett's formula will be quite suitable)

Everett's formula is

$$
\begin{aligned}
y_p = qy_0 \quad & + \frac{q(q^2-1^2)}{3!}\Delta^2 y_{-1} + \frac{q(q^2-1^2)(q^2-2^2)}{5!}\Delta^4 y_{-2} + \cdots \\
& + py_1 + \frac{p(p^2-1^2)}{3!}\Delta^2 y_0 + \frac{p(p^2-1^2)(p^2-2^2)}{5!}\Delta^4 y_{-1} + \cdots \\
= \quad & 0.25 \times 2.51851 + \frac{0.25(0.0625-1)}{6} \times (-0.00039) \\
& + \frac{0.25(0.0625-1)(0.0625-4)}{120} \times (-0.00003) \\
+ \quad & 0.75 \times 2.53148 + \frac{0.75(0.5625-1)}{6} \times (-0.00038) \\
+ \quad & \frac{0.75(0.5625-1)(0.5625-4)}{6} \times (-0.00001) \\
= 0.62963 \quad & +0.00002 - 0.0000002 + 1.89861 + 0.00002 + 0.0000001 \\
= 2.52828 \quad & \text{nearly.}
\end{aligned}
$$

1.3 INTERPOLATION WITH UNEQUAL INTERVALS

Newton’s forward and backward interpolation formulae are applicable only when the values of n are given at equal intervals but in case of unequal intervals, we use Lagrange’s formula for interpolation.

1.3.0 LAGRANGE’S INTERPOLATION FORMULA

Let y = f(x) be a real-valued continuous function defined in an interval [a, b]. Let $x_0, x_1, x_2, \ldots, x_n$ be (n+1) distinct points that are not necessarily equally spaced and the corresponding values of the function are $y_0, y_1, \ldots, y_n$. Since (n + 1) values of the function are given corresponding to the (n+1) values of the independent variable x, we can represent the function $y = f(x)$ as a polynomial in x of degree n.

Let the polynomial is represented by

$f(x) = a_0(x - x_1)(x - x_2)\ldots\ldots(x - x_n) + a_1(x - x_0)(x - x_2)\ldots\ldots.(x - x_n) + a_2(x - x_0)(x - x_1)(x - x_3)\ldots\ldots.(x - x_n) + \ldots\ldots. + a_n(x - x_0)(x - x_1)\ldots\ldots.(x - x_{n-1})$ …(3)

Each term in (3) being a product of n factors in x of degree n, putting $x = x_0$ in (3) we obtain

$$f(x_0) = a_0(x_0 - x_1)(x_0 - x_2)\ldots\ldots\ldots\ldots\ldots\ldots(x_0 - x_n)$$

or
$$a_0 = \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)........(x_0 - x_n)}$$

Putting $x = x_2$ in (3) we obtain

$$f(x_1) = a_1(x_1 - x_0)(x_1 - x_2)\ldots\ldots\ldots\ldots\ldots\ldots(x_1 - x_n)$$

or
$$a_1 = \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)........(x_1 - x_n)}$$

Similarly putting $x = x_2$, $x = x_3$, $x = x_n$ in (3) we obtain

$$a_2 = \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)........(x_2 - x_n)}$$

…… ……. ……..

and
$$a_n = \frac{f(x_n)}{(x_n - x_0)(x_n - x_1)(x_n - x_2)........(x_n - x_{n-1})}$$

Substituting the values of a_0, a_1, ..., a_n in (3) we get

$$y = f(x) = \frac{(x - x_1)(x - x_2).......(x - x_n)}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)........(x_0 - x_n)} f(x_0) +$$

$$\frac{(x - x_0)(x - x_2).......(x - x_n)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)........(x_1 - x_n)} f(x_1) + \ldots\ldots\ldots\ldots\ldots +$$

$$\frac{(x - x_0)(x - x_1).......(x - x_{n-1})}{(x_n - x_0)(x_n - x_1)(x_n - x_2)........(x_n - x_{n-1})} f(x_n) \qquad \ldots(4)$$

The formula given by (4) is known as Lagrange’s interpolation formula.

Example 1.11 Given the values

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

evaluate $f(9)$, using Lagrange's formula

Solution: Here $x_0 = 5, x_1 = 7, x_2 = 11, x_3 = 13, x_4 = 17$

and $y_0 = 150, y_1 = 392, y_2 = 1452, y_3 = 2366, y_4 = 5202.$

Putting $x = 9$ and substituting the above values in Lagrange's formula, we get

$$f(9) = \frac{(9-7)(9-11)(9-13)(9-17)}{(5-7)(5-11)(5-13)(5-17)} \times 150 + \frac{(9-5)(9-11)(9-13)(9-17)}{(7-5)(7-11)(7-13)(7-17)} \times 392$$
$$+ \frac{(9-5)(9-7)(9-13)(9-17)}{(11-5)(11-7)(11-13)(11-17)} \times 1452$$
$$+ \frac{(9-5)(9-7)(9-11)(9-17)}{(13-5)(13-7)(13-11)(13-17)} \times 2366$$
$$+ \frac{(9-5)(9-7)(9-11)(9-13)}{(17-5)(17-7)(17-11)(17-13)} \times 5202$$
$$= -\frac{50}{3} + \frac{3136}{15} + \frac{3872}{3} + \frac{2366}{3} + \frac{578}{5} = 810$$

Example 1.12 Find the polynomial $f(x)$ by using Lagrange's formula and hence find $f(3)$ for

x:	0	1	2	5
$f(x)$:	2	3	12	147

Solution: Here $x_0 = 0, x_1 = 1, x_2 = 2, x_3 = 5$

and $y_0 = 2, \mathrm{y}_1 = 3, \mathrm{y}_2 = 12, \mathrm{y}_3 = 147.$

Lagrange's formula is

$$y = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}y_0 + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}y_1$$
$$+ \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}y_2 + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}y_3$$
$$= \frac{(x-1)(x-2)(x-5)}{(0-1)(0-2)(0-5)}(2) + \frac{(x-0)(x-2)(x-5)}{(1-0)(1-2)(1-5)}(3)$$
$$+ \frac{(x-0)(x-1)(x-5)}{(2-0)(2-1)(2-5)}(12) + \frac{(x-0)(x-1)(x-2)}{(5-0)(5-1)(5-2)}(147)$$

Hence $f(x) = x^3 + x^2 - x + 2$

$\therefore\ f(3) = 27 + 9 - 3 + 2 = 35$

1.3.1 HERMITE'S INTERPOLATION FORMULA

This formula is similar to Lagrange's interpolation formula. In Lagrange's method, the interpolating polynomial $P(x)$ agrees with $y(x)$ at the points $x_0, x_1, \dots\dots, x_n$, whereas in Hermite's method $P(x)$ and $y(x)$ as well as $P'(x)$ and $y'(x)$ coincide at the $(n+1)$ points, i.e.,

$$P(x_i) = y(x_i) \text{ and } P'(x_i) = y'(x_i); i = 0,1, \dots, n \qquad \dots (5)$$

As there are $2(n+1)$ conditions in $(1), (2n+2)$ coefficients are to be determined.

Therefore $P(x)$ is a polynomial of degree $(2n+1)$.

We assume that $P(x)$ is expressible in the form

$$p(x) = \sum_{i=0}^{n} U_i(x)y(x_i) + \sum_{i=0}^{n} V_i(x)y'(x_i) \qquad \dots (6)$$

where $U_i(x)$ and $V_i(x)$ are polynomials in x of degree $(2n+1)$. These are to be determined. Using conditions (5), we get

$$U_i(x_j) = \begin{cases} 0 \text{ when } i \neq j; V_i(x_j) = 0 \text{ for all } i \\ \qquad 1 \text{ when } i = j \end{cases}$$
$$U_i'(x_j) = 0 \text{ for all } i; \mathrm{V}_i(x_j) = \begin{Bmatrix} 0 \text{ when } i \neq j \\ 1 \text{ when } i = j \end{Bmatrix} \qquad \dots (7)$$

We now write

$$\begin{aligned} U_i(x) &= A_i(x)[L_i(x)]^2; V_i(x) = B_i(x)[L_i(x)]^2 \\ \text{where} \quad L_i(x) &= \frac{(x-x_0)(x-x_1)\cdots(x-x_{i-1})(x-x_{i+1})\cdots(x-x_n)}{(x_i-x_0)(x_i-x_1)\cdots(x_i-x_{i-1})(x_i-x_{i+1})\cdots(x_i-x_n)} \end{aligned}$$

Since $[L_i(x)]^2$ is of degree $2n$ and $U_i(x), V_i(x)$ are of degree $(2n+1)$, therefore $A_i(x)$ and $B_i(x)$ are both linear functions

∴ We can write

$$\left.\begin{aligned} U_i(x) &= (a_i + b_i x)[L_i(x)]^2 \\ V_i(x) &= (c_i + d_i x)[L_i(x)]^2 \end{aligned}\right\} \qquad \ldots (8)$$

Using conditions (7) in (8), we get $a_i + b_i x = 1, c_i + d_i x = 0$ and

$$b_i + 2L_i'(x_i) = 0, d_i = 1\}$$

Solving these equations, we obtain

$$\left.\begin{aligned} & b_i = -2L_i'(x_i), a_i = 1 + 2x_i L_i'(x_i) \\ & d_i = 1 \text{ and } c_i = -x_i \end{aligned}\right\}$$

Now putting the above values in (8), we get

$$\begin{aligned} U_i(x) &= [1 + 2x_i L_i'(x_i) - 2xL_i'(x_i)][L_i(x)]^2 \\ &= [1 - 2(x - x_i)L_i'(x_i)][L_i(x)]^2 \end{aligned}$$

and $V_i(x) = (x - x_i)[L_i(x)]^2$

Finally substituting $U_i(x)$ and $V_i(x)$ in (6), we obtain

$$p(x) = \sum_{i=0}^{n} [1 - 2(x - x_i)\mathrm{Li}(x_i)][Li(x)]^2 y(x_i) + \sum_{i=0}^{n} (x - x_i)[\mathrm{Li}(x)]^2 y'(x_i)$$

This is the required Hermite's interpolation formula which is sometimes known as the osculating interpolation formula.

Example 1.13 For the following data:

x:	$f(x)$	$f'(x)$
0.5	4	-16
1	1	-2

Find Hermite's interpolating polynomial.

Solution: We have $x_0 = 0.5, x_1 = 1, y(x_0) = 4, y(x_1) = 1; y'(x_0) = -16, y'(x_1) = -2$

Also $L_i(x_0) = \frac{(x-x_0)}{(x_i-x_0)} = \frac{x-1}{-0.5} = -2(x-1); L_i'(x_0) = -2$

$$L_i(x_1) = \frac{(x-x_0)}{(x_i-x_0)} = \frac{x-0.5}{1-0.5} = 2x-1; L_i'(x_1) = 2$$

Hermite's interpolation formula, in this case, is

$$\begin{aligned}
P(x) &= [1-2(x-x_0)L'(x_0)][L(x_0)]^2y(x_0) + (x-x_0)[L(x_0)]^2y'(x_0) \\
&+[1-2(x-x_1)L'(x_1)][L(x_1)]^2y(x_1) + (x-x_1)[L(x_1)]^2y'(x_1) \\
&= [1-2(x-0.5)(-2)][-2(x-1)]^2(4) + (x-0.5)[-2(x-1)]^2(-16) \\
&+[1-2(x-1)(2)](2x-1)^2(1) + (x-1)(2x-1)^2(-2) \\
&= 16[1+4(x-0.5](x^2-2x+1) - 164(x-0.5)(x^2-2x+1) \\
&+[1-4(x-1)](4x^2-4x+1) - 2(x-1)(4x^2-4x+1)
\end{aligned}$$

Hence $P(x) = -24x^3 + 324x^2 - 130x + 23$

Example 1.14 Determine the Hermite polynomial of degree 4 which fits the following data:

x:	0	1	2
$y(x)$:	0	1	0
$y'(x)$:	0	0	0

Solution: Here $x_0 = 0, x_1 = 1, x_2 = 2, y(x_0) = 0, y(x_1) = 1, y(x_2) = 0$ and $y'(x_0) = 0$, $y'(x_1) = 0, y'(x2) = 0$. Hermite's formula in this case is

$$\begin{aligned} P(x) \quad &= [1-2L_0'(x_0)(x-x_0)][L_0(x)]^2 y(x_0) + (x-x_0)[L_0(x)]^2 y'(x_0) \\ &+[1-2L_1'(x_1)(x-x_1)][L1(x)]^2 \times y(x_1) + (x-x_1)[L1(x)]^2 y'(x_1) \\ &+[1-2L_2'(x_2)(x-x_2)] \times [L_2(x)]^2 y(x_2) + (x-x_2)[L_2(x)]^2 y'(x_2) \end{aligned}$$

Substituting the above values in $P(x)$, we get

$$P(x) = [1-2L_1'(x_1)(x-1)][L_1(x)]^2$$

Where $L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_2)(x_1-x_2)} = 2x - x^2$ and $L_1{}'(x_1) = (2-2x)_{x-1} = 0$ Hence $p(x) = [L_1(x)]^2 = (2x-x^2)^2$.

Example 1.15 Using Hermite's interpolation, find the value of $f(-0.5)$ from the following

x:	-1	0	1
$f(x)$:	1	1	3
$f'(x)$:	-5	1	7

Solution: Here $x_0 = -1, x_1 = 0, x_2 = 1; f(x_0) = 1, f(x_1) = 1, f(x_2) = 3$ and $f'(x_0) = -5$, $f'(x_1) = 1, f'(x_2) = 7$.

Hermite's formula in this case is

$$P(x) = U_0 f(x_0) + V_0 f'(x_0) + U_1 f(x_1) + V_1 f'(x_1) + U_2 f(x_2) + V_2 f'(x_2)$$

where $U_0 = [1-2L_0'(x_0)(x-x_0)][L_0(x)]^2, V_0 = (x-x_0)[L_0(x)]^2$

$U_1 = [1-2L_1'(x_1)(x-x_1)][L_1(x)]^2, V_1 = (x-x_1)[L_1(x)]^2$

$U_2 = [1-2L_2'(x_2)(x-x_2)][L_2(x_2)]^2, V_2 = (x-x_2)[L_2(x)]^2$

and $L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{x(x-1)}{2}, L_0'(x) = x - \frac{1}{2}$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = 1 - x^2 = L_1'(x) = -2x$$
$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{x(x+1)}{2} = L_2'(x) = x + \frac{1}{2}$$

Substituting the values of $L_0, L_0'; L_1, L_1'$ and L_2, L_2', we get

$$U_0 = [1 + 3(x+1)]\frac{x^2(x-1)^2}{4} = \frac{1}{4}(3x^5 - 2x^4 - 5x^3 + 4x^2)$$
$$V_0 = (x+1)\frac{x^2(x-1)^2}{4} = \frac{1}{4}(x^5 - x^4 - x^3 + x^2)$$
$$U_1 = x^4 - 2x^2 + 1, V1 = x^5 - 2x^3 + x$$
$$U_2 = \frac{1}{4}(3x^5 - 2x^4 - 5x^3 + 4x^2), V_2 = \frac{1}{4}(x^5 - x^4 - x^3 + x^2)$$

Substituting the values of $U_{0,}, V_0, U_1, V_1; U_2, V_2$ in (i), we get

$$\begin{aligned} P(x) = \; & \frac{1}{4}(3x^5 - 2x^4 - 5x^3 + 4x^2)(1) + \frac{1}{4}(x^5 - x^4 - x^3 + x^2) \\ & +(x^4 - 2x^2 + 1)(1) + (x^5 - 2x^3 + x)(1) \\ & -\frac{1}{4}(3x^5 - 2x^4 - 5x^3 + 4x^2)(3) + \frac{1}{4}(x^5 - x^4 - x^3 + x^2)(7) \\ = \; & 2x^4 - x^2 + x + 1 \end{aligned}$$

Hence $f(-0.5) = 2(-0.5)^4 - (-0.5)^2 + (-0.5) + 1 = 0.375$

1.4. DIVIDED DIFFERENCES

Lagrange's formula has the drawback that if another interpolation value were inserted, then the interpolation coefficients are required to be recalculated. This labor of recomputing the interpolation coefficients is saved by using Newton's general interpolation formula which employs what is called "divided differences." Before deriving this formula, we shall first define these differences.

If $(x_0, y_0), (x_1, y_1), (x_2, y_2), \cdots$ be given points, then the first divided difference for the arguments x_0, x_1 is defined by the relation $[x_0, x_1] = \frac{y_1 - y_0}{x_1 - x_0}$

Similarly $[x_1, x_2]$ or $\Delta y_{x_2} = \frac{y_2 - y_1}{x_2 - x_1}$ and $[x_2, x_3] = \frac{y_3 - y_2}{x_3 - x_2}$

The second divided difference for x_0, x_1, x_2 is defined as $[x_0, x_1, x_2] = \frac{[x_1,x_2]-[x_0,x_1]}{x_2-x_0}$

The third divided difference for x_0, x_1, x_2, x_3 is defined as $[x_0, x_1, x_2, x_3] = \frac{[x_1,x_2,x_3]-[x_0,x_1,x_2]}{x_2-x_0}$

PROPERTIES OF DIVIDED DIFFERENCES

I. The divided differences are symmetrical in their arguments, i.e, independent of the order of the arguments. For it is easy to write

$$\begin{aligned}
[x_0, x_1] &= \frac{y_0}{x_0 - x_1} + \frac{y_1}{x_1 - x_0} = [x_1, x_0], [x_0, x_1, x_2] \\
&= \frac{y_0}{(x_0 - x_1)(x_0 - x_2)} + \frac{y_1}{(x_1 - x_0)(x_1 - x_2)} + \frac{y_2}{(x_2 - x_0)(x_2 - x_1)} \\
&= [x_1, x_2, x_0] \text{ or } \left[x_{2,}x_0, x_1\right] \text{ and so on}
\end{aligned}$$

II. The nth divided differences of a polynomial of the nth degree are constant.

Let the arguments be equally spaced so that

$$x_1 - x_0 = x_2 - x_1 = \cdots = x_n - x_{n-1} = h. \text{ Then}$$

$$\begin{aligned}
[x_0, x_1] &= \frac{y_1 - y_0}{x_1 - x_0} = \frac{\Delta y_0}{h} \\
[x_0, x_1, x_2] &= \frac{[x_1, x_2] - [x_0 - x_1]}{x_2 - x_0} = \frac{1}{2h}\left\{\frac{\Delta y_1}{h} - \frac{\Delta y_0}{h}\right\} \\
&= \frac{1}{2!\,h^2}\Delta^2 y_0 \text{ and in general, } [x_0, x_1, x_2, \dots\dots, x_n] = \frac{1}{n!\,h^n}\Delta^n y_0
\end{aligned}$$

If the tabulated function is a nth degree polynomial, then $\Delta^n y_0$ will be constant. Hence the nth divided differences will also be constant.

1.4.0 NEWTON'S DIVIDED DIFFERENCE FORMULA

Let $y_0, y_1, \cdots, y_n$ be the values of $y = f(x)$ corresponding to the arguments $x_0, x_1, \cdots, x_n$. Then from the definition of divided differences, we have

$$[x, x_0] = \frac{y - y_0}{x - x_0}$$

So that

$$y = y_0 + (x - x_0)[x, x_0] \qquad \dots (9)$$

Again $[x, x_0, x_1] = \frac{[x, x_0] - [x_0, x_1]}{x - x_1}$

which gives $[x, x_0] = [x_0, x_1] + (x - x_1)[x, x_0, x_1]$ Substituting this value of $[x, x_0]$ in (9), we get

$$y = y_0 + (x - x_0)[x_0, x_1] + (x - x_0)(x - x_1)[x, x_0, x_1] \qquad \dots (10)$$

Also $[x, x_0, x_1, x_2] = \frac{[x \cdot x_0, x_1] - [x \cdot x_0, x_2]}{x - x_2}$

which gives $[x, x_0, x_1] = [x_0, x_1, x_2] + (x - x_2)[x, x_0, x_1, x_2]$

Substituting this value of $[x, x_0, x_1]$ in (10), we obtain

$$\begin{aligned} y = y_0 \quad & +(x - x_0)[x_0, x_1] + (x - x_0)(x - x_1)[x_0, x_1, x_2] \\ & +(x - x_0)(x - x_1)(x - x_2)[x, x_0, x_1, x_2] \end{aligned}$$

Proceeding in this manner, we get

$$\begin{aligned} y = y_0 \quad & +(x - x_0)[x_0, x_1] + (x - x_0)(x - x_1)[x_0, x_1, x_2] \\ & +(x - x_0)(x - x_1) \cdots (x - x_n)[x, x_0, x_1, \cdots x_n] \\ & +(x - x_0)(x - x_1)(x - x_2)[x, x_0, x_1, x_2] + \cdots \end{aligned}$$

which is called Newton's general interpolation formula with divided differences.

RELATION BETWEEN DIVIDED AND FORWARD DIFFERENCES

If $(x_0, y_0), (x_1, y_1), (x_2, y_2), \cdots$ be the given points, then

$$[x_0, x_1] = \frac{y_1 - y_0}{x_1 - x_0}$$

Also $\Delta y_0 = y_1 - y_0$

If $x_0, x_1, x_2, \cdots$ are equispaced, then $x_1 - x_0 = h$, so that

$$[x_0, x_1] = \frac{\Delta y_0}{h}$$

Similarly $[x_1, x_2] = \frac{\Delta y_1}{h}$

Now $[x_0, x_1, x_2] = \frac{[x_1, x_2] - [x_0, x_1]}{x_2 - x_0}$

$$= \frac{\Delta y_1/h - \Delta y_0/h}{2h}$$
$$= \frac{\Delta y_1 - \Delta y_0}{2h^2}$$

$[\because x_2 - x_0 = 2h]$

Thus $[x_0, x_1, x_2] = \frac{\Delta^2 y_0}{2!h^2}$

Similarly

$$[x_0, x_1, x_2] = \frac{\Delta^2 y_1}{2!\,h^2}$$
$$\therefore [x_0, x_1, x_2, x_3] = \frac{\Delta^2 y_1/2h^2 - \Delta^2 y_0/2h^2}{x_3 - x_0} = \frac{\Delta^2 y_1 - \Delta^2 y_0}{2h^2(3)} \ [\because x_3 - x_0 = 3h]$$

Thus

$$[x_0, x_1, x_2, x_3] = \frac{\Delta^3 y_0}{3!\,h^3}$$

In general, $[x_0, x_1, \cdots x_n] = \frac{\Delta^n y_0}{n!\,h^n}$

This is the relation between divided and forward differences.

Example 1.16 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

Solution: The divided differences table is

x	y	First Diff	Second Diff	Third Diff
5	150	$\frac{392-150}{7-5}=121$		
7	392		$\frac{265-121}{11-5}=24$	
11	1452	$\frac{1452-392}{11-7}=265$		$\frac{32-24}{13-5}=1$
13	2366	$\frac{2366-1452}{13-11}=457$	$\frac{457-265}{13-7}=32$	
			$\frac{709-457}{17-11}=42$	
17	5202			

Taking $x = 9$ in Newton's divided difference formula, we obtain

$$\begin{aligned} f(9) &= 150 + (9-5)\times 121 + (9-5)(9-7)\times 24 + (9-5)(9-7)(9-11)\times 1 \\ &= 150 + 484 + 192 - 16 = 810. \end{aligned}$$

Example 1.17 Using Newton's divided differences formula, evaluate $f(8)$ and $f(15)$ given:

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

Solution: The divided differences table is

x	$f(x)$	First Diff	Second Diff	Third Diff	Fourth Diff
4	48				0
		52			
5	100		15		

		97		1	
7	294		21		0
		202		1	
10	900		27		0
		310		1	
11	1210		33		
		409			
13	2028				

Taking $x = 8$ in Newton's divided difference formula, we obtain

$$\begin{aligned} f(8) &= 48 + (8-4)52 + (8-4)(8-5)15 + (8-4)(8-5)(8-7)1 \\ &= 448. \end{aligned}$$

Similarly $f(15) = 3150$.

1.4.1 INTERPOLATION BY ITERATION

We now describe the method due to Aitken, which has the advantage of being very easily programmed for a digital computer. Suppose we are given a set of $(n+1)$ data points $(x_i, y_i), i = 0,1,2,3,\cdots n$ of $y = f(x)$, where the value of x need not necessarily be equally spaced. Then to find the value of y corresponding to any given value of x, we proceed iteratively as follows: We obtain a first approximation to y by considering the first two points only. Then obtain its second approximation by considering the first there points and so on, The different interpolations are polynomials denoted by $\Delta(x)$ with suitable subscripts then at the first stage of approximation we have

$$\Delta_{01}(x) = y_0 + (x - x_0)[\mathrm{x}_0, x_1] = \frac{1}{x_1 - x_0}\begin{vmatrix} \mathrm{y}_0 & \mathrm{x}_0 - x \\ y_1 & \mathrm{x}_1 - x \end{vmatrix}$$

Similarly, we can form $\Delta 02(x), \Delta_{03}(x), \cdots$

Next Δ_{012} is formed by considering the first three points as

$$\Delta_{012}(x) = \frac{1}{\mathrm{x}_2 - x_1}\begin{vmatrix}\Delta_{01} & \mathrm{x}_1 - x \\ \Delta_{02} & \mathrm{x}_2 - x\end{vmatrix}$$

and similarly $\Delta 013(x), \Delta_{014}(x)$, etc are formed. At the nth stage of approximation, we obtain

$$\Delta_{012} \ldots n^{(x)} = \frac{1}{x_n - x_{n-1}}\begin{vmatrix}\Delta_{0123\cdots n-1}^{(x)} & x_n - x \\ \Delta_{0123\cdots n-2n}^{(x)} & x_n - x\end{vmatrix}$$

the computation can be conveniently arranged in the table below

Table 1: Aitken's scheme

x	y				
x_0	y_0				
		$\Delta_{01}(x)$			
x_1	y_1		$\Delta_{012}(x)$		
		$\Delta_{02}(x)$		$\Delta_{0123}(x)$	
x_2	y_2				$\Delta_{01234}(x)$
			$\Delta_{013}(x)$		
		$\Delta_{03}(x)$		$\Delta_{0124}(x)$	
x_3	y_3		$\Delta_{014}(x)$		
		$\Delta_{04}(x)$			
x_4	y_4				

A modification of this scheme suggested by Neville is given in Table 2 which is particularly suited for iterated inverse interpolation

Table 2: Neville's scheme

x	y				
x_0	y_0				
		$\Delta_{01}(x)$			
x_1	y_1		$\Delta_{012}(x)$		
		$\Delta_{12}(x)$		$\Delta_{0123}(x)$	

x_2	y_2		$\Delta_{123}(x)$		$\Delta_{1234}(x)$
		$\Delta_{23}(x)$		$\Delta_{1234}(x)$	
x_3	y_3		$\Delta_{124}(x)$		
		$\Delta_{24}(x)$			
x_4	y_4				

An obvious advance of Aitken's method is that it gives a good idea of the accuracy of the result at any stage.

Example 1.18 Use Aitken's method to complete $\log_{10} 301$ from the data

x	300	304	305	307
$\log_{10} x$	2.4771	2.4829	2.4843	2.4871

Also compare the result with those of Lagrange's and Newton's divided difference formulae.

Solution: Aitken's scheme is given by

x	$\log_{10} x$			
300	2.4771			
		2.47855		
304	2.4829		2.47858	
		2.47854		2.47860
2305	2.4843		2..47857	
		2.47854		
307	2.4871			

Hence $\log_{10} 301 = 2.4786$

Using Lagrange's interpolation formula, we get

$$\log_{10} 301 = \frac{-3(-4)(-6)}{-4(-5)(-7)}(2.4771) + \frac{1(-4)(-6)}{4(-1)(-3)}(2.4829) + \frac{1(-3)(-6)}{5.1(-2)}(2.4843)$$
$$+ \frac{-(-3)(-4)}{7(3)(2)}(2.4871) = 1.2739 + 4.9658 - 4.471 + 0.7106 = 2.4786$$

which is same as above. The divided difference table is

x	$\log_{10} x$	1st	2nd
300	2.4771		
		0.00145	
304	2.4829		0.00001
		0.00140	
305	2.4843		0.00000
		0.00140	
307	2.4871		

Using Netwon's divided formula, we get $\log_{10} 301 = 2.4771 + 0.00145 + (-3)(-0.00001) = 2.4786$, which is again the same as obtain above. It is clear that the arithmetic method is simpler than Lagrange's method. The Aitken's scheme has the advantage to given better estimate at each stage in addition the simplest arithmetic.

1.5 DOUBLE INTERPOLATION

So far, we have derived interpolation formulae to approximate a function of a single variable. In the case of functions, of two variables, we interpolate with respect to the first variable keeping the other variable constant. Then interpolate with respect to the second variable. Similarly, we can extend the said procedure for functions of three variables.

1.6 INVERSE INTERPOLATION

So far, given a set of values of x and y, we have been finding the value of y corresponding to a certain value of x. On the other hand, the process of estimating the value of x for a value of y (which is not in the table) is called inverse interpolation. When the values of x are unequally spaced Lagrange's method is used and when the values of x are equally spaced, the Iterative method should be employed.

1.6.0 LAGRANGE'S METHOD

This procedure is similar to Lagrange's interpolation formula (4), the only difference being that x is assumed to be expressible as a polynomial in y.

Lagrange's formula is merely a relation between two variables either of which may be taken as the independent variable. Therefore, by interchanging x and y in Lagrange's formula, we obtain

$$x = \frac{(y-y_1)(y-y_2)\cdots(y-y_n)}{(y-y_1)(y-y_2)\cdots(y-y_n)}x_0 + \frac{(y-y_0)(y-y_2)\cdots(y-y_n)}{(y_1-y_0)(y_1-y_2)\cdots(y1-y_n)}x_1 + \frac{(y-y_0)(y-y_1)\cdots(y-y_{n-1})}{(y_n-y_0)(y_n-y_1)\cdots(y_n-y_{n-1})}x_\mathrm{n} \quad \dots (11)$$

Example 1.19 The following table gives the values of x and y

x:	1.2	2.1	2.8	4.1	4.9	6.2
y:	4.2	6.8	9.8	13.4	15.5	19.6

Find the value of x corresponding to $y = 12$, using Lagrange's technique.

Solution: Here $x_0 = 1.2, x_1 = 2.1, x_2 = 2.8, x_3 = 4.1, x_4 = 4.9, x_5 = 6.2$ and $y_0 = 4.2$, $y_1 = 6.8, y_2 = 9.8, y_3 = 13.4, y_4 = 15.5, y_5 = 19.6$.

Taking $y = 12$, the above formula (11) gives

$$
\begin{aligned}
x = \quad & \frac{(12-6.8)(12-9.8)(12-13.4)(12-15.5)(12-19.6)}{(4.2-6.8)(4.2-9.8)(4.2-13.4)(4.2-15.5)(4.2-19.6)} \times 1.2 \\
& + \frac{(12-4.2)(12-9.8)(12-13.4)(12-15.5)(12-19.6)}{(6.8-4.2)(6.8-9.8)(6.8-13.4)(6.8-15.5)(6.8-19.6)} \times 2.1 \\
& + \frac{(12-4.2)(12-6.8)(12-13.4)(12-15.5)(12-19.6)}{(9.8-4.2)(9.8-6.8)(9.8-13.4)(9.8-15.5)(9.8-19.6)} \times 2.8 \\
& + \frac{(12-4.2)(12-6.8)(12-9.8)(12-15.5)(12-19.6)}{(13.4-4.2)(13.4-6.8)(13.4-9.8)(13.4-15.5)(13.4-19.6)} \times 4.1 \\
& + \frac{(12-4.2)(12-6.8)(12-9.8)(12-13.4)(12-19.6)}{(15.5-4.2)(15.5-6.8)(15.5-9.8)(15.5-13.4)(15.5-19.6)} \times 4.9 \\
& + \frac{(12-4.2)(12-6.8)(12-9.8)(12-13.4)(12-15.5)}{(19.6-4.2)(19.6-6.8)(19.6-9.8)(19.6-13.4)(19.6-15.5)} \times 6.2 \\
= \quad & 0.022 - 0.234 + 1.252 + 3.419 - 0.964 + 0.055 = 3.55
\end{aligned}
$$

Example 1.20 Apply Lagrange's formula inversely to obtain a root of the equation $f(x) = 0$, given that $f(30) = -30, f(34) = -13, f(38) = 3$, and $f'(42) = 18$.

Solution: Here $x_0 = 30, x_1 = 34, x_2 = 38, x_3 = 42$
and $y_0 = -30, y_1 = -13, y_2 = 3, y_3 = 18$

It is required to find x corresponding to $y = f(x) = 0$.

Taking $y = 0$, Lagrange's formula gives

$$
\begin{aligned}
x = \quad & \frac{(y-y_1)(y-y_2)(y-y_3)}{(y_0-y_1)(y_0-y_2)(y_0-y_3)} x_0 + \frac{(y-y_0)(y-y_2)(y-y_3)}{(y_1-y_0)(y_1-y_2)\cdot(y1-y_3)} x_1 \\
& + \frac{(y-y_0)(y-y_1)\cdot(y-y_3)}{(y_2-y_0)(y_2-y_1)(y_2-y_3)} x_2 + \frac{(y-y_0)(y-y_1)(y-y_2)}{(y_3-y_0)(y_3-y_1)(y_3-y_2)} x_3 \\
= \quad & \frac{13(-3)(-18)}{(-17)(-33)(-48)} \times 30 + \frac{30(-3)(-18)}{17(-16)(-31)} \times 34 \\
& + \frac{30(13)(-18)}{33(16)(-15)} \times 38 + \frac{30(13)(-3)}{48(31)(15)} \times 42 \\
= \quad & -0.782 + 6.532 + 33.682 - 2.202 = 37.23.
\end{aligned}
$$

Hence the desired root of $f(x) = 0$ is 37.23.

1.6.1 ITERATIVE METHOD

Newton's forward interpolation formula is

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

From this, we get

$$p = \frac{1}{\Delta y_0}\left[y_p - y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots\right] \qquad \ldots (12)$$

Neglecting the second and higher differences, we obtain the first approximation to p as

$$p_1 = (y_p - y_0)/\Delta y_0$$

To find the second approximation, retaining the term with second differences in (12) and replacing p by p_1, we get

$$p_2 = \frac{1}{\Delta y_0}\left[y_p - y_0 + \frac{p_1(p_1-1)}{2!}\Delta^2 y_0\right]$$

To find the third approximation, retaining the term with third differences in (12) and replacing every p by p_2, we have

$$p_3 = \frac{1}{\Delta y_0}\left[y_p - y_0 + \frac{p_2(p_2-1)}{2!}\Delta^2 y_0 + \frac{p_2(p_2-1)(p_2-2)}{3!}\Delta^3 y_0\right]$$

and so on. This process is continued till two successive approximations of p agree with each other

This method is a powerful iterative procedure for finding the roots of an equation to a good degree of accuracy.

Example 1.21 The following values of $y = f(x)$ are given

x:	10	15	20
y:	1754	2648	3564

Find the value of x for $y = 3000$ by an iterative method.

Solution: Taking $x_0 = 10$ and $h = 5$, the difference table is

x	y	Δy	$\Delta^2 y$
10	1754		
15	2648	894	
20	3564		22

Here $y_p = 3000, y_0 = 1754, \Delta y_0 = 894$ and $\Delta^2 y0 = 22$.

∴ The successive approximations to p are

$$p_1 = \frac{1}{894}(3000 - 1754) = 1.39$$
$$p_2 = \frac{1}{894}\left[3000 - 1754 - \frac{1.39(1.39 - 1)}{2} \times 22\right] = 1.387$$
$$p_3 = \frac{1}{894}\left[3000 - 1754 - \frac{1.387(1.387 - 1)}{2} \times 22\right] = 1.3871$$

We, therefore, take $p = 1.387$ correct to three decimal places. Hence the value of x (corresponding to $= 3000) = x_0 + ph = 10 + 1.387 \times 5 = 16.935$.

1.7 CHECK YOUR PROGRESS

1. Use Stirling's formula to interpolate the value of $y = e^x$ at $x = 1.91$ from the data

x:	1.7	1.8	1.9	2.0	2.1	2.2
$y = e^x$	5.4739	6.0496	6.6859	7.3891	8.1662	9.0250

2. Use Stirling's formula to find u_{32} form the data

$$u_{20} = 14.035, u_{25} = 13.674, u_{30} = 13.257, u_{35} = 12.734, u_{40} = 12.089, u_{45} = 11.309.$$

3. Using Gauss's forward formula, find the value of $f(32)$ given that

$$f(25) = 0.2707, f(30) = 0.3027, f(35) = 0.3386, f(40) = 0.3794$$

4. Using Gauss's backward formula, find the value of $\sqrt{12.516}$ given that

$\sqrt{12500} = 111.803399, \sqrt{12510} = 111.848111, \sqrt{12520} = 111.892806, \sqrt{1230}$
$= 111.937483$

5. Evaluate $\sin(0.197)$ form the following table :

x:	0.15	0.17	0.19	0.21	0.23
$\sin x$:	0.14944	0.16918	0.18886	0.20846	0.22798

6. If $y(1) = -3, y(3) = 9, y(4) = 30$ and $y(6) = 132$, find the four point Lagrange's interpolation polynomial that takes the same values as y at the given points.

7. Evaluate $\sqrt{155}$ using Lagrange's interpolation formula from the data:

x:	150	152	154	156
$y = \sqrt{x}$:	12.247	12.329	12.410	12.490

8. Using Hermit's interpolation formula estimate the value of $\log(3.2)$ from the following table:

x	:	3	3.5	4.0
$y = \log_x$	:	1.09861	1.25276	1.38629
$y' = \frac{1}{x}$	?	0.33333	0.28571	0.25000

.

1.8 SUMMARY

- The students are made familiar with some preliminary definitions and fundamental results of interpolation.
- Different types of interpolations with Lagrange, Hermite, Bessel, and Stirling formulae etc. have been developed to get the solution in various conditions.

1.9 KEYWORDS

Lagrange's interpolation, Lagrange's inverse interpolation, Bessel's interpolation, Stirling's interpolation, Gauss's backward interpolation, Newton's forward and backward interpolation.

1.10 ANSWERS TO CHECK YOUR PROGRESS

1. 6.7531
2. 13.062
3. 0.3165
4. 111.8749
5. 0.19573
6. $x^3 - 3x^2 + 5x - 6$
7. 12.45
8. 1.16314

1.11 SELF-ASSESSMENT TEST:

1. Find the unique polynomial P(x) of degree 2 or less such that P(1) = 1, P(3) = 27, P(4) = 64 using each of the following methods :
   (i) Lagrange interpolation formula,
   (ii) Newton divided the difference formula and evaluate P(1.5).
2. Calculate the nth divided difference of f (x) = 1 / x.
3. Use Everett's interpolation formula to find the value of y when x = 3.5 from the following table:

X	1	2	3	4	5	6
Y = f(x)	1.2567	1.4356	1.5678	1.6547	1.7658	1.8345

4. Find the zero of the function y(x) from the following data:

X	1.0	0.8	0.6	0.4	0.2
Y = f(x)	-1.049	-0.0266	0.377	0.855	1.15

1.12 REFERENCES/ SUGGESTED READINGS:

1. James F. Epperson; An Introduction to Numerical Methods and analysis. Second Edition Mathematical Reviews, John Wiley & Sons, Inc., Hoboken, New Jersey.
2. B S Grewal; Numerical Methods in Engineering and Science: C, C++, and MATLAB®. ISBN: 978-1-68392-128-8
3. M K Jain, SRK Iyengar, R K Jain; Numerical Methods, New Age International (P) Limited, Publishers, New Delhi
4. S S Shastry; Introductory Methods of Numerical Analysis, Fifth Edition ISBN-978-81-203-4592-8, Asoke K. Ghosh, PHI Learning Pvt. Ltd, M-97, Connaught Circus, New Delhi.

MAL-526: M. Sc. Mathematics (Advanced Numerical Methods)

LESSON No. 2 Written by- Dr. Joginder Singh

APPROXIMATION OF THE FUNCTIONS

STRUCTURE

2.0 LEARNING OBJECTIVES

- This chapter will be devoted to explaining the approximation of a function.
- It also briefs spline interpolation.
- Various ways of approximation of function have been discussed with their suitable examples.

2.1 INTRODUCTION

Often engineers, scientists, organizers, and sociologists have to take some decisions concerning the phenomena of which they know only the behavior from experimentally measured values. In certain cases, for example in physics, the fundamental knowledge of the phenomena in question allows us in proposing a precise, deterministic mathematical model which we call the model of knowledge. In many branches of applied mathematics, it is required to express a given data, obtained from observations in form of the law connecting the two variables involved. Such a law inferred by some scheme is known as an empirical law. Several equations of different types can be obtained to express the given data approximately. But the problem is to find the equation of the curve of 'best fit' which may be most suitable for predicting the unknown values. The process of finding such an equation of 'best fit' is known as curve fitting. The method of least squares is probably the best to fit a unique curve to a given data. It is widely used in applications and can be easily implemented on a computer. There are several cases when we have information or data ' y ' available at several discrete locations 'x' for example tabulated values of the steam, trigonometric, logarithmic, and other functions, etc. Till the use of online measurement devices and recorders became popular, experimental results taken in a laboratory were available in a similar form. We may be required to interpolate or extrapolate these data or may at times, be interested in computing slopes or integrals of functions described by them. This chapter is devoted to the discussion of several techniques for doing this.

2.2 APPROXIMATION OF THE FUNCTIONS

The graphical method and the method of group averages have the obvious drawback of being unable to give a unique curve fit. The principle of least squares, however, provides an elegant procedure for fitting a unique curve to a given data. A French mathematician Adrian Marie Legendre in 1806 suggested the "Principle of least squares," which states that the curve of best fit is that for which the errors (or residuals) are as small as possible i.e., the sum of the squares of the errors is a minimum. The principle of least squares does not help us to determine the form of the appropriate curve which can fit a given data. It only determines the least possible values of the constants in the equation when the form of the curve is known beforehand. The selection of the curve is a matter of experience and practical consideration. Here we shall discuss the fitting of various types of curves by the method of least squares.

2.2.0 STRAIGHT LINE FITTING

Suppose it is required to fit a straight line

$$y = a + bx \qquad \ldots(2.1)$$

to a given set of observations $(x_1, y_1), (x_2, y_2) \ldots (x_n, y_n)$. Since (2.1) passes through the data points (x_i, y_i), we have

$$y_i = a + bx_i$$

The error e_i between the observed and expected values of $y = y_i$ is defined as

$$e_i = y_i - (a + bx_i) \text{i} = 1,2,3, \ldots \text{n}$$

Therefore the sum of the squares of these errors is

$$\text{E} = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} [y_i - (a + bx_i)]^2$$

Now for E to be minimum, we must have

$$\frac{\partial \text{E}}{\partial a} = 0, \frac{\partial \text{E}}{\partial \text{b}} = 0$$

There provide us

and

$$\sum_{i=1}^{n} y_i = na + b \sum_{i=1}^{n} x_i$$

$$\sum_{i=1}^{n} x_i y_i = a \sum_{i=1}^{n} x_i + b \sum_{i=1}^{n} x_i^2$$

These equations are called normal equations. Solving these equations for a and b, we obtain

$$a = \frac{1}{n}\left[b\sum_{i=1}^{n} x_i - \sum_{i=1}^{n} y_i\right]$$
$$b = \frac{n\sum_{i=1}^{n} x_i y_i - (\sum_{i=1}^{n} x_i)(\sum_{i=1}^{n} y_i)}{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}$$

Upon substitution of the values of a and b in (2.1) we obtain the required line of "best fit".

2.2.1 PARABOLIC CURVE FITTING

Suppose the equation of the parabola to fit is given by

$$y = a + bx + cx^2 \qquad \ldots(2.2)$$

Let the data points be $(x_i, y_i), i = 1,2,3, \ldots n$. Since (2.2) passes through these data points, we have

$$y_i = a + bx_i + cx_i^2$$

The error e_i between the observed and expected values of $y = y_i$ is defined as

$$e_i = y_i - (a + bx_i + cx_i^2), i = 1,2,3, \ldots n$$

Therefore, the sum of the squares of these errors is

$$\mathrm{E} = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a - bx_i - cx_i^2)^2$$

For E to be minimum, we have

$$\frac{\partial \mathrm{E}}{\partial a} = 0, \frac{\partial \mathrm{E}}{\partial b} = 0, \frac{\partial \mathrm{E}}{\partial c} = 0$$

which leads to the normal equations

$$\sum y_i = na + b\sum x_i + c\sum x_i{}^2$$
$$\sum x_i y_i = a\sum x_i + b\sum x_i{}^2 + c\sum x_i{}^3$$
$$\sum x_i{}^2 y_i = a\sum x_i{}^2 + b\sum x_i{}^3 + c\sum x_i{}^4$$

Solving these equations for a, b, and c, and using these values in equation (2.2), we obtain the desired curve of best fit.

2.2.2 FITTING OF OTHER CURVES

1. Power curve: Let the curve be given by

$$y = ax^b$$

Taking logarithms, we get

$$\log_{10} y = \log_{10} a + b\log_{10} x \qquad \ldots(2.3)$$
$$Y = A + bX$$

where

$$X = \log_{10} x\,, Y = \log_{10} y$$

Therefore normal equations for (2.3) are

$$\sum Y_i = nA + b\sum X_i$$
$$\sum X_i Y = A\sum X_i + b\sum X_i^2$$

From these A and b can be determined. Then a can be calculated from $A = \log_{10} a$. The values of a and b so obtained are used in (2.3) to get the required curve of best fit.

2. Exponential curve: Let the curve given by,

$$y = ae^{bx}$$

Taking logarithms, we get

i.e.

$$\log_{10} y = \log_{10} a + bx \log_{10} e$$
$$Y = A + Bx \qquad \ldots(2.4)$$

where

$$Y = \log_{10} y, \text{ A} = \log_{10} a, \text{ and B} = b \log_{10} e$$

Here the normal equations are

$$\begin{aligned} \sum Y_i &= nA + B \sum x_i \\ \sum x_i Y_i &= A \sum x_i + B \sum x_i^{\ 2} \end{aligned}$$

From these A and B can be found and consequently a, b can be calculated and used in (2.4) to obtain the desired curve of 'best fit'.

Example 2.1 Fit a second-degree curve to the following data

x:	1.0	1.5	2.0	2.5	3.0	3.5	4.0
y:	1.1	1.3	1.6	2.0	2.7	3.4	4.1

Solution: Let the required curve be $y = a + bx + cx^2$

We put $X = 2x - 5$ so that this equation becomes

$$y = a + bX + cX^2$$

x	y	Y	Xy	X^2	X^2y	X^3	X^4
1.0	-3	1.1	-3.3	9	9.9	-27	81
1.5	-2	1.3	-2.6	4	5.2	-8	16
2.0	-1	1.6	-1.6	1	1.6	-1	1
2.5	0	2.0	0.0	0	0.0	0	0

3.0	1	2.7	2.7	1	2.7	1	1
3.5	2	6.8	6.8	4	13.6	8	16
4.0	3	12.3	12.3	9	36.9	27	81
Tota1	0	16.2	14.3	28	69.9	0	196

The normal equations are

$$7a + 28c = 16.2, 28b = 14.3, 28a + 196c = 69.9$$

Solving these equations leads to $a = 2.07$, $\mathrm{b} = 0.511$, $\mathrm{c} = 0.061$

Therefore,

$$y = 2.07 + 0.511X + \quad 0.061X^2 = 2.07 + 0.511(2x - 5) + 0.061(2x - 5)^2$$
$$= 1.04 - 0.198x + 0.244x^2$$

Thus the required second-degree curve (parabola) is

$$y = 1.04 - 0.198x + 0.244x^2$$

Example 2.2 Fit a straight line to the following data:

Year (x):	1951	1961	1971	1981	1991
Production (y): in thousand tons	8	10	12	10	16

Also, find the expected production in 1996.

Solution: Suppose the equation of the required straight line be $y = a + bx$

x	y	xy	x^2
1951	8	15608	3806401

1961	10	19610	3845521
1971	12	23652	3884841
1981	10	19810	3924361
1991	16	31856	3964081
$\sum x = 9855$	$\sum y = 56$	$\sum xy = 110536$	19425205

The normal equations are

$$\sum y = na + b \sum x$$
$$\sum xy = a \sum x + b \sum x^2$$

imply that

$$5a + 9855b = 56$$
$$9855\text{a} + 19425205\ \text{b} = 110536$$

Solving these equations, we get $a = 304.16, b = .16$

∴ The required straight line is $y = .16x - 304.16$

2.2.3 GENERAL LEAST SQUARE METHOD

Here we propose the following model in terms of the unknown coefficients $c_j, j = 1,2,3, \dots m$ as

$$y_i = c_1 f_1(x_i) + c_2 f_2(x_i) + \cdots + c_m f_m(x_i), i = 1,2,3, \cdots n \qquad \dots(2.5)$$

where $x_i \in R^1$ or R^n. The error committed at the i th point in approximating the observed value y_i for the expected value y_i^* is

$$e_i = y_i - y_i^*, \text{ for i} = 1,2,3, \dots n$$
$$= y_i - \sum_{j=1}^{m} c_j f_j(x_i), i = 1,2,3, \dots n$$

This is a system of n equations in $(n + m)$ unknowns $\mathrm{c_j}, j = 1,2,3, \dots m$ and $\mathrm{e_i}, \mathrm{i} = 1,2,3, \dots \mathrm{n}$, and hence it has an infinite number of solutions. Among all these solutions, we define the best solution as the one that minimizes the scalar quantity

$$E = \sum_{i=1}^{n} w_i e_i^2$$

where $w_i \geq 0$ are the weights so that

$$\|y - y^*\|_2 = \sum_{i=1}^{n} (y_i - y_i)^2 w_i$$

defines the weighted least squares norm. We look for minimizing E with respect to the parameters $\{c_1, c_2, c_3, \dots, c_m\}$. The necessary condition in which E is minimum in the space of $\{c_1, c_2, \dots c_m\}$ is that

$$\frac{\partial E}{\partial c_k} = 0, \mathrm{k} = 1,2,3 \dots n$$

Permuting the summation and partial derivative operation and taking the derivative, we obtain

$$2 \sum_{i=1}^{n} w_i e_i \frac{\partial e_i}{\partial c_k} = 0, k = 1,2, \dots, m \qquad \dots(2.6)$$

Using equation (2.5) in (2.6), we obtain

$$\sum_{i=1}^{n} w_i \left[y_i - \sum_{j=1}^{m} c_j f_j(x_i) \right] f_k(x_i) = 0, k = 1,2, \dots m$$

This implies that

$$\sum_{j=1}^{m} c_j \sum_{i=1}^{n} w_i f_j(x_i) f_k(x_i) = \sum_{i=1}^{n} w_i y_i f_k(x_i),\ k = 1,2,3 \dots m$$

$$\sum_{j=1}^{m} a_{kj} c_j = b_k, k = 1,2 \dots m$$

where

$$\begin{aligned} a_{kj} &= \sum_{i=1}^{n} f_j(x_i) f_k(x_i) w_{i,} k = 1,2,\dots m, j = 1,2,3 \dots m \\ b_k &= \sum_{i=1}^{n} w_i y_i f_k(x_i), k = 1,2 \dots m \end{aligned} \qquad \dots(2.7)$$

In matrix form we have

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} C_1 \\ \vdots \\ C_m \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix} \qquad \dots(2.8)$$

The quantities a_{kj} and b_k defined in (2.7) are completely determined because the pairs (x_i, y_i) and the function $f_j(x)$ are known in the linear system (2.8), it remains only to determine these m unknowns $\{c_1, c_2, \dots, c_m\}$.

Algorithm for Least squares method: Linear model

The n pairs (x_i, y_i) of data points are given along with their weights w_i

1. Define the function $f_j(x)$ composing the model so that $y_i^* = \sum_{j=1}^{m} c_j f_j(x_i)$

2. For $k = 1,2,3, \cdots m$, calculate the terms

$$a_{kj} = \sum_{i=1}^{n} f_j(x_j) f_k(x_i) w_{i,j} j = 1,2,3, \dots m$$

and

$$b_k = \sum_{i=1}^{n} w_i y_\mathrm{i} f_k(x_i)$$

3. Solve the linear system of the symmetric matrix equation

$$\sum_{j=1}^{m} a_{kj} c_{j=b_k}, k = 1,2,3, \dots m$$

2.3 SPLINE INTERPOLATION

In the interpolation methods so far explained, a single polynomial has been fitted to the tabulated points. If the given set of points belongs to the polynomial, then this method works well, otherwise, the results are rough approximations only. If we draw lines through every two closest points, the resulting graph will not be smooth. Similarly, we may draw a quadratic curve through points A_i, A_{i+1} and another quadratic curve through A_{i+1}, A_{i+2}, such that the slopes of the two quadratic curves match at A_{i+1} (Fig. 2.1). The resulting curve looks better but is not quite smooth. We can ensure this by drawing a cubic curve through A_i, A_{i+1} and another cubic through A_{i+1}, A_{i+2} such that the slopes and curvatures of the two curves match at A_{i+1}. Such a curve is called a cubic spline. We may use polynomials of higher order but the resulting graph is not better. As such, cubic splines are commonly used. This technique of "spline-fitting" is of recent origin and has important applications.

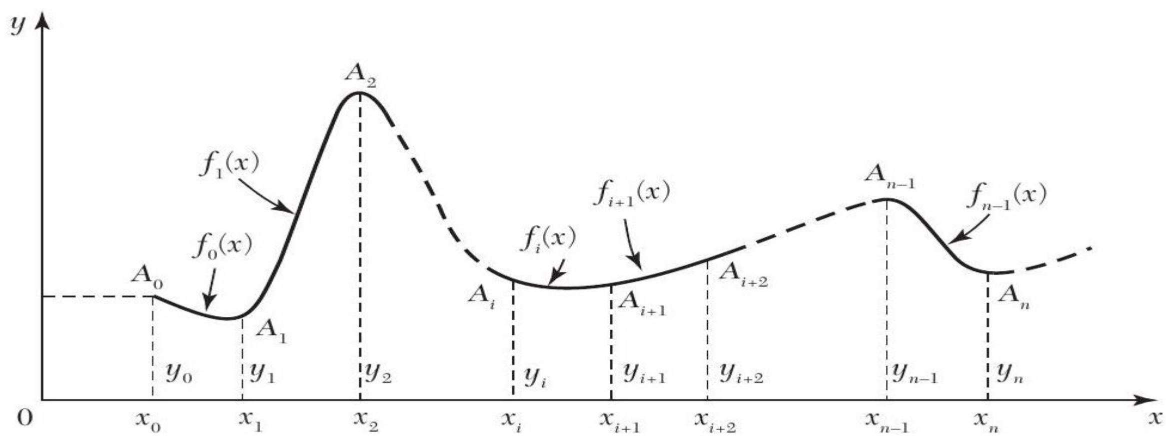

FIGURE 2.1

CUBIC SPLINE

Consider the problem of interpolating between the data points (x_0, y_0), $(x_1, y_1), \cdots (x_n, y_n)$ using spline fitting.

Then the cubic spline $f(x)$ is such that

(i) $f(x)$ is a linear polynomial outside the interval (x_0, x_n),

(ii) $f(x)$ is a cubic polynomial in each of the subintervals,

(iii) $f'(x)$ and $f''(x)$ are continuous at each point.

Since $f(x)$ is cubic in each of the subintervals $f''(x)$ shall be linear. $\therefore$ Taking equally-spaced values of x so that $x_{i+1} - x_i = h$, we can write

$$f''(x) = \frac{1}{h}[(x_{i+1} - x)f''(x_i) + (x - x_i)f''(x_{i+1})]$$

Integrating twice, we have

$$f(x) = \frac{1}{h}\left[\frac{(x_{i+1}-x)}{3!}f''(x_i) + \frac{(x-x_i)}{3!}f''(x_{i+1})\right]a_i(x_{i+1} - x) + b_i(x - x_i) \qquad \ldots(2.9)$$

The constants of integration a_i, b_i are determined by substituting the values of $y = f(x)$ at x_i and x_{i+1}. Thus,

$$a_i = \frac{1}{h}\left[y_i - \frac{h^2}{3!}f''(x_i)\right] \text{ and } b_i = \frac{1}{h}\left[y_{i+1} - \frac{h^2}{3!}f''(x_{i+1})\right]$$

Substituting the values of ai, bi, and writing $f''(x_i) = M_i$, (2.9) takes the form $f(x) = \frac{(x_{i+1}-x)^3}{6h}M_i + \frac{(x-x_i)^3}{6h}M_{i+1}$

$$+\frac{x_{i+1}-x}{h}\left(y_i - \frac{h^2}{6}M_i\right) + \frac{x-x_i}{h}\left(y_{i+1} - \frac{h^2}{6}M_{i+1}\right) \qquad \ldots(2.10)$$

$$\therefore f'(x) = -\frac{(x_{i+1} - x)^2}{2h}M_i + \frac{(x - x_i)^2}{6h}M_{i+1} - \frac{h}{6}(M_{i+1} - M_i) + \frac{1}{h}(y_{i+1} - y_i)$$

To impose the condition of continuity of $f'(x)$, we get $f'(x - \varepsilon) = f'(x + \varepsilon)$ as $\varepsilon \to 0$

$$\begin{aligned} \therefore \quad & \frac{h}{6}(2M_i + M_{i-1}) + \frac{1}{h}(y_i - y_{i-1}) = -\frac{h}{6}(2M_i + M_{i+1}) + \frac{1}{h}(y_{i+1} - y_i) \\ & M_{i-1} + 4M_i + M_{i+1} = \frac{6}{h^2}(y_{i-1} - 2y_i + y_{i+1}), i = 1 \text{ to } n - 1 \end{aligned} \qquad \ldots(2.11)$$

Now since the graph is linear for $x < x_0$ and $x > x_n$, we have

$$M_0 = 0, M_n = 0 \qquad \ldots(2.12)$$

(2.11) and (2.12) give $(n + 1)$ equations in $(n + 1)$ unknowns $M_i(i = 0,1, \cdots n)$ which can be solved. Substituting the value of M_i in (2) gives the concerned cubic spline.

Example 2.3 Obtain the cubic spline for the following data

x:	0	1	2	3
y:	2	-6	-8	2

Solution: Since the points are equispaced with $h = 1$ and $n = 3$, the cubic spline can be determined from $M_{i-1} + 4M_i + M_{i+1} = 6(y_{i-1} - 2y_i + y_{i+1}), i = 1,2.$

$$\therefore\ M_0 + 4M_1 + M_2 = 6(y_0 - 2y_1 + y_2)$$

$$M_1 + 4M_2 + M_3 = 6(y_1 - 2y_2 + y_3)$$

i.e., $4M_1 + M_2 = 36; M_1 + 4M_2 = 72$ $[\because M_0 = 0, M_3 = 0]$

Solving these, we get $M_1 = 4.8, M_2 = 16.8.$

Now the cubic spline in $(x_i \leq x \leq x_i + 1)$ is

$$f(x) = \frac{1}{6}(x_{i+1} - x)^3 M_i + \frac{1}{6}(x - x_i)^3 M_{i+1} \quad +(x_{i+1} - x)\left(y_i - \frac{1}{6}M_i\right) + \quad (x - x_i)\left(y_{i+1} - \frac{1}{6}M_{i+1}\right)$$

Taking $i = 0$, the cubic spline in $(0 \leq x \leq 1)$ is

$$\begin{aligned} f(x) \quad &= \frac{1}{6}(1 - x)^3(0) + \frac{1}{6}(x - 0)^3(4.8) + (1 - x)(x - 0) + x\left[-6 - \frac{1}{6}(4.8)\right] \\ &= 0.8x^3 - 8.8x + 2\ (0 \leq x \leq 1) \end{aligned}$$

Taking $i = 1$, the cubic spline in $(1 \leq x \leq 2)$ is

$$\begin{aligned} f(x) = &\quad \frac{1}{6}(2 - x)^3(4.8) + \frac{1}{6}(x - 1)^3(16.8) + (2 - x)\left[-6 - \frac{1}{6}(4.8)\right] \\ &\quad +(x - 1)[-8 - 1(16.8)] \\ = &\quad 2x^3 - 5.84x^2 - 1.68x + 0.8 \end{aligned}$$

Taking $i = 2$, the cubic spline in $(2 \leq x \leq 3)$ is

$$
\begin{aligned}
f(x) = & \frac{1}{6}(3-x)^3(4.8) + \frac{1}{6}(x-2)^3(0) + (3-x)[-8-1(16.8)] \\
+ & +(x-2)[2-1(2)] \\
= -0.8x^3 + & 2.64x^2 + 9.68x - 14.8
\end{aligned}
$$

Example 2.4 The following values of x and y are given:

x:	1	2	3	4
y:	1	2	5	11

Find the cubic splines and evaluate $y(1.5)$ and $y'(3)$.

Solution: Since the points are equispaced with $h = 1$ and $n = 3$, the cubic splines can be obtained from

$$
\begin{aligned}
M_{i-1} + 4M_i + M_{i+1} &= 6(y_{i-1} - 2y_i + y_{i+1}), i = 1,2. \\
M_0 + 4M_1 + M_2 &= 6(y_0 - 2y_1 + y_2) \\
M_1 + 4M_2 + M_3 &= 6(y_1 - 2y_2 + y_3)
\end{aligned}
$$

i.e.,

$$4M_1 + M_2 = 12, M_1 + 4M_2 = 18$$

$$[\because M_0 = 0, M_3 = 0]$$

which give,

$$M_1 = 2, M_2 = 4.$$

Now the cubic spline in $(x_i \leq x \leq x_{i+1})$ is

$$
\begin{aligned}
f(x) = \frac{1}{6}(x_{i+1} - x)^3 M_i & + \frac{1}{6}(x - x_i)^3 M_{i+1} + (x_{i+1} - x)\left(y_i - \frac{1}{6}M_i\right) \\
& + (x - x_i)\left(y_{i+1} - \frac{1}{6}M_{i+1}\right)
\end{aligned}
$$

Thus, taking $i = 0, i = 1, i = 2$, the cubic splines are

$$f(x) = \begin{cases} \frac{1}{3}(x^3 - 3x^2 + 5x) 1 \le x \le 2 \\ \frac{1}{3}(x^3 - 3x^2 + 5x) 2 \le x \le 3 \\ \frac{1}{3}(-2x^3 - 24x^2 - 76x + 81) 3 \le x \le 4 \end{cases}$$

$$\therefore y(1.5) = f(1.5) = 11/8$$

Example 2.5 Find the cubic spline interpolation for the data:

x:	1	2	3	4	5
$f(x)$:	1	0	1	0	1

Solution: Since the points are equispaced with $h = 1, n = 4$, the cubic spline can be found using

$$M_{i-1} + 4M_i + M_{i+1} = 6(y_{i-1} - 2y_i + y_{i+1}), i = 1,2,3$$
$$M_0 + 4M_1 + M_2 = 6(y_0 - 2y_1 + y_2) = 12$$
$$M_1 + 4M_2 + M_3 = 6(y_1 - 2y_2 + y_3) = -12$$
$$M_2 + 4M_3 + M_4 = 6(y_2 - 2y_3 + y_4) = 12$$

Since $M_0 = y_0'' = 0$ and $M_4 = y_4'' = 0$

$$\therefore \ 4M_1 + M_2 = 12; M_1 + 4M_2 + M_3 = -12; M_1 + 4M_3 = 12$$

Solving these equations, we get $M_1 = 30/7, M_2 = -36/7, M_3 = 30/7$

Now the cubic spline in $(xi \le x \le xi + 1)$ is

$$f(x) = \frac{1}{6}(x_{i+1} - x)^3 M_i + \frac{1}{6}(x - x_i)^3 M_{i+1} + (x_{i+1} - x)$$
$$\left(y_i - \frac{1}{6}M_i\right) + (x - x_i)\left(y_{i+1} - \frac{1}{6}M_{i+1}\right)$$

Taking $i = 0$, the cubic spline in $(1 \le x \le 2)$ is

$$y = \frac{1}{6}[(x_1 - x)^3 M_0 + (x - x_0)^3 M_1] + (x_1 - x)\left(y_0 - \frac{1}{6}M_0\right)$$
$$+(x - x_0)\left(y_1 - \frac{1}{6}M_1\right)$$
$$= \frac{1}{6}[(2 - x)^3(0) + (x - x_0)^3(30/7)] + (2 - x)\left(1 - \frac{1}{6}(0)\right)$$
$$+(x - 1)\left(0 - \frac{1}{6}\left(\frac{30}{7}\right)\right)$$

i.e., $y = 0.71x^3 - 2.14x^2 + 0.42x + 2 \ (1 < x \leq 2)$

Taking $i = 1$, the cubic spline in $(2 \leq x \leq 3)$ is

$$y = \frac{1}{6}\left[(3 - x)^3 \frac{30}{7} + (x - 2)^3\left(-\frac{36}{7}\right)\right] + (3 - x)\left(0 - \frac{1}{6}\left(\frac{30}{7}\right)\right)$$
$$+(x - 2)\left(1 - \frac{1}{6}\left(-\frac{36}{7}\right)\right)$$

i.e., $y = -1.57x^3 + 11.57x^2 - 27x + 20.28. \ (2 \leq x \leq 3)$

Taking $i = 2$, the cubic spline in $(3 \leq x \leq 4)$ is

$$y = \frac{1}{6}(4 - x)^3\left(-\frac{36}{7}\right) + \frac{1}{6}(x - 3)^3 \frac{30}{7} + (4 - x)\left(1 - \frac{1}{6}\left(-\frac{36}{7}\right)\right) + (x - 3)\left(0 - \frac{5}{7}\right)$$

i.e., $y = 1.57x^3 - 16.71x^2 + 57.86x - 64.57 \ (3 \leq x \leq 4)$

Taking $i = 3$, the cubic spline in $(4 \leq x \leq 5)$ is

$$y = \frac{1}{6}(1 - x)^3\left(\frac{30}{7}\right) + (5 - x)^3\left(-\frac{5}{7}\right) + (x - 4)(1)$$

i.e., $y = -0.71x^3 + 2.14x^2 - 0.43x - 6.86. \ (4 \leq x \leq 5)$

2.4 CHEBYSHEV POLYNOMIALS

The Chebyshev polynomials of the first kind, $T_n(x)$ are defined by

$$T_n(x) = \cos(n\cos^{-1} x)$$

where n is a non-negative integer.

Remark. Chebyshev polynomials are also known as Tchebicheff, Tchebieheff, or Tschebysheff.

RECURRENCE RELATIONS (FORMULAE)

I. $T_{n+1}(x) - 2xT_n(x) + T_{n-1}(x) = 0.$

II. $(1 - x^2)T_n{}'(x) = -nxT_n(x) + nT_{n-1}(x).$

Proof I. We have, by definition $T_n(x) = \cos(n\cos^{-1} x)$

$\therefore$ $T_n(\cos\theta) = \cos(n\cos^{-1}\cos\theta) = \cos n\theta$ …(2.13)

so that $T_{n+1}(\cos\theta) = \cos(n+1)\theta$ and $T_{n-1}(\cos\theta) = \cos(n-1)\theta$ …(2.14)

We are to show that $T_{n+1}(x) - 2xT_n(x) + T_{n-1}(x) = 0.$ …(2.15)

Replacing x by $\cos\theta$ in (2.15), we must now prove that

$$T_{n+1}(\cos\theta) - 2\cos\theta T_n(\cos\theta) + T_{n-1}(\cos\theta) = 0$$

i.e.

$$\cos(n+1)\theta - 2\cos\theta\cos n\theta + \cos(n-1)\theta = 0, \text{ by (2.13) and (2.14)}$$

i.e.,

$$\cos(n+1)\theta + \cos(n-1)\theta - 2\cos\theta\cos n\theta = 0. \qquad \text{…(2.16)}$$

Now, L.H.S. (2.16) $= 2\cos n\theta\cos\theta - 2\cos\theta\cos n\theta = 0,$

which proves (2.16) and hence (2.14) is true.

II. We have $T_n'(x) = -\sin(n\cos^{-1} x) \cdot \frac{-n}{\sqrt{(1-x^2)}}$

or $T_n'(\cos\theta) = \sin(n\cos^{-1}\cos\theta) \cdot \frac{n}{\sqrt{(1-\cos^2\theta)}}$

Thus,

$$T_n'(\cos\theta) = (n\sin n\theta)/\sin\theta \qquad \text{…(2.17)}$$

We are to show that

$$(1-x^2)T_n'(x) = -nxT_n(x) + nT_{n-1}(x). \qquad \ldots(2.18)$$

Putting $x = \cos\theta$ and using (2.14) and (2.17), (2.18) may be re-written as

$$\sin^2\theta \frac{n\sin n\theta}{\sin\theta} = -n\cos\theta\cos n\theta + n\cos(n-1)\theta$$

or $\quad \sin\theta\sin n\theta = \cos(n-1)\theta - \cos\theta\cos n\theta. \qquad \ldots(2.19)$

R.H.S. of (2.19) $= \cos(n\theta - \theta) - \cos\theta\cos n\theta$

$$= \cos n\theta\cos\theta + \sin n\theta\sin\theta - \cos\theta\cos n\theta$$

$= \sin n\theta\sin\theta =$ L.H.S. of (2.19),

which proves (2.19) and hence (2.18) is true.

Example 2.6 Show that $T_n(x)$ is the solution to Chebyshev's equation

$$(1-x^2)(d^2y/dx^2) - x(dy/dx) + n^2y = 0. \qquad \ldots(2.20)$$

Solution: Chebyshev's equation is $(1-x^2)(d^2y/dx^2) - x(dy/dx) + n^2y = 0$

To show that $T_n(x)$ is a solution of (2.20), by definition we have

$$T_n(x) = \cos(n\, cos^{-1} x) \qquad \ldots(2.21)$$

$$\therefore \frac{d}{dx}T_n(x) = \frac{d}{dx}\cos(n\cos^{-1}x) = -\sin(n\cos^{-1}x)\cdot n\cdot\frac{-1}{(1-x^2)^{1/2}}$$

or

$$\frac{d}{dx}T_n(x) = \frac{n}{(1-x^2)^{1/2}}\sin(n\cos^{-1}x) \qquad \ldots(2.22)$$

and

$$\frac{d^2}{dx^2}T_n(x) = \frac{d}{dx}\left(\frac{d}{dx}T_n(x)\right) = n\frac{d}{dx}\left[(1-x^2)^{-1/2}\sin(n\cos^{-1}x)\right]$$

$$= n\begin{bmatrix} -\frac{1}{2}(1-x^2)^{-\frac{3}{2}}(-2x)\cdot\sin(n\cos^{-1}x) \\ +(1-x^2)^{-1/2}\cos(n\cos^{-1}\cdot x)\cdot n\cdot\frac{1}{(1-x^2)^{1/2}} \end{bmatrix}$$

Thus, $\frac{d^2}{dx^2}T_n(x) = \frac{nx}{(1-x^2)^{3/2}}\sin(n\cos^{-1}x) - \frac{n^2}{1-x^2}\cos(n\cos^{-1}x)$. …(2.23)

Using (2.21), (2.22), and (2.23), we have

$$(1-x^2)\frac{d^2}{dx^2}T_n(x) - x\frac{d}{dx}T_n(x) + n^2T_n(x)$$

$$= \frac{nx}{(1-x^2)^{\frac{1}{2}}}\sin(n\cos^{-1}x) - n^2\cos(n\cos^{-1}x)$$

$$-\frac{nx}{(1-x^2)^{1/2}}\sin(n\cos^{-1}x) + n\cos(n\cos^{-1}x)$$

$= 0$

showing that $T_n(x)$ is a solution of (2.20).

ORTHOGONAL PROPERTY OF CHEBYSHEV POLYNOMIALS

Show that

$$\int_{-1}^{1}\frac{T_m(x)T_n(x)}{\sqrt{(1-x^2)}}dx = \begin{cases} 0, m \neq n \\ \pi/2, m = n \neq 0 \\ \pi, m = n = 0 \end{cases}$$

Proof. We have, by definition

$T_m(x) = \cos(m\cos^{-1}x)$ and $T_n(x) = \cos(n\cos^{-1}x)$.

$\therefore\ T_m(\cos\theta) = \cos(m\cos^{-1}\cos\theta) = \cos m\theta$

Let $I = \int_{-1}^{1}\frac{T_m(x)T_n(x)}{\sqrt{(1-x^2)}}dx$. ... (2.24)

Putting $x = \cos\theta$ so that $dx = -\sin\theta d\theta$ and (2.24), reduces to

$$I = \int_{\pi}^{0} \frac{\cos m\theta \cos n\theta}{\sin\theta}(-\sin\theta)d\theta \text{ or } I = \int_{\pi}^{0} \cos m\theta \cos n\theta d\theta$$

Case 1. Let $m \neq n$ so that $(m-n) \neq 0$. then, (2.24) gives

$$I = \frac{1}{2}\int_0^{\pi} 2\cos m\theta \cos n\theta d\theta = \frac{1}{2}\int_0^{\pi} [\cos(m+n)\theta + \cos(m-n)\theta]d\theta$$
$$= \frac{1}{2}\left[\frac{\sin(m+n)\theta}{m+n} + \frac{\sin(m-n)\theta}{m-n}\right]_0^{\pi} = 0$$

Case 2. Let $m = n \neq 0$. Then (2.24) gives

$$I = \int_0^{\pi} \cos^2 m\theta d\theta = \int_0^{\pi} \frac{1+\cos 2m\theta}{2} d\theta = \frac{1}{2}\left[\theta + \frac{\sin 2m\theta}{2m}\right]_0^{\pi} = \frac{\pi}{2}.$$

Case 3. Let $m = n = 0$. Then $\cos m\theta = \cos n\theta = 1$. Then (2.24) gives

$$I = \int_0^{\pi} (1)(1)dx = [\theta]_0^{\pi} = \pi$$

From cases 1, 2, and 3, the required result follows.

Example 2.7 Show that $T_n(x) = (1/2) \times \left[\left\{x + i(1-x^2)^{1/2}\right\}^n + \left\{x - i(1-x^2)^{1/2}\right\}^n\right]$.

Solution: Putting $x = \cos\theta$, and using the definition, we have

$$\begin{aligned} T_n(x) &= \cos(n\cos^{-1} x), = \cos(n\cos^{-1}\cos\theta) = \cos n\theta = \left(e^{in\theta} + e^{-in\theta}\right)/2 \\ &= (1/2) \times \left\{\left(e^{i\theta}\right)^n + \left(e^{-i\theta}\right)^n\right\} = (1/2) \times \{(\cos\theta + i\sin\theta)^n + (\cos\theta - i\sin\theta)^n\} \\ &= (1/2) \times \left[\left\{\cos\theta + i(1-\cos^2\theta)^{1/2}\right\}^n + \left\{\cos\theta - i(1-\cos^2\theta)^{1/2}\right\}^n\right] \\ &= (1/2) \times \left[\left\{x + i(1-x^2)^{1/2}\right\}^n + \left\{x - i(1-x^2)^{1/2}\right\}^n\right], \text{ as } x = \cos\theta \end{aligned}$$

Example 2.8 Show that $T_m\{T_n(x)\} = T_n\{T_m(x)\} = T_{nm}(x)$.

Solution: We have, by definition

$$\begin{aligned} T_m\{T_n(x)\} &= T_m[\cos(n\cos^{-1} x)] \\ &= \cos[m\cos^{-1}\{\cos(n\cos^{-1} x)\}], \text{ by definition again} \\ &= \cos(nm\cos^{-1} x). \qquad \text{... (2.25)} \end{aligned}$$

Again, $T_n\{T_m(x)\} = T_n[\cos(m\cos^{-1} x)]$, by definition

$= \cos[n\cos^{-1}\{\cos(m\cos^{-1} x)\}]$, by definition again

$= \cos(nm\cos^{-1} x)$, …(2.26)

Finally,

$T_{mn}(x) = \cos(mn\cos^{-1} x)$, by definition …(2.27)

From (2.25), (2.26), and (2.27), we get the required result.

2.5 CHECK YOUR PROGRESS

1. Fit a straight line by the method of least squares to the data:

x:	1	2	3	4	5
y:	14	27	40	55	68

2. Fit a least square geometric curve $y = ax^6$ to the data:

x:	1	2	3	4	5
y:	0.5	2	4.5	8	12.5

3. Use the method of least squares to fit a relation of the form $y = ab^x$ to the data :

x:	2	3	4	5	6
y:	144	172.8	207.4	248.8	298.5

4. Find the parabola of the form $y = a + bx + cx^2$ which fits most closely with the observations:

x:	-3	2	-1	0	1	2	3
y:	4.63	2.11	0.67	0.09	0.63	2.15	4.58

5. Obtain the natural cubic spline which agrees with $y(x)$ at the set of data points:

x:	2	3	4

y:	11	49	12

Hence compute $y(2.5)$ and $y'(2)$

6. Determine the cubic spline valid in the interval $\lfloor x_{i-1}, x_1 \rfloor$ for the following data:

x	6.2	6.5
$y = x\log x$	11.3119	14.1014

2.6 SUMMARY

- The students are made familiar with the approximation of functions.
- Different types of approximation have been developed for the functions.

2.7 KEYWORDS

Approximation, Least Square method, Spline interpolation, Chebyshev's approximation

2.8 SELF-ASSESSMENT TEST

1. Show that

$$T_{m+n}(x) + T_{m-n}(x) = 2T_m(x)T_n(x).$$

2. and

$$2\{T_n(x)\}^2 = 1 + T_{2n}(x).$$

3. Show that the set of Chebyshev polynomials $T_n(x) = \cos(n\cos^{-1}x)$, (n = 0,1,2 ....) is orthogonal on the interval $(-1,1)$ with respect to the weight function $p(x) = 1/(1-x^2)^{1/2}$.
4. Show that Chebyshev's polynomials $T_n(x) = \cos(n\cos^{-1}x)$ are solutions of
5. $(1-x^2)(d^2y/dx^2) - x(dy/dx) + n^2y = 0.$
6. Prove that $T_n(x) - 2xT_{n-1}(x) + T_{n-2}(x) = 0$

2.9 ANSWERS TO CHECK YOUR PROGRESS

1. y = 13.6x

2. $a = 0.5012, b = 1.9977$

3. $a = 99.86, b = 1.2$

4. $y = 1.243 - 0.004x + 0.22x^2$

5. $y(x) = \begin{cases} 3x^2 - 9x^2 + 11x - 11 & 2 \leq x \leq 3 \\ -3x^2 + 27x^2 - 61x + 37 & 3 \leq x \leq 4 \end{cases}$

$$y(2.5) = -4.625, y'(2) = 11$$

2.10 REFERENCES/ SUGGESTED READINGS

1. JAMES F. EPPERSON; An Introduction to Numerical Methods and analysis. Second Edition Mathematical Reviews, John Wiley & Sons, Inc., Hoboken, New Jersey.

2. B S Grewal; Numerical Methods in Engineering and Science: C, C++, and MATLAB®. ISBN: 978-1-68392-128-8

3. M K Jain, SRK Iyengar, R K Jain; Numerical Methods, New Age International (P) Limited, Publishers, New Delhi

4. S S Shastry; Introductory Methods of Numerical Analysis, Fifth Edition ISBN-978-81-203-4592-8, Asoke K. Ghosh, PHI Learning Pvt. Ltd, M-97, Connaught Circus, New Delhi.

MAL-526: M. Sc. Mathematics (Advanced Numerical Methods)

LESSON No. 3 Written by- Dr. Joginder Singh

NUMERICAL DIFFERENTIATION

STRUCTURE

3.0 LEARNING OBJECTIVES

- This chapter will be devoted to explaining the main concepts of the numerical differentiation of functions.
- Some methods concerning the numerical differentiation of the functions will be established.

3.1 INTRODUCTION

The process, by which we can find the derivative of a function at some assigned value of the independent variable when we are given a set of values of that function, is called "numerical differentiation". The problems of numerical differentiation are solved by first approximating the function by an interpolating formula and then differentiating this formula as many times as desired. In case the values of the argument are equally spaced, and we desire to find the derivatives of the function at a point near the beginning (end) of a set of tabular values, we use Newton Gregory's forward (backward) formula. To find the derivative at a point near the middle of the table, we should use a central different formula. For calculating the derivatives of a function whose argument values are unequally spaced, we should use Newton's divided difference formula to represent the function. While using these formulae, it must be observed that the table of values defines the function at these points only and does not completely define the function hence the function may not be differentiable at all. As such the process of numerical differentiation should be used only if the tabulated values are such that the differences of the same order are constants. Otherwise, errors are bound to creep in which go on to increase as derivatives of higher order are found. This is because the difference between the actual function $f(x)$ and the approximating polynomial $\phi(x)$ may be small at the data points but $f'(x) - \phi'(x)$ maybe large.

3.2 NUMERICAL DIFFERENTIATION

The general method for deriving the numerical differentiation formula is to differentiate the interpolating polynomial. We illustrate the derivation with Newton's forward formula only because the method of derivation about other formulae is the same. Consider the function $y = f(x)$ which is tabulated for the values $x_i (= x_0 + ih)$, i $= 0,1,2,3, \ldots$ n. Then Newton's forward difference formula is given by

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

where $x = x_0 + uh$.

Then

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx} \quad = \frac{1}{h}\frac{d}{du}\left[y_0 + u\Delta y_0 + \frac{u^2-u}{2!}\Delta^2 y_0 + \frac{u^3-3u^2+2u}{3!}\Delta^3 y_0 + \cdots\right.$$

$$= \frac{1}{h}\left[\Delta y_0 + \frac{2u-1}{2!}\Delta^2 y_0 + \frac{3u^2-6u+2}{3!}\Delta^3 y_0 + \cdots\right. \qquad \ldots (3.1)$$

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

$$= \frac{1}{h^2}\left[\Delta^2 y_0 + \frac{6u-6}{3!}\Delta^3 y_0 + \frac{12u^2-36u+22}{4!}\Delta^4 y_0 + \cdots\right. \qquad \ldots (3.2)$$

The formulae (3.1) and (3.2) are used for computing the values of $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ for nontabulated values of x respectively. For tabular values of x, these formulae take simple forms, for by setting $x = x_0$, we obtain $u = 0$ and hence expressions (3.1) and (3.2) give us

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

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \cdots\right]$$

The higher derivates may be computed from the formulae, which can be obtained by successive differentiation. Alternatively, we know that $1 + \Delta = E = e^{hD}$ which implies that

$$D = \frac{1}{h}\log(1+\Delta) = \frac{1}{h}\left[\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \cdots\right]$$

and

$$D^2 = \frac{1}{h^2}\left[\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \cdots\right]^2 = \frac{1}{h^2}\left[\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 + \cdots\right]$$

and so on higher order derivatives formulae can be obtained by applying these identities to y_0. Similarly, different formulae can be derived by interpolation formulae

(a) Newton's backward difference formula

$$\frac{dy}{dx} = \frac{1}{h}\left[\nabla y_n + \frac{2u+1}{2!}\nabla^2 y_n + \frac{3u^2+6u+2}{3!}\nabla^3 y_n + \cdots\right]$$

and

$$\frac{d^2y}{dx^2} = \frac{1}{h^2} = \left[\nabla^2 y_n + \frac{6u+6}{3!}\nabla^3 y_n + \frac{12u^2+36u+22}{4!}\nabla^4 y_n + \cdots\right]$$

for non-tabular values of x, where $x = x_n + uh$. For tabular values, we obtain.

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

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \cdots\right] \qquad \text{... (3.3)}$$

Alternatively, we also know that $1 - \nabla = E^{-1} = e^{-hD}$ which implies that

$$\Rightarrow\ D = -\frac{1}{h}\log(1-\nabla) = \frac{1}{h}\left[\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \cdots\right]$$

and

$$D^2 = \frac{1}{h^2}\left[\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \cdots\right]^2 = \frac{1}{h^2}\left[\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \cdots\right]$$

and so on. Applying these identities to y_n, we get a formula similar to (3.3)

(b) Stirling's formula

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

where $x = x_0 + uh$.

Differentiating, we get

$$\frac{dy}{dx} = \frac{1}{h}\left[\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + u\Delta^2 y_{-1} + \frac{3u^2-1}{3!}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{4u^3-2u}{4!}\Delta^4 y_{-2} + \cdots\right]$$

At $x = x_0, u = 0$, we get

$$\left(\frac{dy}{dx}\right) = \frac{1}{h}\left[\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) - \frac{1}{6}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{1}{30}\left(\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2}\right) + \cdots\right] \qquad \ldots(3.4)$$

Similarly,

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \frac{1}{90}\Delta^6 y_{-3} + \cdots\right] \qquad \ldots(3.5)$$

We can similarly also use other interpolation formulae for computing the derivatives.

Example 3.1 Given that

x:	1.0	1.1	1.2	1.3	1.4	1.5	1.6
y:	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 $x = 1.1$

Solution: The difference table is

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
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		0.000		-0.001
		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						

Here $h = 0.1$ and $x_0 = 1.1$. Therefore at $x = 1.1$ we get.

$$\left[\frac{dy}{dx}\right]_{x=1.1} = \frac{1}{0.1}\left[0.378 - \frac{1}{2}(-0.03) + \frac{1}{3}(0.004) - \frac{1}{4}(0) + \frac{1}{5}(0.001)\right] = 3.946$$

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.1} = \frac{1}{(0.1)^2}\left[-0.03 - (0.004) + \frac{11}{12}(0) - \frac{5}{6}(0.001)\right] = 3.545$$

3.3 ERRORS IN NUMERICAL DIFFERENTIATION

There are two types of errors, viz. Truncation errors and round-off errors, which generally occur in the numerical computation of derivatives. The truncation error is caused by replacing the tabulated function with an interpolation polynomial. This error can usually be estimated by a formula of error estimation in polynomial interpolation. However, the truncation error in any numerical differentiation formula can easily be estimated as below.

Suppose that the tabulated function is such that its differences of a certain order are small and that the tabulated function is well approximated by the polynomial. We consider, for example, Stirling's formula (3.4), which can be written in the form

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{\Delta y_{-1}+\Delta y_0}{2h} + T_1 = \frac{y_1 - y_{-1}}{2h} + T_1$$

…(3.6)

where T_1 the truncation error is given by

$$T_1 = \frac{1}{6h}\left|\frac{\Delta^3 y_{-2}+\Delta^3 y_{-1}}{2}\right| \quad \text{…(3.7)}$$

Similarly, formula (3.5) leads to

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\Delta^2 y_{-1} + T_2$$

where

$$T_2 = \frac{1}{12h^2}|\Delta^4 y_{-2}| \quad \text{…(3.8)}$$

The round-off error, on the other hand, is inversely proportional to h in the case of first-order derivatives and inversely proportional to h^2 in the case of second-order derivatives and so on. Thus the round-off error increases as h decreases. In the case of Stirling's formula (3.6), the roundoff error does not exceed $2 \in/2h = \epsilon/h$, where $\in$ the maximum error in the value is y_i. On the other hand the formula (3.4) viz.

$$\left[\frac{dy}{dx}\right]_{x=0.x_0} = \frac{\Delta y_{-1}+\Delta y_0}{2h} - \frac{\Delta^3 y_{-2}+\Delta^3 y_{-1}}{12h} + \cdots = \frac{y_{-2}-8y_{-1}+8y_1-y_2}{12h} + \cdots \qquad \ldots(3.9)$$

has the maximum rounding error $\frac{18\epsilon}{12h} = \frac{3\epsilon}{2h}$, whereas the formula (3.5)

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{\Delta^2 y-1}{h^2} + \cdots = \frac{y_{-1}-2y_0+y_1}{h^2} + \cdots \qquad \ldots(3.10)$$

has the maximum rounding error $\frac{4\epsilon}{h^2}$. This shows that in the case of higher derivatives, the round-off error in cases is rather rapid.

Example 3.2 Estimate the errors in the values of $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at $x = 1.6$ for the data given

x:	1.0	1.2	1.4	1.6	1.8	2.0	2.2
y:	2.7183	3.3201	4.0552	4.9530	6.0496	7.3891	9.0250

Solution: Form equation (3.7), we have

Truncation error $= \frac{1}{6h}\left|\frac{\Delta^3 y_{-1}-\Delta^3 y_0}{2}\right| = \frac{1}{6(0.2)}\frac{00361+0.0441}{2} = 0.03342.$

Also from equation (3.9), we have

Round-off error $= \frac{3\epsilon}{2h} = \frac{3(0.5)10^{-4}}{2(0.2)} = 0.00038,$

Here $\in < 0.00005 = 0.5 \times 10^{-4}$.

$\therefore$ Total error $= 0.03342 + 0.00038 = 0.0338$

From Stirling's formula (3.6) with first-order differences, we get

$$\left(\frac{dy}{dx}\right)_{x=1.6} = \frac{\Delta y_{-1} + \Delta y_o}{2h} = \frac{0.8978 + 1.0966}{0.4} = \frac{1.9944}{0.4} = 4.9860$$

The exact value is 4.9530 as the tabulated function is e^x so that the error in the above solution is $(4.9.860 - 4.9530) = 0.0330$, which agrees with the total error obtained above. Using (3.10), we obtain

$$\left(\frac{d^2y}{dx^2}\right)_{x=1.6} = \frac{\Delta^2 y - 1}{h^2} = \frac{0.1988}{0.04} = 4.9700$$

so that error $= 4.9700 - 4.9530 = 0.0170.$

Also, the truncation error $= \frac{1}{12h^2}|\Delta^4 y_{-2}| = \frac{1}{12(0.04)}0.0080 = 0.01667$

and the round-off error $= \frac{4\epsilon}{h^2} = \frac{4\times 0.5\times 10^{-4}}{0.04} = 0.0050.$

Hence, total error in $\left(\frac{d^2y}{dx^2}\right)_{x=1.6} = 0.0167 + 0.0050 = 0.0217$

3.4 Maximum and minimum values of a tabulated function

Consider Newton's forward difference formula

$$y = y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{6}\Delta^3 y_0 + \cdots$$

Differentiating with respect to p we get

$$\frac{dy}{dp} = \Delta y_0 + \frac{2p-1}{2}\Delta^2 y_0 + \frac{3p^2 - 6p + 2}{6}\Delta^3 y_0 + \cdots$$

We know that for maxima or minima $\frac{dy}{dp} = 0$. Hence, terminating the right-hand side for simplicity, after the third-order differences and equating it to zero, we obtain

where

$$c_0 + c_1 p + c_2 p^2 = 0 \qquad \text{... (3.11)}$$

$$c_0 = \Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0$$

$$c_1 = \Delta^2 y_0 - \Delta^3 y_0$$

$$c_2 = \frac{1}{2}\Delta^3 y_0$$

The equation (3.11) being a quadratic, can be solved for p and the corresponding values of x are then found from $x = x_0 + ph$, at which y is maximum or minimum.

Example 3.3 Find the minimum values of y from the table

x:	3	4	5	6	7	8
y:	0.205	0.240	0.259	0.262	0.250	0.224

Solution: The difference table is

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5
3	0.205					
		0.035				
4	0.240		-0.016			
		0.019		0.000		
5	0.259		-0.016		0.001	
		0.003		0.001		-0.001
6	0.262		-0.015		0.000	
		-0.012		0.001		
7	0.250		-0.014			
		-0.026				
8	0.224					

Taking $x_0 = 3$ and $h = 1$, Newton's forward difference formula gives us

$$y = 0.205 + p(0.035) + \frac{p(p-1)}{2}(-0.016) \qquad \ldots(3.12)$$

Differentiating this with respect to p, we get

$$\frac{dy}{dp} = 0.035 + \frac{2p-1}{2}(-0.016)$$

For y to be minimum, $\frac{dy}{dp} = 0$, which implies that $p = 2.6875$

$\therefore\ x = x_0 + ph = 3 + 2.6875(1) = 5.6875$

Using the values in equation (3.12) we get

$$y_{\min} = 0.205 + 2.6875(0.035) + \frac{1}{2}(2.6875)(1.6875)(-0.016) = 0.2628$$

Example 3.4 Find the maximum value of $f(x)$ in the range of x from the following table of values

x:	60	75	90	105	120
$f(x)$:	28.2	38.2	43.2	40.9	37.7

Solution: The difference table is

x	$y = f(x)$	Δ	Δ^2	Δ^3	Δ^4
60	28.2				
		10.0			
75	38.2		-5.0		
		5.0		-2.3	
90	43.2		-7.3		8.7
		-2.3		6.4	
105	40.9		-0.9		
		-3.2			
120	37.7				

From Stirling's formula, we have

$$y = f(x) = y_0 + \frac{p}{1!}\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + \frac{p^2}{2!}\Delta^2 y_{-1} + \frac{p(p^2-1)}{3!}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{p^2(p^2-1)}{4!}\Delta^4 y_{-2} + \cdots \quad \ldots(3.13)$$

where $x = x_0 + ph$ and $y_0 = f(x_0), x_0 = 90$ and $h = 15$.

Therefore, we have

$$\frac{dy}{dx} = \frac{dy}{dp} \cdot \frac{dp}{dx} = \frac{1}{h}\frac{dy}{dp}$$

To have $y = f(x)$ maximum, we solve the equation

$$\frac{dy}{dx} = f'(x) = 0 \Rightarrow \frac{dy}{dp} = 0 \Rightarrow f'(p) = 0.$$

i.e.

$$\frac{\Delta y_0 + \Delta y_{-1}}{2} + \frac{2p}{2!}\Delta^2 y_{-1} + \frac{3p^2 - 1}{3!}\frac{\Delta^3 y_{-1} + \Delta^3 y - 2}{2} + \frac{4p3 - 24}{4!}\Delta^4 y_{-2} = 0$$
$$17.4p^3 + 12.3p^2 - 96.3p + 12.10 = 0$$

Solving this equation by the Newton-Raphson method, we have $p = 0.128126$

$\therefore\ x = 90 + 15p = 90 + 15(0.128126) = 91.92189$

Using these values of x and p in (3.13), we get

$$y_{\max} = f(91.92189) = 43.2641$$

which is the required maximum value of $f(x)$.

Example 3.5 From the following table find the maximum value of y correct to two decimal places

x:	1,2	1.3	1.4	1.5	1.6
y:	0.9320	0.9636	0.9855	0.9975	0.9996

Solution: The difference table is

x	y	Δ	Δ^2	Δ^3	Δ^4
1.2	0.9320				
		0.0316			
1.3	0.9636		−0.0097		
		0.0219		−0.0002	
1.4	0.9855		−0.0099		0.0002
		0.0120		0.0000	
1.5	0.9975		−0.0099		
		0.0021			
1.6	0.9996				

Let $x_0 = 1.2$. Thus from Newton's forward difference formula, we have

$$0 = 0.0316 + \frac{2p-1}{2}(-0.0097)$$

$\Rightarrow\ p = 3.8$

$\therefore\ x = x_0 + ph = 1.2 + (3.8)(0.1) = 1.58$

For this values of x, Newton's backward difference formula at $x_n = 1.6$, gives us

$$\begin{aligned} y(1.58) &= 0.9996 - 0.2(0.0021) + \frac{-0.2(-0.2+1)}{2}(-0.0099) \\ &= 0.9996 - 0.0004 + 0.0008 = 1.0 \end{aligned}$$

which is the required maximum value.

3.5 CHECK YOUR PROGRESS

1. Given that

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

find $\frac{dy}{dx}$ dx and $\frac{d^2y}{dx^2}$ at (a) x = 1.1 (b) x = 1.6.

2. Find the value of cos (1.74) from the following table:

X	1.7	1.74	1.78	1.82	1.86
Sin x	0.9916	0.9857	0.9781	0.9691	0.9584

3. A slider in a machine moves along a fixed straight rod. Its distance x cm. along the rod is given below for various values of the time t seconds. Find the velocity of the slider and its acceleration when t = 0.3 seconds.

t:	0	0.1	0.2	0.3	0.4	0.5	0.6
x:	30.13	31.62	32.87	3364	33.95	33.81	33.24

4. The elevation above a datum line of seven points of a road is given below:

x:	0	300	600	900	1200	1500	1800
y:	135	149	157	183	201	205	193

Find the gradient of the road at the middle point.

5. From the table below, for what value of x, y is minimum? Also, find this value of y.

x:	3	4	5	6	7	8
y:	0.205	0.240	0.259	0.262	0.250	0.224

3.6 SUMMARY

- The students are made familiar with some preliminary definitions and fundamental results of numerical differentiation of various functions.
- Application of the numerical differentiation of the functions has been developed.

- Lastly, maxima-minima and partial differentiation of the function have been explained in detail.

3.7 KEYWORDS

Numerical Differentiation, maxima-minima of tabulated function, Optimum choice of step Length, partial differentiation, Methods Based on Undetermined Coefficients.

3.8 SELF-ASSESSMENT TEST

1. Find the first, second, and third derivatives of f(x) at x = 1.5 if

X	1.5	2.0	2.5	3.0	3.5	4.0
f(x)	3.375	7.000	13.625	24.000	38.875	59.000

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(x)	0.000	0.128	0.544	1.296	2.432	4.000

3. Given the following table of values of x and y

X	1.00	1.05	1.10	1.15	1.20	1.25	1.30
Y	1.000	1.025	1.049	1.072	1.095	1.118	1.140

find dy/dx and d^2y/dx^2 at (a) x = 1.05. (b) x = 1.25 (c) x = 1.15.

4. For the following values of x and y, find the first derivative at x = 4.

X	1	2	4	8	10
Y	0	1	5	21	27

5. Find the derivative of f(x) at x = 0.4 from the following table:

X	0.1	0.2	0.3	0.4
f(x)	1.10517	1.22140	1.34986	1.49182

6. From the following table, find the values of dy/dx and 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

7. Using the following data, find x for which y is the minimum and find this value of y.

x:	0.60	0.65	0.70	0.75
y:	0.6221	0.6155	0.6138	0.6170

8. Find the value of x for which f (x) is maximum, using the table

x:	9	10	11	12	13	14
f (x):	1330	1340	1320	1250	1120	930

Also, find the maximum value of f (x).

3.9 ANSWERS TO CHECK YOUR PROGRESS

1. 3.952, -3.74 (ii) 2.75, -0.715
2. 0.175
3. The required velocity is 5.33 cm/sec and acceleration is – 45.6 cm/sec^2.
4. The gradient of the road at the middle point is 0.085.
5. y is minimum when x = 5.6875, y = 0.2628

3.10 REFERENCES/ SUGGESTED READINGS

1. JAMES F. EPPERSON; An Introduction to Numerical Methods and analysis. Second Edition Mathematical Reviews, John Wiley & Sons, Inc., Hoboken, New Jersey.

2. B S Grewal; Numerical Methods in Engineering and Science: C, C++, and MATLAB®. ISBN: 978-1-68392-128-8

3. M K Jain, SRK Iyengar, R K Jain; Numerical Methods, New Age International (P) Limited, Publishers, New Delhi

4. S S Shastry; Introductory Methods of Numerical Analysis, Fifth Edition ISBN-978-81-203-4592-8, Asoke K. Ghosh, PHI Learning Pvt. Ltd, M-97, Connaught Circus, New Delhi.

MAL-526: M. Sc. Mathematics (Advanced Numerical Methods)

LESSON No. 4 **Written by- Dr. Joginder Singh**

NUMERICAL INTEGRATION

STRUCTURE

4.0 LEARNING OBJECTIVES

- This chapter will be devoted to explaining the main concepts of the numerical integration of functions.
- Some methods concerning the numerical integration of the functions will be established.

4.1 INTRODUCTION

Numerical integration is primary tool used by engineers and scientists to obtain approximate answers for definite integrals that cannot be solved analytically. The process of evaluating a definite integral from a set of tabulated values of the integrand $y = f(x)$ is called numerical integration. The general problem of numerical integration may be stated as follows:

Given a set of data points $(x_i, y_i), i = 0,1,2,3, \dots$ n of a function $y = f(x)$, where $f(x)$ is not known explicitly, it is required to compute the value of the definite integral

$$I = \int_a^b y dx \qquad \dots(4.1)$$

As in the case of numerical differentiation, we here again replace $y = f(x)$, by an interpolating polynomial $\phi(x)$ in order to obtain an approximate value of the definite integral. Thus different integration formulae can be obtained depending upon the type of the interpolation formula used. Here we derive a general formula for numerical integration by using Newton's forward difference formula. Let the interval $[a, b]$ be divided into n - equal subintervals such that

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b, \text{ with } x_n = x_0 + nh, h = \frac{b-a}{n}$$

Hence, the integral (4.1) becomes

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

Using Newton's forward difference formula, we get

$$I \quad = \int_{x_0}^{x_n} \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \right] dx, \text{ where } x = x_0 + ph.$$

$$= h\int_0^n \left(y_0 + p\Delta y_0 + \frac{p^2-p}{2}\Delta^2 y_0 + \frac{p^3-3p^2+2p}{6}\Delta^3 y_0 + \cdots \right) dp$$

Therefore, on simplification, we have

$$I = \int_{x_0}^{x_n} y dx = nh\left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_o + \frac{n(n-2)^2}{24}\Delta^3 y_o + \cdots \right] \qquad \ldots(4.2)$$

From the general formula (4.2), we can find different integration formulae by putting $n = 1,2,$ 3... etc. This formula is also knows as Newton's -cotes closed quadrature formula.

4.2.0 TRAPEZOIDAL RULE

Putting $n = 1$ in (4.2) and taking the curve $y = f(x)$ through the points (x_0, y_0) and (x_1, y_1) as a straight line i.e. a polynomial of first degree so that differences of order higher than first become zero, we get

$$1_1 = \int_{x_0}^{x_1} y dx = h\left[y_0 + \frac{1}{2}\Delta y_0 \right] = h\left[y_0 + \frac{1}{2}(y_1 - y_0) \right] = \frac{h}{2}(y_0 + y_1)$$

Similarly, $I_2 = \int_{x_1}^{x_2} y dx = \frac{h}{2}(y_1 + y_2)$

$$I_3 = \int_{x_2}^{x_3} y dx = \frac{h}{2}(y_2 + y_3)$$

and so on. In general, we get

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

Adding all these expressions and using interval additive property of the definite integrals, we obtain.

$$I = \sum_{i=1}^{n} I_i = \int_{x_0}^{x_n} y dx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + y_3 + \cdots + y_{n-1}) + y_n] = \frac{h}{2}(X + 2I)$$

where X = sum of end ordinates, I = sum of intermediate ordinates. This expression is known as the trapezoidal rule. Geometrically this rule signifies that the curve $y = f(x)$ is replaced by n straight lines joining the points $(x_i, y_i), i = 0,1,2,3, \dots n$. The area bounded by the curve $y = f(x)$ the ordinates $x = x_0, x = x_n$, and the x-axis is then approximately equivalent to the sum of the areas of the n-trapeziums so obtained.

4.2.1 SIMPSON'S 1/3 RULE

Putting $n = 2$ in (4.2) and taking the curve through the points $(x_0, y_0), (x_1, y_1)$ and (x_2, y_2) as a parabola i.e. a polynomial of second degree so that differences of order higher than second vanish, we get

$$I_1 = \int_{x_0}^{x_2} y dx = 2h\left(y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0\right) = \frac{h}{3}(y_0 + 4y_1 + y_2)$$

Similarly, $I_2 = \int_{x_2}^{x4} y dx = \frac{h}{3}(y_2 + 4y_3 + y_4)$

$$I_3 = \int_{x_4}^{x_6} y dx = \frac{h}{3}(y_4 + 4y_5 + y_6)$$

and so on. In general, we have

$$I_n = \int_{x_{2n-2}}^{x_{2n}} y dx = \frac{h}{3}(y_{2n-2} + 4y_{2n-1} + y_{2n})$$

Summing up these integrals, we get

$$\begin{aligned} I = \int_{x_0}^{x_n} y dx \quad &= \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5 + \cdots y_{2n-1}) + 2(y_2 + y_4 + y_6 + \cdots y_{2n-2}) + y_{2n}] \\ &= \frac{h}{3}(X + 4O + 2E) \end{aligned}$$

where X = sum of end ordinates, O = sum of odd ordinates and E = sum of even ordinates.

This expression is known as Simpson's 1/3-rule, or simply Simpson's rule and is most commonly used. It is observed that this rule requires the whole range i.e. the given interval must be divided into even number of equal sub-intervals, since we find the area of two strips at a time.

4.2.2 SIMPSON'S $3/8$ RULE

Setting $n = 3$ in (4.2) above and taking the curve through $(x_i, y_i), i = 0,1,2,3$ as a polynomial of degree three so that the differences higher than the third order vanish, we get

$$I_1 = \int_{x_0}^{x_3} y dx = 3h\left(y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{2}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0\right) = \frac{3}{8}h(y_0 + 3y_1 + 3y_2 + y_3)$$

Similarly,

$$I_2 = \int_{x3}^{x_6} y dx = \frac{3}{8}h(y_3 + 3y_4 + 3y_5 + y_6)$$
$$I_3 = \int_{x_6}^{x_9} y dx = \frac{3}{8}h(y_6 + 3y_7 + 3y_8 + y_9)$$

and so on. In general, we have

$$I_n = \int_{x_{3n-3}}^{x_{3n}} y dx = \frac{3}{8}h(y_{3n-3} + 3y_{3n-2} + 3y_{3n-1} + y_{3n})$$

Summing up all these expressions, we get

$$I = \int_{x_0}^{x_{3n}} y dx = \frac{3}{8}h \quad [y_0 + 3(y_1 + y_2 + y_4 + y_5 + y_7 + y_8 + \cdots + y_{3n-2} + y_{3n-1})$$
$$+2(y_3 + y_6 + y_9 + \cdots + y_{3n-3}) + y_{3n}]$$

This expression is known as Simpson's $3/8$ rule. It is noticed that in order to apply this formula the number of sub-intervals should be taken as multiples of 3. This rule is not as accurate as Simpson 1/3 rule, the dominant term in the error of this formula being $\frac{-3}{80}h^5 y^{iv}(\bar{x})$

4.2.3 BOOLE'S RULE

Putting $n = 4$ in (4.2) above and taking the curve through $(x_i, y_i), i = 0,1,2,3,4$ as a polynomial of degree 4 , so that the difference of order higher than four are neglected, we get

$$\int_{x_0}^{x_4} ydx \quad = 4h\left(y_0 + 2\Delta y_0 + \frac{5}{3}\Delta^2 y_0 + \frac{2}{3}\Delta^3 y_0 + \frac{7}{90}\Delta^4 y_0\right)$$
$$= \frac{2h}{45}(7y_0 + 32y_1 + 12y_2 + 32y_3 + 7y_4)$$

Similarly, $\int_{x_4}^{x_8} ydx = \frac{2h}{45}(7y_4 + 32y_5 + 12y_6 + 32y_7 + 7y_8)$ and so on.

Adding all these integrals from x_0 to x_n, where n is a multiple of 4 , we get

$$I = \int_{x_0}^{x_n} ydx = \frac{2h}{45}[7y_0 \quad +32(y_1 + y_3 + y_5 + y_7 + \cdots) + 12(y_2 + y_6 + y_{10} + \cdots)$$
$$+14(y_4 + y_8 + y_{12} + \cdots) + 7y_n]$$

This expression is known as Boole's rule. While applying this result the number of subintervals should be taken as a multiple of 4. The leading term in the error of formula can be shown as $\frac{-8h^7}{945} y(\bar{x})$.

4.2.4 WEDDLE'S RULE

Putting $n = 6$ in (4.2) above and taking the curve $y = f(x)$ through the points $(x_i, y_i), i = 0,1,$ 2,3,4,5,6 as a polynomial of degree six so that the differences of order higher than six are neglected, we obtain.

$$\int_{x_0}^{x_6} ydx = 6h\left(y_0 + 3\Delta y_0 + \frac{9}{2}\Delta^2 y_0 + 4\Delta^3 y_0 + \frac{123}{60}\Delta^4 y_0 + \frac{11}{20}\Delta^5 y_0 + \frac{41}{840}\Delta^6 y_0\right)$$

$$= \frac{3h}{10}[y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + y_6],$$

since if we replace $\frac{41}{140}\Delta^6 y_0$ by $\frac{3}{10}\Delta^6 y_0$, the error made will be negligible.

Similarly,

$$\int_{x_6}^{x_{12}} ydx = \frac{3h}{10}(y_6 + 5y_7 + y_8 + 6y_9 + y_{10} + 5y_{11} + y_{12}) \text{ and so on.}$$

Adding these integrals from x_0 to x_n, where x is a multiple of 6 , we get

$$\int_{x_0}^{x_n} ydx = \frac{3h}{10}[y_0 + 5(y_1 + y_5 + y_7 + y_{11} + \cdots) + (y_2 + y_4 + y_8 + y_{10} + \cdots)$$
$$+6(y_3 + y_9 + y_{15} + \cdots) + 2(y_6 + y_{12} + y_{18} + \cdots) + y_n]$$

This expression is known as Weddle's rule. It is generally, more accurate than any of the other rules and the error in this is given by $\frac{-h^7}{140}y^{vi}(\bar{x})$. While applying this result the number of subintervals should be taken as multiply of 6.

Example 4.1 Evaluate $\int_0^6 \frac{dx}{1+x^2}$ by using (i) Trapezoidal rule, (ii) Simpson's $1/3$ rule, (iii) Simpson's rule and (iv) Weddle's rule and command the result the results

Solution: We divide the interval (0,6) into six parts with $h = 1$. The values of x and $y = \frac{1}{1+x^2}$ are given by

x:	0	1	2	3	4	5	6
y:	1	0.5	0.2	0.1	0.0588	0.0385	0.027

(i) Trapezoidal rule

$$I = \int_0^6 \frac{dx}{1+x^2} = \frac{1}{2}[(1 + 0.027) + 2(.5 + .2 + .1 + 0588 + .0385)] = 1.4108$$

(ii) Simpson's $1/3$ rule

$$I = \int_0^6 \frac{dx}{1+x^2} = \frac{1}{3}[(1 + .027) + 4(0.5 + 0.1 + 0.0385) + 2(0.2 + 0.0588)] = 1.3662$$

(iii) Simpson's $3/8$ rule

$$I = \int_0^6 \frac{dx}{1+x^2} = \frac{3}{8}[(1 + 0.027) + 3(0.5 + 0.2 + .0.0588 + 0.0385) + 2(0.1)] = 1.3571$$

(iv) Weddle's rule

$$I = \int_0^6 \frac{dx}{1+x^2} = \frac{3}{10}[1 + 5(0.5) + 0.2 + 6(0.1) + 0.0588 + 5(0.0385) + 0.027] = 1.3735$$

Also $I = \int_0^6 \frac{dx}{1+x^2} = |\tan^{-1} x|_0^6 = \tan^{-1} 6 = 1.4056$

This shows that the values of the integral found by Weddle's rule is the nearest to the actual value followed by Simpson's $1/3$ rule.

Example 4.2 A solid of revolution is formed by rotating about the x-axis, the area between the lines $x = 0$ and $x = 1$ and a curve through the points with following coordinates.

x:	0.00	0.25	0.50	0.75	1.00
y:	1.0000	0.9896	0.9589	0.9089	0.8415

Estimate the volume of the solid formed by using Simpson's $\frac{1}{3}$ rule.

Solution: Here $h = 0.25$, $y_0 = 1$, $y_1 = 0.9896 y_2 = .09589$, $y_3 = 0.9089$ and $y_4 = 0.8415$. Therefore, the required volume of the solid generated, by Simpson's rule is given by

$$\begin{aligned} V &= \int_0^1 \pi y^2 dx = \frac{\pi h}{3}[(y_0^2 + y_4^2) + 4(y_1^2 + y_3^2) + 2y_2^2] \\ &= \frac{0.25\pi}{3}[\{1 + (0.8415)^2\} + 4\{(0.9896)^2 + (0.9089)^2\} + 2(0.9589)^2] \\ &= \frac{0.25(3.1416)}{3}[1.7081 + 7.2216 + 1.839] = 2.8192 \end{aligned}$$

which is the required volume.

4.3 ROMBERG INTEGRATION

Romberg's method provides a simple modification to the approximate quadrature formula derived with the help if finite differences method in order to find their better approximations. As an illustration, we improve upon the value of the integral

$$I = \int_a^b y dx = \int_a^b f(x) dx \qquad \ldots(4.3)$$

by trapezoidal rule. We evaluate (4.3) by trapezoidal rule with two different widths h_1 and h_2 to obtain the approximate values I_1 and I_2 respectively. The corresponding errors E_1 and E_2 are then given by

$$E_1 = -\frac{(b-a)h_1^2}{12} y''(\bar{x}), E_2 = -\frac{(b-a)h_2^2}{12} y''(\bar{\bar{x}})$$

Since $y''(\bar{\bar{x}})$ is also the largest value of $y''(x)$, so it is reasonable to assume that the quantities $y''(\bar{x})$ and $y''(\bar{\bar{x}})$ are very nearly equal. Therefore we have

$$\frac{E_1}{E_2} = \frac{h_1^2}{h_2^2} \Rightarrow \frac{E_2}{E_2 - E_1} = \frac{h_2{}^2}{h_2^2 - h_1^2} \qquad \ldots(4.4)$$

Now since $I = I_1 - E_1 = I_2 - E_2$, therefore

$$E_2 - E_1 = I_2 - I_1 \qquad \ldots(4.5)$$

From (4.4) and (4.5), we have

$$E_2 = \frac{h_2^2}{h_2^2 - h_1^2}(E_2 - E_1) = \frac{h_2^2}{h_2^2 - h_1{}^2}(I_2 - I_1)$$

$$I_3 = I_2 - E_2 = \frac{I_1 h_2{}^2 - I_2 h_1{}^2}{h_2{}^2 - h_1{}^2} \qquad \ldots(4.6)$$

which is a better approximation of I. In order to evaluate I systematically, we take $h_1 = h$ and $h_2 = \frac{1}{2}h$ so that (4.6) gives

$$I = \frac{I_1 \frac{h^2}{4} - I_2 h^2}{\frac{h^2}{4} - h^2} = \frac{4I_2 - I_1}{3}$$

$$\text{i.e. } I\left(h, \frac{h}{2}\right) = \frac{4\mathrm{I}\left(\frac{h}{2}\right) - \mathrm{I}(h)}{3} \qquad \ldots(4.7)$$

Now we use the trapezoidal rule several times successively halving h and apply (4.7) to each pair of values as per the following scheme.

$$
\begin{array}{llll}
I(h) & & & \\
I\left(\frac{h}{2}\right) & I\left(h,\frac{h}{2},\frac{h}{4}\right) & & \\
I\left(\frac{h}{4}\right) & I\left(\frac{h}{2},\frac{h}{4}\right) & I\left(h,\frac{h}{2},\frac{h}{4},\frac{h}{8}\right) & \\
I\left(\frac{h}{8}\right) & I\left(\frac{h}{4},\frac{h}{8}\right) & & \\
I\left(\frac{h}{8}\right) & & &
\end{array}
$$

The computation is continued till successive values are close to each other. This method, due to L.F. Richardson, is called the deferred approach to the limit and the systematic tabulation of this is called Romberg integration.

Example 4.3 Use Romberg's method to compute $\int_0^1 \frac{dx}{1+x^2}$, correct to 4 decimal places, by taking $h = 0.5, 0.25$ and 0.125.

Solution: We evaluate the given integral by using trapezoidal rule

(i) When h $= 0.5$, we have

$$
\begin{array}{llll}
x: & 0 & 0.5 & 1.0 \\
y = \dfrac{1}{1+x^2}: & 1 & 0.8 & 0.5
\end{array}
$$

$$I = \int_0^1 \frac{dx}{1+x^2} = \frac{.5}{2}[1 + 2(.8) + 0.5] = 0.775 \text{ by Trapezoidal rule}$$

(ii) When h $= 0.25$, the values of x and y are

(iii)

$$
\begin{array}{llllll}
x: & 0 & 0.25 & 0.5 & 0.75 & 1.0 \\
y = \dfrac{1}{1+x^2}: & 1 & 0.9412 & 0.8 & 0.64 & 0.5
\end{array}
$$

Therefore by trapezoidal rule, we have

$$I = \int_0^1 \frac{dx}{1+x^2} = \frac{.25}{2}[1 + 2(0.9412 + 0.8 + 0.64) + 0.5] = 0.7828$$

(iv) When $h = 0.125$, we find that $I = 0.7848$. Now using formula (4.7) we obtain the table of values as

$$\begin{array}{llll}
0.5 & 0.775 & & \\
 & & 0.7854 & \\
0.25 & 0.7828 & & 0.7855 \\
 & & 0.7855 & \\
0.125 & 0.7848 & &
\end{array}$$

Hence the value of the integral is 0.7855.

Example 4.4 Use Romberg's method to compute $I = \int_0^1 \frac{dx}{1+x}$, correct to three decimal places.

Solution: We take $h = 0.5, 0.25$ and 0.125 and use trapezoidal rule successively to obtain.

$$I(h) = I(0.5) = 0.7084, I\left(\frac{h}{2}\right) = I(0.25) = 0.6970$$

and

$$I\left(\frac{h}{4}\right) = I(0.125) = 0.6941$$

Now using formula (4.7) we obtain

$$\begin{aligned}
I\left(h, \frac{h}{2}\right) &= \frac{4(0.6970) - 0.7084}{3} = 0.6932 \\
I\left(h, \frac{h}{2}, \frac{h}{4}\right) &= \frac{4(0.6941) - 0.6970}{3} = 0.6931 \\
I\left(\frac{h}{2}, \frac{h}{4}\right) &= \frac{4(0.6931) - 0.6932}{3} = 0.6931
\end{aligned}$$

The table of values is therefore

$$\begin{array}{llll}
0.5 & 0.7084 & & \\
 & & 0.6932 & \\
0.25 & 0.6970 & & 0.6931 \\
0.125 & 0.6941 & & \\
06931 & & &
\end{array}$$

Hence the value of the given integral is 0.6931

4.4 GAUSSIAN INTEGRATION

Consider the integral

$$I = \int_a^b y dx = \int_a^b f(x) dx \qquad \ldots (4.8)$$

Setting $x = \frac{1}{2}u(b-a) + \frac{1}{2}(a+b)$ the integral (4.8) takes the form

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

Gauss derived a formula, which uses the same number of function values, but with different spacing in contrast to other integration formulae, which require values of the function at equally spaced points of the interval and it gives better accuracy. This formula is expressed in the form

$$\int_{-1}^{1} F(u) du = W_1 F(u_1) + W_2 F(u_2) W_3 F(u_3) + \cdots + W_n F(u_n) = \sum_{i=1}^{n} W_i F(u_i) \qquad \ldots (4.9)$$

where W_i and u_i are called the weights and abscissas respectively, which are symmetrical with respect to the middle points of the interval. The weights and abscissa can be determined such that the formula is exact when $F(u)$ is a polynomial of degree not exceeding $2n-1$ as there are total $2n$ arbitrary constants. Hence we have

$$F(u) = c_0 + c_1 u + c_2 u^2 + c_3 u^3 + \cdots + c_{2n-1} u^{2n-1} \qquad \ldots (4.10)$$

Then from (4.9) we have

$$\int_{-1}^{1} F(u) du = \int_{-1}^{1} [c_0 + c_1 u + c_2 u^2 + c_3 u^3 + \cdots + c_{2n-1} u^{2n-1}] du = 2c_0 + \frac{2}{3}c_2 + \frac{2}{5}c_4 + \cdots \qquad \ldots (4.11)$$

Now (4.10) implies that $F(u_i) = \vec{c}_0 + c_1 u_i + c_2 u_i^3 + \cdots + c_{2n-1} u_i^{2n-1}$ so that from (5.7.3) we have

$$\int_{-1}^{1} F(u)du = \int_{-1}^{1} F(u)du = w_1(c_0 + c_1u_1 + c_2u_1^2 + \cdots + c_{2n-1}u_1^{2n-1})$$
$$+w_2(c_0 + c_1u_2 + c_2u_2^2 + \cdots + c_{2n-1}u_1^{2n-1})$$
$$+w_3(c_0 + c_1u_3 + c_2u_3^2 + \cdots + c_{2n-1}u_3^{2n-1})$$
$$+\cdots + w_n(c_0 + c_1u_n + c_2 + \cdots + c_{2n-1}u_n^{2n-1}) \quad \ldots (4.12)$$

Therefore, we get

$$\int_{-1}^{1} F(u)du = c_0(w_1 + w_2 + \cdots + w_n) + c_1(w_1u_1 + w_2u_2 + \cdots w_nu_n)$$
$$+c_2(w_1u_1^2 + w_2u_2^2 + \cdots + w_nu_n^2)$$
$$+\cdots + c_{2n-1}(w_1u_1^{2n-1} + w_2u_1^{2n-1} + \cdots + w_nu_n^{2n-1}) \quad \ldots (4.13)$$

Now comparing expressions (4.11) and (4.13) we get

$$\left.\begin{array}{l} w_1 + w_2 + w_3 + \cdots + w_n = 2 \\ w_1u_1 + w_2u_2 + w_3u_3 + \cdots + w_nu_n = 0 \\ w_1u_1^2 + w_2u_2^2 + w_3^2 + \cdots + w_nu_n^2 = 2/3 \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ w_1u_1^{2n-1} + w_2u_2^{2n-1} + w_3u_3^{2n-1} + \cdots + w_nu_n^{2n-1} = 0 \end{array}\right\} \quad \ldots (4.14)$$

a system of $2n$ equations in $2n$ unknowns w_i and $u_i, (i = 1,2,3, \ldots, n)$.

In order to illustrate, we take $n = 2$. Then the formula is

$$\int_{-1}^{1} F(u)du = w_1F(u_1) + w_2F(u_2) \quad \ldots (4.15)$$

This formula is exact when $F(u)$ a polynomial of degree not exceeding 3 is, we put successively

$F(u) = 1, u, u^2$ and u^3 Then (4.15) provides us

$$\left.\begin{array}{l} w_1 + w_2 = 2 \\ w_1u_1 + w_2u_2 = 0 \\ w_1u_1^2 + w_2u_2^2 = 2/3 \\ w_1u_1^3 + w_2u_2^3 = 0 \end{array}\right\} \quad \ldots (4.16)$$

This system of equations gives us

$$w_1 = w_2 = 1, \mathrm{u}_2 = -u_1 = 1/\sqrt{3}$$

This method when applied to the general system (4.14) above will be extremely complicated difficult and an alternative method must be chosen to solve the non-linear system (4.14). It can be shown that u_i are the zeros of the $(n+1)$ Legendre polynomial $P_{n+1}(u)$, which can be generated by using the recurrence relation

$$(n+1)P_{n+1}(u) = (2n+1)uP_n(u) - nP_{n-1}(u)$$

where $P_0(u) = 1$ and $P_1(u) = u$. The first five Legendre polynomials are given by

$$P_0(u) = 1, P_1(u) = u, P_2(u) = \frac{1}{2}(3u^2 - 1)$$

$$P_0(u) = 1, P_1(u) = u, P_2(u) = \frac{1}{2}(3u^2 - 1), P_3(u) = \frac{1}{2}(5u^3 - 3u),$$
$$P_4(u) = \frac{1}{8}(35u^4 - 30u^2 + 3)$$

It can also be shown that the corresponding weights w_i are given by

$$w_{\mathrm{i}} = \int_{-1}^{1} \prod_{\substack{j=0 \\ j\neq i}}^{n} \left(\frac{u-u_j}{u_i-u_j}\right) du \qquad \dots (4.17)$$

where $u_i\,'s$ are the abscissas. For example when $n = 1$ we solved $P_2(u) = 0$ i.e., $\frac{1}{2}(3u^2 - 1) = 0$ which implies that $u_0 = -\frac{1}{\sqrt{3}} = -\sqrt{3}/3$ and $u_1\,\frac{1}{\sqrt{3}} = \sqrt{3}/3$

The corresponding weights are given by

$$w_0 = \int_{-1}^{1} \frac{u-u_1}{u_0-u_1} du = \frac{1}{u_0-u_1'}\left[\frac{u^2}{2} - u_1 u\right]_{-1}^{1} = 1$$
$$w_1 = \int_{-1}^{1} \frac{u-u_0}{u_1-u_0} du = \frac{1}{u_1-u_0}\left[\frac{u^2}{2} - u_0 u\right]_{-1}^{1} = 1$$

Similarly, for $n = 3$ we solve $P_4(u) = 0$ i.e. $\frac{1}{8}(35u^4 - 30u^2 + 3) = 0$

which implies that $u_i = \pm\left[\frac{15\pm2\sqrt{30}}{35}\right]^{1/2}$ The weights w_i can then be found from (4.17).

Example 4.5 Evaluate $I = \int_0^1 x dx$, by Gauss's formula

Solution: Put $x = \frac{1}{2}(u+1)$, we get $I = \frac{1}{4}\int_{-1}^{1}(u+1)du = \frac{1}{4}\sum_{i=1}^{n} W_i F(u_i)$ where $F(u_i) = u_i + 1$. For simplicity, we take $n = 4$, we obtain

$$I = \frac{1}{4}[(-0.86114+1)(0.34785) + (-0.33998+1)(0.65214) + (0.33998+1)(0.65214) + (0.86114+1)(0.34785)] = 0.49999 \ldots$$

where the abscissae and weights have been rounded to five decimal places.

4.5 EULER-MACLAURINS FORMULA

We consider $\Delta f(x) = g(x)$ and define inverse operator Δ^{-1} as

$$f(x) = \Delta^{-1} g(x)$$

Now

$$\begin{aligned} &f(x_1) - f(x_0) = \Delta f(x_0) = g(x_0) \\ &f(x_2) - f(x_1) = g(x_1) \\ &f(x_3) - f(x_2) = g(x_2) \\ &\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\ &f(x_n) - f(x_{n-1}) = g(x_{n-1}) \end{aligned}$$

On addition these lead to

$$f(x_n) - f(x_0) = \sum_{i=0}^{n-1} g(x_i) \qquad \ldots (4.18)$$

where $x_i = i = 0,1,2, \ldots n$ are $(n+1)$ equally spaced values such that $x_i = x_0 + ih$.

Now, we have

$$f(x) = \Delta^{-1} g(x) = (E+1)^{-1} g(x) = (e^{hD} - 1)^{-1} g(x), \forall: E = e^{hD}]$$
$$= \left[\left(1 + hD + \frac{h^2D^2}{2!} + \frac{h^3D^3}{3!} + \cdots\right) - 1\right]^{-1} g(x)$$
$$= \frac{1}{h} D^{-1} \left[1 - \frac{hD}{2} + \frac{h^2D^2}{12} - \frac{h^4D^4}{720} + \cdots\right] g(x)$$
$$= \frac{1}{h}\int \; g(x)dx - \frac{1}{2} g(x)dx + \frac{h}{12} g'(x) - \frac{h^3}{720} g''(x) + \cdots \qquad \ldots (4.19)$$

Upon putting $x = x_n$ and $\text{x} = x_0$ in (4.19) and then subtracting, we get

$$f(x_n) - f(x_0) = \frac{1}{h}\int_{x_0}^{x_n} g(x)dx - \frac{1}{2}[g(x_n) - g(x_0)] + \frac{h}{12}[g'(x_n) - g'(x_0)]$$
$$- \frac{h^3}{720}[g''(x_n) - g''(x_0)] + \cdots \qquad \ldots (4.20)$$

Now (4.18) and (4.20) provide us

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

which implies that

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

$$= \frac{1}{2}\{g(x_0) + 2[g(x_1) + g(x_2) + \cdots g(x_{n-1})] + g(x_n)\} - \frac{h}{12}[g'(x_n) - g'(x_0)]$$
$$+ \frac{h^3}{720}[g^{m\prime}(x_n) - g^m(x_0)]$$

Hence

$$\int_{x_0}^{x_n} ydx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + y_3 + \cdots + y_{n-1}) + y_n] - \frac{h^2}{12}(y_n' - y_0')$$
$$+ \frac{h^4}{720}(y_n'' - y_0^m) \qquad \ldots (4.21)$$

where $y = g(x)$ and $x_n = x_0 nh$.

This is called Euler-Maclaurins formula. The first term on the right hand side of (4.21) represents the approximate value of the integral obtained from trapezoidal rule and other terms denote the successive corrections to this value. This formula is often used to find the sum of series of the form

$$y(x_0) + y(x_1) + y(x_2) + y(x_3) + \cdots + y(x_n) + .. \text{ where } x_i = x_0 + ih.$$

Example 4.6 Use Euler-Maclaurins formula to find the value of $\log_e^2$ from $\int_0^1 \frac{dx}{1+x}$.

Solution: Here we take $y = \frac{1}{1+x}, x_0 = 0, \mathrm{n} = 10, \mathrm{h} = 0.1$ so that

$$y' = \frac{-1}{(1+x)^2}, \text{ and } y'' = \frac{-6}{(1+x)^4}.$$

Then Euler-Maclaurin's formula gives us

$$\int_0^1 \frac{dx}{1+x} = \frac{0.1}{2}\left[\frac{1}{1+0} + 2\left(\frac{1}{1+0.1} + \frac{1}{1+0.2} + \frac{1}{1+0.3} + \cdots + \frac{1}{1+0.9}\right) + \frac{1}{1+1}\right]$$
$$= \frac{(0.1)^2}{2}\left[\frac{-1}{(1+1)^2} - \frac{-1}{(1+0)^2}\right] + \frac{(0.1)^4}{720}\left[\frac{-6}{(1+1)^4} - \frac{6}{(1+0)^4}\right]$$
$$= 0.693773 - 0.000625 + 0.000001 = 0.693149$$

Also $\int_0^1 \frac{dx}{1+x} = |\log(1+x)|_0^1 = \log_e 2$.

Hence $\log_e 2 = 0.693149$, approximately.

Example 4.7 Use Euler-Maclaurins formula to prove that $\sum_1^n x^3 = \frac{n^2(n+1)^2}{4}$

Solution: Here $y = x^3, y' = 3x^2, y''' = 6$ and $h = 1$.From Euler-Maclaurins formula we have

$$\frac{1}{2}[y_0 + 2(y_1 + y_2 + y_3 + \cdots + y_{n-1}) + y_n]$$

$$= \frac{1}{h}\int_{x_0}^{x_n} ydx + \frac{h}{12}(y_n' - y_0') - \frac{h^3}{720}(y_n^m - y_0^m) + \frac{h^5}{30240}\left(y_n^{(v)} - y_e^{(v)}\right) - \cdots$$

This leads to

$$\sum_1^n x^3 = \int_1^n x^3 dx + \frac{1}{2}(n^3+1) + \frac{1}{12}(3n^2-3) - \frac{1}{720}(6-6) = \frac{n^4-1}{4} + \frac{n^3+1}{2} + \frac{n^2-1}{4}$$

$$= \frac{n^4-1}{4} + \frac{n^3+1}{2} + \frac{n^2-1}{4}$$

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

$$= \frac{1}{4}(n+1)[n^3 - n^2 + n - 1 + 2n^2 - 2n + 2 + n - 1]$$

$$= \frac{1}{4}(n+1)[n^3 + n^2] = \frac{n^2(n+1)^2}{4}.$$

Example 4.8 Evaluate $I = \int_0^{\frac{\pi}{2}} \sin x \mathrm{dx}$ by using Euler-Maclaurins formula.

Solution: Here $y = \sin x, x_0 = 0$ and $\mathrm{x_n} = \frac{\pi}{2}$.

Then Euler-Maclaurins formula for $h = \pi/4$ provides us

$$\int_0^{\pi/2} \sin x\mathrm{dx} = \frac{\mathrm{h}}{2}[\mathrm{y}_0 + 2(y_1 + y_2 + \cdots + y_{n-1}) + y_n]\frac{\mathrm{h}^2}{12} + \frac{h^4}{720} + \frac{h^6}{3240} + \cdots$$

$$= \frac{\pi}{8}(0+2+0) + \frac{\pi^2}{192} + \frac{\pi^4}{184320} + \cdots = \frac{\pi}{4} + \frac{\pi^2}{192} + \frac{\pi^4}{184320}, \text{ approximately}$$

$$= 0.785398 + 0.051404 + 0.000528 = 0.83733$$

For $h = \frac{\pi}{8}$, we obtain

$$\int_0^{\frac{\pi}{2}} \sin x\mathrm{dx} = \frac{\pi}{16}[0 + 2(0.382683 + 0.707117 + 0.923879) + 1.000000]$$

$$= 0.987119 + 0.012851 + 0.000033 = 1.000003.$$

4.6 EVALUATION OF SINGULAR INTEGRALS

We have so for considered the integration of the function $y = f(x)$, which can be represented either by a polynomial or can be expanded in a Taylor's series in the interval of integration $[a, b]$. A function $f(x)$ is said to be singular at a point if $f(x)$ or any of its derivatives is infinite at that point. In such cases the formulae discussed earlier cannot be applied, and some special methods will have to be adopted. The approach depends, in general, on the type of the problem under consideration. We describe below some methods which can be applied in certain situations.

4.6.0 PRINCIPAL VALUE INTEGRALS

Consider the integral

$$I = \int_a^b \frac{f(x)dx}{x-t} \qquad \dots (4.22)$$

which is singular at $t = x$. The principal value $P(I)$ of integral (4.22) is defined as

$$P(I) = \text{Lim}_{\epsilon \to 0}\left[\int_a^{t-\epsilon} \frac{f(x)}{x-t}dx + \int_{t+\epsilon}^b \frac{f(x)}{x-t}dx\right], a < t < b$$
$$= I, \text{ for } t < a \text{ or } t > b$$

We take $x = a + uh$ and $t = a + \text{k}h$ in (4.22) so that

$$P(I) = P\int_0^p \frac{f(a+uh)}{u-k}du, p = \frac{b-a}{h}$$

Upon replacing $f(a + uh)$ by Newton's forward difference formula at $x = a$ and simplifying, we have

$$I = \sum_{j=0}^{\infty} \frac{\Delta^j f(a)}{j!} c_j \qquad \dots (4.23)$$

$$c_j = P\int_0^p \frac{(u)_j}{u-k}du$$

Here $(u)_0 = 1, (u)_1 = u, (u)_2 = u(u-1)$, etc. Various approximate formulae can be obtained by truncating the series on the right hand side of (4.23). Hence we can write (4.23) as

$$I_n = \sum_{j=0}^{n} \frac{\Delta^j f(a)}{j!} c_j$$

to obtain rule of orders 1,2,3, ... by setting $n = 1,2,3, \ldots$ respectively.

(a) Two point rule ($n = 1$)

$$I_1 = \sum_{j=0}^{1} \frac{\Delta^j f(a)}{j^j!} c_j = c_0 f(a) + c_1 \Delta f(a) = (c_0 - c_1) f(a) + c_1 f(a+h)$$

(b) Three point rule ($n = 2$)

$$I_2 = \sum_{j=0}^{2} \frac{\Delta^j f(a)}{j!} c_j = c_0 f(a) + c_1 \Delta f(a) + c_2 \Delta^2 f(a)$$
$$= \left(c_0 - c_1 + \frac{1}{2} c_2\right) f(a) + (c_1 - c_2) f(a+h) + \frac{1}{2} c_2 f(a+2h)$$

In the above relations, we have

$$c_0 = \log_e \left|\frac{p-k}{k}\right|, c_1 = p + c_0 k, c_2 = \frac{p^2}{2} + p(k-1) + c_0 k(k-1)$$

4.6.1 GENERALIZED QUADRATURE

Consider the integral

$$I(s) = \int_a^b f(t)\phi(t-s)dt \qquad \ldots (4.24)$$

where $f(t)$ is continuous but $\phi(u)$ may have an integrable singularity by adopting the forms of the type $|s-t|^\alpha, \alpha > -1$ or $\log|s-t|$ etc. For the numerical evaluation, we divide the range (a, b) such that $t_j = a + jh, j = 0,1,2, \ldots n$ with $nh = b - a$.

Then (4.24) becomes

$$I(s) = \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} f(t)\phi(t-s)dt \qquad \ldots (4.25)$$

Now we approximate $f(t)$ by a linear interpolating function $f_n(t)$ as

$$f_n(t) = \frac{1}{h}\left[\left(t_{j+1} - t\right)f\left(t_j\right) + \left(t - t_j\right)f\left(t_{j+1}\right)\right]$$

so that (4.25) takes the form

$$\begin{aligned} I(s) \quad &= \frac{1}{h}\sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \left[\left(t_{j+1} - t\right)f\left(t_j\right) + \left(t - t_j\right)f\left(t_{j+1}\right)\right]\phi(t-s)dt \\ &= h\sum_{j=0}^{n-1} \int_0^1 \left[(1-p)f\left(t_j\right) + pf\left(t_{j+1}\right)\right]\phi\left(t_j + ph - s\right)dp \end{aligned}$$

where $t = t_j + ph$. This can be rewritten as

$$I(s) \quad = \sum_{j=0}^{n-1} \left[\alpha_j f\left(t_j\right) + \beta_j f\left(t_{j+1}\right)\right] \qquad \text{... (4.26)}$$

$$\begin{aligned} where \qquad \alpha_j \quad &= h\int_0^1 (1-p)\phi\left(t_j + ph - s\right)dp \\ and \qquad \beta_j \quad &= h\int_0^1 p\phi\left(t_j + ph - s\right)dp \qquad \text{... (4.27)} \end{aligned}$$

Clearly if $\phi(u) = 1$, then $\alpha_j = \beta_j = \frac{h}{2}$ and hence (4.26) gives us

$$I(s) = \frac{h}{2}\left[f(t_0) + 2\{f(t_1) + f(t_2) + \cdots + f(t_{n-1})\} + f(t_n)\right]$$

which is the trapezoidal rule. Therefore the rule defined by (4.26) and (4.27) is called generalized trapezoidal rule due to K. E. Atkinson. For $\phi(u) = \log|u|$, this rule finds important applications in the numerical solution of certain singular integral equations. In general, the computation of the weights α_j and β_j may be difficult but they can be evaluated once and for all, for a given $\phi(u)$. In a similar fashion we can also deduce the generalized Simpson's rule, analogous to the ordinary Simpson's rule, by approximating $f(t)$ by means of a quadratic interpolating function in the interval $\left(t_j, t_{j+1}\right)$. The error in generalized quadrature can also be estimated by the method used in case of ordinary quadrature formulae. For example it can be shown that the error in the generalized trapezoidal rule is of order h^2, assuming that f'' is continuous in $[a, b]$.

4.7 DOUBLE INTEGRATION

The double integral of the type

$$I = \int_c^d \int_a^b f(x, y) dx dy$$

is evaluated numerically by two successive integration in x and y direction considering one variable at a time by repeated applications of trapezoidal or Simpson's rule.

4.7.0 TRAPEZOIDAL RULE

We divide intervals (a, b) and (c, d) into n and m equal subintervals each of length h and k respectively, so that we have

$$x_i = x_0 + ih, x_0 = a, x_n = b, i = 0,1,2, \dots n$$
$$y_j = y_0 + jk, y_0 = c, y_m = d, j = 0,1,2, \dots m$$

Using trapezoidal rule in both direction, we get

$$\begin{aligned} I &= \int_{y_0}^{y_m} \int_{x_0}^{x_n} f(x, y) dx dy \\ &= \frac{h}{2} \int_{y_0}^{y_m} \{f(x_0, y) + f(x_n, y) + 2[f(x_1, y) + f(x_2, y) + \dots + f(x_{n-1}, y)]\} dy \\ &= \frac{hk}{4} \Big[(f_{00} + f_{om}) + 2\big(f_{01} + f_{02} + \dots + f_{0,m-1}\big) + (f_{n0} + f_{nm}) + 2\big(f_{n1} + f_{n2} + \dots + f_{n,m-1}\big) \\ &+2 \sum_{i=1}^{n-1} \{(f_{i0} + f_{im}) + 2\big(f_{i1} + f_{i2} + \dots + f_{i,m-1}\big)\} \Big], \; f_{ij} = f\big(x_i, y_j\big) \end{aligned}$$

4.7.1 SIMPSON'S RULE

In this case we divide the interval (a, b) in $2n$ equal subintervals each of width h and the interval (c, d) into $2m$ equal subintervals each of width k so that we have

$$x_i = x_0 + ih, \; y_j = y_0 + jk, x_0 = a, x_{2n} = b, y_0 = c, y_{2m} = d$$

Then by Simpson's rule in both directions, we have

$$\int_{y_{j-1}}^{y_{j+1}}\int_{x_{i-1}}^{x_{i+1}} f(x,y)dxdy = \frac{h}{3}\int_{y_{j-1}}^{y_{j+1}} [f(x_{i-1},y) + 4f(x_i,y) + f(x_{i+1},y)]dy$$

$$= \frac{hk}{9}\left[\left(f_{i-1,j-1} + 4f_{i-1,j} + f_{i-1,j+1}\right) + 4\left(f_{i,j-1} + f_{i,j} + f_{i,j+1}\right) + \left(f_{i+1,j-1} + 4f_{i+1,j} + f_{i=1,j+1}\right)\right]$$

$$= \frac{hk}{9}\left[f_{i-1,j-1} + f_{i-1,j+1} + f_{i+1,j-1} + f_{i+1,j+1} + 4\left(f_{i-1,j} + f_{i,j-1} + +f_{i,j+1} + f_{i+1,j}\right) + 16f_{i,j}\right]$$

Adding all such intervals, we obtain the value of

$$I = \int_{y_0}^{y_{2m}}\int_{x_0}^{x_{2n}} f(x,y)dxdy$$

Example 4.9 Evaluate the integral $I = \int_0^1\int_0^1 e^{x+y}dxdy$

by using (i) trapezoidal rule and (ii) Simpson's rule

Solution: We take $h = k = 0.5$ and $f(\mathrm{x,y}) = \mathrm{e}^{\mathrm{x+y}}$.

(i) Trapezoidal rule

$$I = \frac{0.25}{4}[1.0 + 4(1.6487) + 6(2.7183) + 4(4.4817) + 7.3891] = \frac{12.3050}{4} = 3.07625$$

(ii) Simpson's rule

$$\begin{aligned} I = \frac{0.25}{9}&[1.0 + 2.7183 + 7.3891 + 2.7183 \\ &+4(1.6487 + 4.4817 + 4.4817 + 1.6487) + 16(2.7183)] \\ &= \frac{26.59042}{9} = 2.9545 \end{aligned}$$

The exact value of the double integral is 2.9525 and thus the result obtained by Simpson's rule is sixty time more accurate than that given by trapezoidal rule.

4.8 CHECK YOUR PROGRESS

1 Find the sum of the series $\frac{1}{51^2}+\frac{1}{53^2}+\frac{1}{55^2}+\cdots+\frac{1}{99^2}$ by using Euler-Maclaurins summation formula.

2 Drive Gauss Ian integration formula when $n=2$ and apply this to evaluate the integral $\int_{-1}^{1}\frac{dx}{1+x^2}$

3 Use there point Gauss-Legendre formula to evaluate the integral $\int_0^{\frac{\pi}{2}}\sin xdx$ Compare this result with that obtained by Simpson's rule using seven points.

4 Use Romberg's method to compute $\int_0^1\frac{dx}{1+x}$ with h $=0.5,0.25$ and 0.125. Hence evaluate $\log_e^2$ correct to four decimal places.

5 Apply Romberg's method to evaluate given that

x:	4.0	4.2	4.4	4.6	4.8	5.0	5.2
$\log_e 2$:	1.3863	1.4351	1.4816	1.526	1.5686	1.6094	1.6486

6 Use Euler-Maclaurins formulae to prove that $\sum x^2=\frac{n(n+1)(2n+1)}{6}$.

7 Evaluate $\int_0^1\int_0^1 xe^y dxdy$ using Trapezoidal rule $(h=k=0.5)$.

8 Apply Trapezoidal rule to evaluate $\int_1^5\int_1^5\frac{dxdy}{\sqrt{x^2+y^2}}$, taking two subintervals.

9 Evaluate $\int_1^{2.6}\int_2^{3.2}\frac{dxdy}{x+y}$, using Simpson's rule.

4.9 SUMMARY

The students are made familiar with various methods for numerical integration.

4.10 KEYWORDS

Numerical Integration, Romberg Integration, Gaussian Integration, Singular Integral, Double Integration.

4.11 SELF-ASSESSMENT TEST

1. Evaluate $\int_0^1 \frac{dx}{1+x^2}$ by using (i) Trapezoidal rule taking $h = 0.25$, (ii) Simpson's $\frac{1}{3}$ rule taking $h = 0.25$, (iii) Simpson's $\frac{3}{8}$ rule taking $h = \frac{1}{6}$, (iv) Weddle's rule taking $h = \frac{1}{6}$.

2. Evaluate $\int_0^1 e^x dx$ by Simpson's rule given that $e = 2.72, e^2 = 7.39, e^3 = 20.09, e^4 = 54.6$ and compare it with the actual value

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

4. Integrate numerically $\int_0^{\frac{\pi}{2}} \sqrt{\cos\theta}\, d\theta$.

4.12 ANSWERS TO CHECK YOUR PROGRESS

1 0.004999

2 1.5

3 1.00002

4 0.6931

5 1.8278

7 0.876

8 4.134

9 0.49

4.13 REFERENCES/ SUGGESTED READINGS

1. JAMES F. EPPERSON; An Introduction to Numerical Methods and analysis. Second Edition Mathematical Reviews, John Wiley & Sons, Inc., Hoboken, New Jersey.
2. S S Shastry; Introductory Methods of Numerical Analysis, Fifth Edition ISBN-978-81-203-4592-8, Asoke K. Ghosh, PHI Learning Pvt. Ltd, M-97, Connaught Circus, New Delhi
3. C.F. Gerald and P.O. Wheatley : Applied Numerical Methods, Low- priced edition, Pearson Education Asia (2002), Sixth Edition.

4. D. Kincaid and W. Cheney, Numerical Analysis: Mathematics of Scientific Computing, 3rd Edn., AMS (2002).
5. D.V. Griffiths and I.M. Smith, Numerical Methods for Engineers, Blackwell Scientific Publications (1991).
6. John H Mathews, Numerical Methods for Mathematics, Science and Engineering, Prentice Hall of India (1994).
7. K. E. Atkinson, Introduction to Numerical Analysis, 2nd Edn., John Wiley (1989).
8. M.K. Jain: Numerical Solution of Differential Equations, 4th Edition, New Age (2018).

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LESSON No. 5 Written by- Dr. Joginder Singh

SYSTEM OF LINEAR EQUATIONS

STRUCTURE

5.0 LEARNING OBJECTIVES

Students are able to

- Solve linear simultaneous equations using various iterative methods : Jacobi's method, Gauss-Seidel method, SOR, Relaxation method.
- Solve Ill-conditioned equations.

5.1 INTRODUCTION

Most problems arising from engineering and applied sciences require the solution of systems of linear algebraic equations and computation of eigenvalues and eigenvectors of a matrix. We assume that the readers are familiar with the theory of determinants and elements of matrix algebra since these provide a convenient way to represent linear algebraic equations. Consider the system of equations.

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

This may be represented as the matrix equation, where

$$AX = b$$
$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \text{ and } b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

To solve this system, we discuss some iterative method such as Jacobi and Gauss-Seidel, SOR, etc. Before proceeding further, we need to define norms on matrices.

VECTOR AND MATRIX NORMS

The distance between a vector and the null vector is a measure of the size or length of the vector. This is called a norm of the vector. The norm of the vector x, written as $\| x \|$, is a real number which satisfies the following conditions or axioms:

$$\| x \| \geq 0 \text{ and } \| x \| = 0 \text{ if and only if } x = 0 \qquad \text{... (5.1)}$$
$$\| \alpha x \| = |\alpha| \, \| x \| \quad \text{for any real } \alpha \qquad \text{... (5.2)}$$
$$\| x + y \| \leq \| x \| + \| y \| \quad \text{(triangle inequality).} \qquad \text{...(5.3)}$$

For the vector

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad \text{... (5.4)}$$

some useful norms are

$$\| x \|_1 = |x_1| + |x_2| + \cdots + |x_n| = \sum_{i=1}^{m} |x_i| \qquad \text{... (5.5)}$$
$$\| x \|_2 = \sqrt{|x_1|^2 + |x_2|^2 + \cdots + |x_n|^2} = \left[\sum_{i=1}^{n} |x_i|^2 \right]^{1/2} = \| x \|_e$$
$$\| x \|_\infty = \max_i |x_i| \qquad \text{... (5.6)}$$

The norm $\|\cdot\|_2$ is called the Euclidean norm since it is just the formula for distance in the three-dimensional Euclidean space. The norm $\|\cdot\|_\infty$ is called the maximum norm or the uniform norm.

It is easy to show that the three norms $\| x \|_1, \| x \|_2$ and $\| x \|_\infty$ satisfy the conditions (5.1) to (5.3), given above. Conditions (5.1) and (5.2) are trivially satisfied. Only condition (5.3), the triangle inequality, needs to be shown to be true. For the norm $\| x \|_1$ we observe that

$$\begin{aligned} \| x + y \| &= \sum_{i=1}^{n} |x_i + y_i| \\ &\leq \sum_{i=1}^{n} (|x_i| + |y_i|) \\ &= \sum_{i=1}^{n} |x_i| + \sum_{i=1}^{n} |y_i| \\ &= \| x \|_1 + \| y \|_1 \end{aligned} \qquad \dots (5.7)$$

Similarly, for $\| x \|_\infty$, we have

$$\begin{aligned} \| x + y \|_\infty &= \max_i |x_i + y_i| \\ &\leq \max_i (|x_i| + |y_i|) \\ &= \| x \|_\infty + \| y \|_\infty . \end{aligned} \qquad \dots (5.8)$$

The proof for the Euclidean norm is left as an exercise to the reader.

To define matrix norms, we consider two matrices A and B for which the operations $\mathrm{A} + \mathrm{B}$ and AB are defined. Then,

$$|A + B| \leq |A| + |B| \qquad \dots (5.9)$$
$$|AB| \leq |A||B| \qquad \dots (5.10)$$
$$|\alpha A| = |\alpha||A| \ (\alpha \text{ a scalar}). \qquad \dots (5.11)$$

From Eq. (3.10) it follows that

$$|A^p| \leq |A|^p,$$

where p is a natural number. In the above equations, $|A|$ denotes the matrix A with absolute values of the elements.

By the norm of a matrix $A = |a_{ij}|$, we mean a nonnegative number, denoted by $\| A \|$, which satisfies the following conditions

$$
\begin{aligned}
\| A \| &\geq 0 \text{ and } \| A \| = 0 \text{ if and only if } A = 0 \\
\| \alpha A \| &= |\alpha| \, \| A \| \quad (\alpha \text{ a scalar}) \\
\| A + B \| &\leq \| A \| + \| B \| \\
\| AB \| &\leq \| A \| \| B \|.
\end{aligned}
$$

From above Eq., it easily follows that

$$\|A^p\| \leq \| A \|^p ,$$

where p is a natural number. Corresponding to the vector norms given in Eqs. (5.5)-(5.6), we have the three matrix norms

$$\| A \|_1 = \max_j \sum_i |a_{ij}| \text{ (the column norm)}$$

$$\| A \|_e = \left[\sum_{i,j} |a_{ij}|^2 \right]^{1/2} \quad \text{(the Euclidean norm)}$$

$$\| A \|_\infty = \max_i \sum_j |a_{ij}| \text{ (the row norm).}$$

In addition to the above, we have $\| A \|_2$ defined by

$$\| A \|_2 = (M\text{aximum eigenvalue of } A^\top A)^{1/2}.$$

The choice of a particular norm is dependent mostly on practical considerations. The row-norm is, however, most widely used because it is easy to compute and, at the same time, provides a fairly adequate measure of the size of the matrix.

The following example demonstrates the computation of some of these norms.

Example 5.1 Given the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

find $\parallel A \parallel_1, \parallel A \parallel_e$ and $\parallel A \parallel_\infty$.

Solution: We have

$$\begin{aligned}
\parallel \mathrm{A} \parallel_1 &= \mathrm{m}\ \ [1 + 4 + 7, 2 + 5 + 8, 3 + 6 + 9] = \mathrm{m}\ \ [12,15,18] = 18 \\
\parallel \mathrm{A} \parallel_l &= (1^2 + 2^2 + 3^2 + 4^2 + 5^2 + 6^2 + 7^2 + 8^2 + 9^2)^{1/2} \\
&= (1 + 4 + 9 + 16 + 25 + 36 + 49 + 64 + 81)^{1/2} \\
&= (285)^{1/2} \\
&= 16.88. \\
\parallel \mathrm{A} \parallel_\infty &= \mathrm{m}\ \ [1 + 2 + 3, 4 + 5 + 6, 7 + 8 + 9] \\
&= \mathrm{m}\ \ [6,15,24] \\
&= 24.
\end{aligned}$$

The concept of the norm of a matrix will be useful in the study of the convergence of iterative methods of solving linear systems. It is also used in defining the 'stability' of a system of equations.

5.2 SOLUTION OF TRIDIAGONAL SYSTEMS

Consider the system of equations defined by

$$\left.\begin{aligned}
b_1 u_1 + c_1 u_2 &= d_1 \\
a_2 u_1 + b_2 u_2 + c_2 u_3 &= d_2 \\
a_3 u_2 + b_3 u_3 + c_3 u_4 &= d_3 \\
&\vdots \\
a_n u_{n-1} + b_n u_n &= d_n.
\end{aligned}\right\} \qquad \ldots (5.12)$$

The matrix of coefficients is

$$A = \begin{bmatrix}
b_1 & c_1 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\
a_2 & b_2 & c_2 & 0 & \cdots & \cdots & \cdots & 0 \\
0 & a_3 & b_3 & c_3 & \cdots & \cdots & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \cdots & 0 & a_{n-1} & b_{n-1} & c_{n-1} \\
0 & 0 & 0 & \cdots & 0 & 0 & a_n & b_n
\end{bmatrix} \qquad \ldots (5.13)$$

Matrices of the type, given in Eq. (5.13), called the tridiagonal matrices, occur frequently in the solution of ordinary and partial differential equations by finite difference methods. The method of factorization described earlier can be conveniently applied to solve the system (5.12). For example, for a (3×3) matrix we have

$$\begin{bmatrix} b_1 & c_1 & 0 \\ a_2 & b_2 & c_2 \\ 0 & a_3 & b_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ 0 & l_{32} & 1 \end{bmatrix} \begin{bmatrix} b_1 & c_1 & 0 \\ 0 & u_{22} & c_2 \\ 0 & 0 & u_{33} \end{bmatrix}$$

This matrix equation gives

$$\left.\begin{aligned} l_{21}b_1 = a_2, \quad l_{21}c_1 + u_{22} = b_2 \\ l_{32}u_{22} = a_3, \quad l_{32}c_2 + u_{33} = b_3 \end{aligned}\right\}$$

From these four equations, we can compute l_{21}, u_{22}, l_{32} and u_{33} and these values are stored in the locations occupied by a_2, b_2, a_3 and b_3, respectively. These computations can be achieved by the following statements:

Do $i = 2(1)N$

$a(i) = a(i)/b(i-1)$

$b(i) = b(i) - a(i)c(i-1)$

Next i

When the decomposition is complete, forward and back substitutions give the required solution. This algorithm is due to Thomas and possesses all the advantages of the LU decomposition.

5.3 ILL-CONDITIONED LINEAR SYSTEMS

In practical applications, one usually encounters systems of equations in which small changes in the coefficients of the system produce large changes in the solution. Such systems are said to be ill-conditioned. On the other hand, if the corresponding changes in the solution are also small, then the system is well-conditioned.

Ill-conditioning can usually be expected when $|A|$, in the system $AX = b$, is small. The quantity $c(A)$ defined by

$$c(A) = \| A \| \, \|A^{-1}\|,$$

where $\| A \|$ is any matrix norm, gives a measure of the condition of the matrix. It is, therefore, called the condition number of the matrix. Large condition numbers indicate that the matrix is ill-conditioned. Again, let $A = [a_{ij}]$ and

$$s_i = [a_{i1}^2 + a_{i2}^2 + \cdots + a_{in}^2]^{1/2}$$

If we define

$$k = \frac{|A|}{s_1 s_2 \cdots s_n},$$

then the system is ill-conditioned if k is very small compared to unity. Otherwise, it is well-conditioned.

Example 5.2 The system

$$\left.\begin{aligned} 2x + y &= 2 \\ 2x + 1.01y &= 2.01 \end{aligned}\right\}$$

has the solution $x = 0.5$ and $y = 1$.

But the system

$$\left.\begin{aligned} 2x + y &= 2 \\ 2.01x + y &= 2.05 \end{aligned}\right\}$$

has the solution $x = 5$ and $y = -8$.

Also,

$$\| A \|_e = 3.165 \text{ and } \|A^{-1}\|_e = 158.273$$

Therefore, condition number $c(A) = \| A \| \, \|A^{-1}\| = 500.974$.

Hence the system is ill-conditioned.

Also

$$|A| = 0.02$$
$$s_1 = \sqrt{5} \text{ and } s_2 = 2.24$$

So,

$$k = 4.468 \times 10^{-3}$$

Hence the system is ill-conditioned.

Example 5.3 Let

$$\mathrm{A} = \begin{bmatrix} \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \\ \frac{1}{8} & \frac{1}{9} & \frac{1}{10} \end{bmatrix}$$

which is called Hilbert's matrix.

Solution: Now

$$|A| = 0.0000297, \text{which is small compared to 1.}$$

Hence A is ill-conditioned.

Example 5.4 Let

$$A = \begin{bmatrix} 25 & 24 & 10 \\ 66 & 78 & 37 \\ 92 & -73 & -80 \end{bmatrix}$$

Solution: Now

$$|A| = 1.0.$$

Also,

$$s_1 = 36.0694,\ s_2 = 108.6692 \text{ and } s_3 = 142.1021.$$

Therefore,

$$k = 1.7954 \times 10^{-6}.$$

which shows that A is ill-conditioned.

METHOD FOR III-CONDITIONED SYSTEMS

In general, the accuracy of an approximate solution can be improved upon by an iterative procedure. This is described below. Let the system be

$$\left.\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_2 &= b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= b_3 \end{aligned}\right\} \qquad \ldots (5.14)$$

Let $x_1^{(1)}, x_2^{(1)}$ and $x_3^{(1)}$ be an approximate solution. Substituting these values in the left side of Eq. (5.14), we get new values of b_1, b_2 and b_3. Let these new values be $b_1^{(1)}, b_2^{(1)}$ and $b_3^{(1)}$. The new system of equations is given by

$$\left.\begin{aligned} a_{11}x_1^{(1)} + a_{12}x_2^{(1)} + a_{13}x_3^{(1)} &= b_1^{(1)} \\ a_{21}x_1^{(1)} + a_{22}x_2^{(1)} + a_{23}x_3^{(1)} &= b_2^{(1)} \\ a_{31}x_1^{(1)} + a_{32}x_2^{(1)} + a_{33}x_3^{(1)} &= b_3^{(1)} \end{aligned}\right\} \qquad \ldots (5.15)$$

Subtracting each equation given in (5.15) from the corresponding equation given in (5.14), we obtain

$$\left.\begin{aligned} a_{11}e_1 + a_{12}e_2 + a_{13}e_3 &= d_1 \\ a_{21}e_1 + a_{22}e_2 + a_{23}e_3 &= d_2 \\ a_{31}e_1 + a_{32}e_2 + a_{33}e_3 &= d_3 \end{aligned}\right\} \qquad \ldots (5.16)$$

where $e_i = x_i - \mathrm{x}_i^{(1)}$ and $d_i = b_i - \mathrm{b}_i^{(1)}$. We now solve the system (5.16) for e_1, e_2 and e_3. Since $e_i = x_i - x_i^{(1)}$, we obtain

$$x_i = x_i^{(1)} + e_i,$$

which is a letter approximation for x_i. The procedure can be repeated to improve upon the accuracy.

Example 5.5   Solve the system

$$\begin{aligned} 2x + y &= 2 \\ 2x + 1.01y &= 2.01 \end{aligned}$$

Solution: Let an approximate solution of the given system be given by

$$x^{(1)} = 1 \text{ and } y^{(1)} = 1.$$

Substituting these values in the given system, we obtain

$$\left.\begin{aligned} 2x^{(1)} + y^{(1)} &= 3 \\ 2x^{(1)} + 1.01y^{(1)} &= 3.01 \end{aligned}\right\} \qquad \dots (i)$$

Subtracting each equation of (i) from the corresponding equation of the given system, we get

$$2\left(x - x^{(1)}\right) + \left(y - y^{(1)}\right) = -1$$

$$2\left(x - x^{(1)}\right) + 1.01\left(y - y^{(1)}\right) = -1.$$

Solving the above system of equations, we obtain

$$x - x^{(1)} = -\frac{1}{2} \text{ and } y - y^{(1)} = 0.$$

Hence

$$x = \frac{1}{2} \text{ and } y = 1,$$

which is the exact solution of the given system.

5.4 SOLUTION OF LINEAR SYSTEMS-ITERATIVE METHODS

We shall now describe the iterative or indirect methods, which start from an approximation to the true solution and, if convergent, derive a sequence of closer approximations - the cycle of computations being repeated till the required accuracy is obtained. This means that in a direct method the amount of computation is fixed, while in an iterative method the amount of computation depends on the accuracy required.

In general, one should prefer a direct method for the solution of a linear system, but in the case of matrices with a large number of zero elements, it will be advantageous to use iterative methods which preserve these elements.

Let the system be given by

$$\left.\begin{array}{c} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \cdots + a_{3n}x_n = b_3 \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n \end{array}\right\} \qquad \ldots (5.17)$$

in which the diagonal elements a_{ii} do not vanish. If this is not the case, then the equations should be rearranged so that this condition is satisfied. Now, we rewrite the system (5.17) as

$$\left.\begin{array}{l} x_1 = \dfrac{b_1}{a_{11}} - \dfrac{a_{12}}{a_{11}}x_2 - \dfrac{a_{13}}{a_{11}}x_3 - \cdots - \dfrac{a_{1n}}{a_{11}}x_n \\ x_2 = \dfrac{b_2}{a_{22}} - \dfrac{a_{21}}{a_{22}}x_1 - \dfrac{a_{23}}{a_{22}}x_2 - \cdots - \dfrac{a_{2n}}{a_{22}}x_n \\ x_3 = \dfrac{b_3}{a_{33}} - \dfrac{a_{31}}{a_{33}}x_1 - \dfrac{a_{32}}{a_{33}}x_2 - \cdots - \dfrac{a_{3n}}{a_{33}}x_n \\ \vdots \\ x_n = \dfrac{b_n}{a_{nn}} - \dfrac{a_{n1}}{a_{nn}}x_1 - \dfrac{a_{n2}}{a_{nn}}x_2 - \cdots - \dfrac{a_{n,n-1}}{a_{nn}}x_{n-1}\,. \end{array}\right\} \qquad \ldots (5.18)$$

Suppose $x_1^{(1)}, x_2^{(1)}, \ldots, x_n^{(1)}$ are any first approximations to the unknowns $x_1, x_2, \ldots, x_n$. Substituting in the right side of Eq. (3.18), we find a system of second approximations

$$\left.\begin{array}{l} x_1^{(2)} = \dfrac{b_1}{a_{11}} - \dfrac{a_{12}}{a_{11}}x_2^{(1)} - \cdots - \dfrac{a_{1n}}{a_{11}}x_n^{(1)}, \\ x_2^{(2)} = \dfrac{b_2}{a_{22}} - \dfrac{a_{21}}{a_{22}}x_1^{(1)} - \cdots - \dfrac{a_{2n}}{a_{22}}x_n^{(1)}, \\ x_3^{(2)} = \dfrac{b_3}{a_{33}} - \dfrac{a_{31}}{a_{33}}x_1^{(1)} - \cdots - \dfrac{a_{3n}}{a_{33}}x_n^{(1)}, \\ \vdots \\ x_n^{(2)} = \dfrac{b_n}{a_{nn}} - \dfrac{a_{n1}}{a_{nn}}x_1^{(1)} - \cdots - \dfrac{a_{n,n-1}}{a_{nn}}x_{n-1}^{(1)}. \end{array}\right\} \qquad \ldots (5.19)$$

Similarly, if $x_1^{(n)}, x_2^{(n)}, \dots, x_n^{(n)}$ are a system of nth approximations, then the next approximation is given by the formula

$$\left.\begin{aligned} x_1^{(n+1)} &= \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}} x_2^{(n)} - \cdots - \frac{a_{1n}}{a_{11}} x_n^{(n)}, \\ x_2^{(n+1)} &= \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}} x_1^{(n)} - \cdots - \frac{a_{2n}}{a_{22}} x_n^{(n)}, \\ &\vdots \\ x_n^{(n+1)} &= \frac{b_n}{a_{nn}} - \frac{a_{n1}}{a_{nn}} x_1^{(n)} - \cdots - \frac{a_{n,n-1}}{a_{nn}} x_{n-1}^{(n)}. \end{aligned}\right\} \quad \dots (5.20)$$

If we write Eq. (5.18) in the matrix form

$$X = HX + C$$

then the iteration formula (5.20) may be written as

$$X^{(n+1)} = HX^{(n)} + C.$$

This method is due to Jacobi and is called the method of simultaneous displacements. It can be shown that a sufficient condition for the convergence of this method is that

$$\| H \| < 1.$$

A simple modification in this method sometimes yields faster convergence and is described below:

In the first equation of Eq. (5.18), we substitute the first approximation $\left(x_1^{(1)}, x_2^{(1)}, x_3^{(1)}, \dots, x_n^{(1)}\right)$ into the right-hand side and denote the result as $x_1^{(2)}$. In the second equation, we substitute $\left(x_1^{(2)}, x_2^{(1)}, x_3^{(1)}, \dots, x_n^{(1)}\right)$ and denote the result as $x_2^{(2)}$. In the third, we substitute $\left(x_1^{(2)}, x_2^{(2)}, x_3^{(1)}, \dots, x_n^{(1)}\right)$ and call the result as $x_3^{(2)}$. In this manner, we complete the first stage of iteration and the entire process is repeated till the values of $x_1, x_2, \dots, x_n$ are obtained to the accuracy required. It is clear, therefore, that this method uses an improved component as soon as it is available and it is called the method of successive displacements, or the Gauss-Seidel method.

The Jacobi and Gauss-Seidel methods converge, for any choice of the first approximation $x_j^{(1)} (j = 1,2, \dots, n)$, if every equation of the system (5.18) satisfies the condition that the sum of the absolute values of the coefficients a_{ij}/a_{ii} is almost equal to, or in at least one equation less than unity, i.e. provided that

$$\sum_{j=1, j\neq i}^{n} \left|\frac{a_{ij}}{a_{ii}}\right| \leq 1,\ (i = 1,2, \dots, n), \qquad \dots(5.21)$$

where the ' $<$ ' sign should be valid in the case of 'at least' one equation. It can be shown that the Gauss-Seidel method converges twice as fast as the Jacobi method.

Let the coefficient matrix **A** be written as

$$\mathbf{A} = \mathbf{L} + \mathbf{D} + \mathbf{U}$$

where $\mathbf{L}, \mathbf{D}, \mathbf{U}$ are the strictly lower triangular, diagonal and strictly upper triangular parts of A respectively. Write the system **Ax=b** as

$$(\mathbf{L} + \mathbf{D} + \mathbf{U})\mathbf{x} = \mathbf{b} \qquad \dots.(a)$$

Jacobi Iteration Method

We rewrite (a) as

$$\mathbf{Dx} = -(\mathbf{L} + \mathbf{U})\mathbf{x} + \mathbf{b}$$

and define an iterative procedure as

$$\mathbf{x}^{(k+1)} = -\mathbf{D}^{-1}(\mathbf{L} + \mathbf{U})\mathbf{x}^{(\boldsymbol{k})} + \mathbf{D}^{-\mathbf{1}}\mathbf{b}.$$

The iteration matrix is given by

$$\mathbf{H} = -\mathbf{D}^{-1}(\mathbf{L} + \mathbf{U}).$$

This method is called the Jacobi Iteration method.

Gauss-Seidel Iteration Method

In this case, we define the iterative procedure as

$$(\mathbf{D}+\mathbf{L})\mathbf{x}^{(k+1)} = -\mathbf{U}\mathbf{x}^{(k)} + \mathbf{b}$$

or

$$\mathbf{x}^{(k+1)} = -(\mathbf{D}+\mathbf{L})^{-1}\mathbf{U}\mathbf{x}^{(k)} + (\mathbf{D}+\mathbf{L})^{-1}\mathbf{b}$$

where $\mathbf{H} = -(\mathbf{D}+\mathbf{L})^{-1}\mathbf{U}$ is the iteration matrix.

Successive Over Relaxation (SOR) Method

The iterative procedure is given by

$$\mathbf{x}^{(k+1)} = (\mathbf{D}+w\mathbf{L})^{-1}[(1-w)\mathbf{D} - w\mathbf{U}]\mathbf{x}^{(k)} + w(\mathbf{D}+w\mathbf{L})^{-1}\mathbf{b}$$

where w is the relaxation parameter.

When $w = 1$, it reduces to the Gauss-Seidel method. The relaxation parameter w satisfies the condition $0 < w < 2$. If $w > 1$ then the method is called an over relaxation method and if $w < 1$, it is called an under relaxation method. Maximum convergence of SOR is obtained when

$$w = w_{\text{opt}} \approx \frac{2}{\mu^2}\left[1 - \sqrt{1-\mu^2}\right] = \frac{2}{1+\sqrt{1-\mu^2}}$$

where $\mu = \rho\left(\mathbf{H}_{\text{Jacobi}}\right)$ and w_{opt} is rounded to the next digit.

The rate of convergence of an iterative method is defined as

$$v = -\ln(\rho(\mathbf{H})), \text{ or also as } v = -\log_{10}(\rho(\mathbf{H})).$$

where $\mathbf{H}$ is the iteration matrix.

The spectral radius of the SOR method is $\mathrm{W}_{\text{opt}} - 1$ and its rate of convergence is

$$v = -\ln\left(\mathrm{W}_{\text{opt}} - 1\right) \text{ or } \mathrm{V} = -\log_{10}\left(\mathrm{W}_{\text{opt}} - 1\right).$$

The working of the methods is illustrated in the following examples:

Example 5.6 We consider the equations:

$$\begin{aligned} 10x_1 - 2x_2 - x_3 - x_4 &= 3 \\ -2x_1 + 10x_2 - x_3 - x_4 &= 15 \\ -x_1 - x_2 + 10x_3 - 2x_4 &= 27 \\ -x_1 - x_2 - 2x_3 + 10x_4 &= -9. \end{aligned}$$

Solution: To solve these equations by the iterative methods, we re-write them as follows:

$$\begin{aligned} x_1 &= 0.3 + 0.2x_2 + 0.1x_3 + 0.1x_4 \\ x_2 &= 1.5 + 0.2x_1 + 0.1x_3 + 0.1x_4 \\ x_3 &= 2.7 + 0.1x_1 + 0.1x_2 + 0.2x_4 \\ x_4 &= -0.9 + 0.1x_1 + 0.1x_2 + 0.2x_3. \end{aligned}$$

It can be verified that these equations satisfy the condition (5.21). The results are given in Tables 5.1 and 5.2:

Table 5.1 Gauss-Seidel Method

n	x_1	x_2	x_3	x_4
1	0.3	1.56	2.886	−0.1368
2	0.8869	1.9523	2.9566	−0.0248
3	0.9836	1.9899	2.9924	−0.0042
4	0.9968	1.9982	2.9987	−0.0008
5	0.9994	1.9997	2.9998	−0.0001
6	0.9999	1.9999	3.0	0.0
7	1.0	2.0	3.0	0.0

Table 5.2 J acobi's Method

n	x_1	x_2	x_3	x_4
1	0.3	1.5	2.7	−0.9
2	0.78	1.74	2.7	−0.18
3	0.9	1.908	2.916	−0.108
4	0.9624	1.9608	2.9592	−0.036
5	0.9845	1.9848	2.9851	−0.0158
6	0.9939	1.9938	2.9938	−0.006
7	0.9975	1.9975	2.9976	−0.0025
8	0.9990	1.9990	2.9990	−0.0010
9	0.9996	1.9996	2.9996	−0.0004
10	0.9998	1.9998	2.9998	−0.0002
11	0.9999	1.9999	2.9999	−0.0001
12	1.0	2.0	3.0	0.0

From Tables 5.1 and 5.2, it is clear that twelve iterations are required by Jacobi's method to achieve the same accuracy as seven Gauss-Seidel iterations.

Example 5.7 Solve the system

$$\begin{aligned} 6x + y + z &= 20 \\ x + 4y - z &= 6 \\ x - y + 5z &= 7 \end{aligned}$$

using both Jacobi and Gauss-Seidel methods.

Solution: (a) Jacobi's method

We rewrite the given system as

$$x = \frac{20}{6} - \frac{1}{6}y - \frac{1}{6}z = 3.3333 - 0.1667y - 0.1667z$$
$$y = 1.5 - 0.25x + 0.25z$$
$$z = 1.4 - 0.2x + 0.2y$$

In matrix form, the above system may be written as

$$X = C + BX$$

where

$$C = \begin{bmatrix} 3.3333 \\ 1.5 \\ 1.4 \end{bmatrix}, B = \begin{bmatrix} 0 & -0.1667 & -0.1667 \\ -0.25 & 0 & 0.25 \\ -0.2 & 0.2 & 0 \end{bmatrix} \text{ and } X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Assuming

$$x^0 = \begin{bmatrix} 3.3333 \\ 1.5 \\ 1.4 \end{bmatrix}, \text{we obtain}$$

$$X^{(1)} = \begin{bmatrix} 3.3333 \\ 1.5 \\ 1.4 \end{bmatrix} + \begin{bmatrix} 0 & -0.1667 & -0.1667 \\ -0.25 & 0 & 0.25 \\ -0.2 & 0.2 & 0 \end{bmatrix} \begin{bmatrix} 3.3333 \\ 1.5 \\ 1.4 \end{bmatrix} = \begin{bmatrix} 2.8499 \\ 1.0167 \\ 1.0333 \end{bmatrix}$$
$$X^{(2)} = \begin{bmatrix} 3.3333 \\ 1.5 \\ 1.4 \end{bmatrix} + \begin{bmatrix} 0 & -0.1667 & -0.1667 \\ -0.25 & 0 & 0.25 \\ -0.2 & 0.2 & 0 \end{bmatrix} \begin{bmatrix} 2.8499 \\ 1.0167 \\ 1.0333 \end{bmatrix} = \begin{bmatrix} 2.9647 \\ 1.0458 \\ 1.0656 \end{bmatrix}$$

Proceeding in this way, we obtain

$$X^{(8)} = \begin{bmatrix} 2.9991 \\ 1.0012 \\ 1.0010 \end{bmatrix} \text{ and } X^{(9)} = \begin{bmatrix} 2.9995 \\ 1.0005 \\ 1.0004 \end{bmatrix}.$$

We, therefore, conclude that

$$x = \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix} \text{ i.e., } x = 3,\ y = 1 \text{ and } z = 1$$

(b) Gauss-Seidel method

As before, we obtain the first approximation as

$$X^{(1)} = \begin{bmatrix} 2.8499 \\ 1.0167 \\ 1.0333 \end{bmatrix}$$

Then

$$\begin{aligned}
x^{(2)} &= 3.3333 - 0.1667 \times 1.0167 - 0.1667 \times 1.0333 = 2.9916 \\
y^{(2)} &= 1.5 - 0.25 \times 2.9916 + 0.25 \times 1.0333 = 1.0104 \\
z^{(2)} &= 1.4 - 0.2 \times 2.9916 + 0.2 \times 1.0104 = 1.0038
\end{aligned}$$

Similarly, we find

$$\begin{aligned}
x^{(3)} &= 2.9975,\ y^{(3)} = 1.0016,\ z^{(3)} = 1.0008, \\
x^{(4)} &= 2.9995,\ y^{(4)} = 1.0003,\ z^{(4)} = 1.0002, \\
x^{(5)} &= 2.9998,\ y^{(5)} = 1.0001,\ z^{(5)} = 1.0001.
\end{aligned}$$

At this stage, we can conclude that

$$x = 3,\ y = 1,\ z = 1.$$

Example 5.8 Solve by Jacobi's iteration method, the equations

$20x + y - 2z = 17; 3x + 20y - z = -18; 2x - 3y + 20z = 25.$

Solution: We write the given equations in the form

$$\left.\begin{aligned}
x &= \frac{1}{20}(17 - y + 2z) \\
y &= \frac{1}{20}(-18 - 3x + z) \\
z &= \frac{1}{20}(25 - 2x + 3y)
\end{aligned}\right\} \quad \dots (i)$$

We start from an approximation $x_0 = y_0 = z_0 = 0$.

Substituting these on the right sides of the equations (i), we get

$$x_1 = \frac{17}{20} = 0.85,\ y_1 = \frac{18}{20} = -0.9,\ z_1 = \frac{25}{20} = 1.25$$

Putting these values on the right sides of the equations (i), we obtain

$$x_2 = \frac{1}{20}(17 - y1 + 2z_1) = 1.02$$
$$y_2 = \frac{1}{20}(-18 - 3x + z1) = -0.965$$
$$z_2 = \frac{1}{20}(25 - 2x1 + 3y_1) = 1.03$$

Substituting these values on the right sides of the equations (i), we have

$$x_3 = \frac{1}{20}(17 - y_2 + 2z_2) = 1.00125$$
$$y_3 = \frac{1}{20}(-18 - 3x_2 + z_2) = 1.0015$$
$$z_3 = \frac{1}{20}(25 - 2x_2 + 3y_2) = 1.00325$$

Substituting these values, we get

$$x_4 = \frac{1}{20}(17 - y_3 + 2z_3) = 1.0004$$
$$y_4 = \frac{1}{20}(-18 - 3x_3 + z_3) = -1.000025$$
$$z_4 = \frac{1}{20}(25 - 2x_3 + 3y_3) = 0.9965$$

Putting these values, we have

$$x_5 = \frac{1}{20}(-17 - y_4 + 2z_4) = 0.999966$$
$$y_5 = \frac{1}{20}(-18 - 3x_4 + z_4) = -1.000078$$
$$z_5 = \frac{1}{20}(25 - 2x_4 + 3y_4) = 0.999956$$

Again substituting these values, we get

$$x_6 \quad = \frac{1}{20}(-17 - y_5 + 2z_5) = 1.0000$$
$$y_6 \quad = \frac{1}{20}(-18 - 3x_5 + z_5) = 0.999997$$
$$z_6 \quad = \frac{1}{20}(25 - 2x_5 + 3y_5) = 0.999992$$

The values in the fifth and sixth iterations being practically the same, we can stop. Hence the solution is $x = 1, y = -1, z = 1$.

Example 5.9 Solve by Jacobi's iteration method, the equations $10x + y - z = 11.19$, $x + 10y + z = 28.08, -x + y + 10z = 35.61$, correct to two decimal places.

Solution: Rewriting the given equations as $x = \frac{1}{10}(11.19 - y + z), y = \frac{1}{10}(28.08 - x - z), z = \frac{1}{10}(35.61 + x - y)$

We start from an approximation, $x_0 = y_0 = z_0 = 0$. First iteration

$$x_1 = \frac{11.19}{10} = 1.119, y_1 = \frac{28.08}{10} = 2.808, z_1 = \frac{35.61}{10} = 3.561$$

Second iteration

$$\begin{aligned} x_2 &= \frac{1}{10}(11.19 - y_1 + z_1) = 1.19 \\ y_2 &= \frac{1}{10}(28.08 - x_1 - z_1) = 2.34 \\ z_2 &= \frac{1}{10}(35.61 + x_1 - y_1) = 3.39 \end{aligned}$$

Third iteration

$$\begin{aligned} x_3 &= \frac{1}{10}(11.19 - y_2 + z_2) = 1.22 \\ y_3 &= \frac{1}{10}(28.08 - x_2 - z_2) = 2.35 \\ z_3 &= \frac{1}{10}(35.61 + x_2 - y_2) = 3.45 \end{aligned}$$

Fourth iteration

$$\begin{aligned} x_4 &= \frac{1}{10}(11.19 - y_3 + z_3) = 1.23 \\ y_4 &= \frac{1}{10}(28.08 - x_3 - z_3) = 2.34 \\ z_4 &= \frac{1}{10}(35.61 + x_3 - y_3) = 3.45 \end{aligned}$$

Fifth iteration

$$x_5 = \frac{1}{10}(11.19 - y_4 + z_4) = 1.23$$
$$y_5 = \frac{1}{10}(28.08 - x_4 - z_4) = 2.34$$
$$z_5 = \frac{1}{10}(35.61 + x_4 - y_4) = 3.45$$

Hence $x = 1.23, y = 2.34, z = 3.45$

Example 5.10 Apply the Gauss-Seidel iteration method to solve the equations $20x + y - 2z = 17; 3x + 20y - z = -18; 2x - 3y + 20z = 25.$

Solution: We write the given equations in the form

$$x = \frac{1}{20}(17 - y + 2z) \qquad \dots(i)$$
$$y = \frac{1}{20}(-18 - 3x + z) \qquad \dots(ii)$$
$$z = \frac{1}{20}(25 - 2x + 3y) \qquad \dots(iii)$$

First iteration

Putting $y = y_0, z = z_0$ in first equation, we get $x_1 = \frac{1}{2}(17 - y_0 + 2z_0) = 0.8500$

Putting $x = x_1, z = z_0$ in second equation, we have $y_1 = \frac{1}{20}(-18 - 3x_1 + z_0) = -1.0275$

Putting $x = x_1, y = y_1$ in third equation, we obtain $z_1 = \frac{1}{20}(25 - 2x_1 + 3y_1) = 1.0109$

Second iteration

Putting $y = y_1, z = z_1$ in (i), we get $x_2 = \frac{1}{20}(17 - y_1 + 2z_1) = 1.0025$

Putting $x = x_2, z = z_1$ in (ii), we obtain $y_2 = \frac{1}{20}(-18 - 3x_2 + z_1) = -0.9998$

Putting $x = x_2, y = y_2$ in (iii), we get $z_2 = \frac{1}{20}(25 - 2x_2 + 3y_2) = 0.9998$ Third iteration, we get

$$
\begin{aligned}
x_3 &= \frac{1}{20}(17 - y_2 + 2z_2) = 1.0000 \\
y_3 &= \frac{1}{20}(-18 - 3x_3 + z_2) = -1.0000 \\
z_3 &= \frac{1}{20}(25 - 2x_3 + 3y_3) = 1.0000
\end{aligned}
$$

The values in the second and third iterations being practically the same, we can stop.

Hence the solution is $x = 1, y = -1, z = 1$.

Example 5.11 Solve the system of equations

$$
\begin{aligned}
4x_1 + x_2 + x_3 &= 2 \\
x_1 + 5x_2 + 2x_3 &= -6 \\
x_1 + 2x_2 + 3x_3 &= -4
\end{aligned}
$$

using the Jacobi iteration method. Take the initial approximation as $x^{(0)} = [0.5, -0.5, -0.5]^T$ and perform three iterations in each case. The exact solution is $x_1 = 1, x_2 = -1, x,= -1$.

Solution: We have

$$
\begin{aligned}
\mathbf{L} &= \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 2 & 0 \end{bmatrix}, \mathbf{D} = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 3 \end{bmatrix}, \mathbf{U} = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{bmatrix} \\
\mathbf{H} &= -\mathbf{D}^{-1}(\mathbf{L} + \mathbf{U}) = -\begin{bmatrix} 4 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 3 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 2 \\ 1 & 2 & 0 \end{bmatrix} \\
&= -\begin{bmatrix} 1/4 & 0 & 0 \\ 0 & 1/5 & 0 \\ 0 & 0 & 1/3 \end{bmatrix} \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 2 \\ 1 & 2 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -1/4 & -1/4 \\ -1/5 & 0 & -2/5 \\ -1/3 & -2/3 & 0 \end{bmatrix} \\
\mathbf{c} &= \mathbf{D}^{-1}\mathbf{b} = \begin{bmatrix} 1/4 & 0 & 0 \\ 0 & 1/5 & 0 \\ 0 & 0 & 1/3 \end{bmatrix} \begin{bmatrix} 2 \\ -6 \\ -4 \end{bmatrix} = \begin{bmatrix} 1/2 \\ -6/5 \\ -4/3 \end{bmatrix}
\end{aligned}
$$

Therefore, Jacobi iteration method becomes

$$\mathbf{x}^{(k+1)} = \begin{bmatrix} 0 & -1/4 & -1/4 \\ -1/5 & 0 & -2/5 \\ -1/3 & -2/3 & 0 \end{bmatrix} \mathbf{x}^{(k)} + \begin{bmatrix} 1/2 \\ -6/5 \\ -4/3 \end{bmatrix}, k = 0,1, \ldots$$

Starting with $\mathbf{x}^{(0)} = [0.5, -0.5, -0.5]^T$, we obtain

$$\mathbf{x}^{(1)} = \begin{bmatrix} 0.75 \\ -1.1 \\ -1.1667 \end{bmatrix}, \mathbf{x}^{(2)} = \begin{bmatrix} 1.0667 \\ -0.8833 \\ -0.8500 \end{bmatrix}, \mathbf{x}^{(3)} = \begin{bmatrix} 0.9333 \\ -1.0733 \\ -1.1000 \end{bmatrix}$$

Alternately, we may write directly

$$x_1^{(k+1)} = \frac{1}{4}\left[2 - x_2^{(k)} - x_3^{(k)}\right], x_2^{(k+1)} = \frac{1}{5}\left[-6 - x_1^{(k)} - 2x_3^{(k)}\right]$$
$$x_3^{(k+1)} = \frac{1}{3}\left[-4 - x_1^{(k)} - 2x_2^{(k)}\right]$$

Starting with $x_1^{(0)} = 0.5, x_2^{(0)} = -0.5, x_3^{(0)} = -0.5$, we get

$$\mathbf{x}^{(1)} = [0.75, -1.1, -1.1667]^T, \mathbf{x}^{(2)} = [1.0667, -0.8833, -0.8500]^T$$
$$\mathbf{x}^{(3)} = [0.9333, -1.0733, -1.1000]^T.$$

Example 5.12 Solve the system of equations

$$2x_1 - x_2 + 0x_3 = 7$$
$$-x_1 + 2x_2 - x_3 = 1$$
$$0x_1 - x_2 + 2x_3 = 1$$

using the Gauss-Seidel method. Take the initial approximation as $\mathbf{x}^{(0)} = \mathbf{0}$ and perform three iterations.

Solution: We have

$$\mathbf{D} + \mathbf{L} = \begin{bmatrix} 2 & 0 & 0 \\ -1 & 2 & 0 \\ 0 & -1 & 2 \end{bmatrix}, \mathbf{U} = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{bmatrix}$$

The Gauss-Seidel method gives

$$\mathbf{x}^{(k+1)} = -(\mathbf{D} + \mathbf{L})^{-1}\mathbf{U}\mathbf{x}^{(k)} + (\mathbf{D} + \mathbf{L})^{-1}\mathbf{b}.$$

We get

$$(\mathbf{D}+\mathbf{L})^{-1} = \begin{bmatrix} 2 & 0 & 0 \\ -1 & 2 & 0 \\ 0 & -1 & 2 \end{bmatrix}^{-1} = \begin{bmatrix} 1/2 & 0 & 0 \\ 1/4 & 1/2 & 0 \\ 1/8 & 1/4 & 1/2 \end{bmatrix}$$

$$(\mathbf{D}+\mathbf{L})^{-1}\mathbf{U} = \begin{bmatrix} 1/2 & 0 & 0 \\ 1/4 & 1/2 & 0 \\ 1/8 & 1/4 & 1/2 \end{bmatrix}\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -1/2 & 0 \\ 0 & -1/4 & -1/2 \\ 0 & -1/8 & -1/4 \end{bmatrix}$$

$$(\mathbf{D}+\mathbf{L})^{-1}\mathbf{b} = \begin{bmatrix} 1/2 & 0 & 0 \\ 1/4 & 1/2 & 0 \\ 1/8 & 1/4 & 1/2 \end{bmatrix}\begin{bmatrix} 7 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 7/2 \\ 9/4 \\ 13/8 \end{bmatrix}$$

Therefore, we obtain the iteration scheme

$$\mathbf{x}^{(k+1)} = \begin{bmatrix} 0 & 1/2 & 0 \\ 0 & 1/4 & 1/2 \\ 0 & 1/8 & 1/4 \end{bmatrix}\mathbf{x}^{(k)} + \begin{bmatrix} 7/2 \\ 9/4 \\ 13/8 \end{bmatrix}$$

Starting with zero initial vector, we get

$$\mathbf{x}^{(1)} = \begin{bmatrix} 3.5 \\ 2.25 \\ 1.625 \end{bmatrix}, \mathbf{x}^{(2)} = \begin{bmatrix} 4.625 \\ 3.625 \\ 2.3125 \end{bmatrix}, \text{ and } \mathbf{x}^{(3)} = \begin{bmatrix} 5.3125 \\ 4.3125 \\ 2.6563 \end{bmatrix}$$

The exact solution is $\mathbf{x} = [6,5,3]^T$.

POWER METHOD

In many engineering problems, it is required to compute the numerically largest eigenvalue and the corresponding eigenvector. In such cases, the following iterative method is quite convenient which is also well-suited for machine computations.

If $X_1, X_2 \cdots X_n$ are the eigenvectors corresponding to the eigenvalues λ_1, $\lambda_2, \cdots \lambda_n$, then an arbitrary column vector can be written as

$$X = k_1X_1 + k_2X_2 + \cdots + k_nX_n$$

Then

$$
\begin{aligned}
AX &= k_1AX_1 + k_2AX_2 + \cdots + k_nAX_n \\
&= k_1\lambda_1X_1 + k_2\lambda_2X_2 + \cdots + k_n\lambda_nX_n
\end{aligned}
$$

Similarly $A^2X = k_1\lambda_1{}^2X_1 + k_2\lambda_2{}^2X_2 + \cdots + k_n\lambda_n{}^2X_n$

and

$$A^rX = k_1\lambda_1rX_1 + k_2\lambda_2rX_2 + \cdots + k_n\lambda_n{}^rX_n$$

If $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$, then λ_1 is the largest root and the contribution of the term $k_1\lambda_1^rX_1$ to the sum on the right increases with r and, therefore, every time we multiply a column vector by A, it becomes nearer to the eigenvector X_1. Then we make the largest component of the resulting column vector unity to avoid the factor k_1.

Thus we start with a column vector X which is as near the solution as possible and evaluate AX which is written as $\lambda^{(1)}X^{(1)}$ after normalization. This gives the first approximation $\lambda^{(1)}$ to the eigenvalue and $X^{(1)}$ to the eigenvector. Similarly we evaluate $AX^{(1)} = \lambda^{(2)}X^{(2)}$ which gives the second approximation. We repeat this process until $\left[X^{(r)} - X^{(r-1)}\right]$ becomes negligible. Then $\lambda^{(r)}$ will be the largest eigenvalue and $X^{(r)}$, the corresponding eigenvector.

This iterative procedure for finding the dominant eigenvalue of a matrix is known as Rayleigh's power method.

NOTE: Rewriting $AX = \lambda X$ as $A^{-1}AX = \lambda A^{-1}X$ or $X = \lambda A^{-1}X$.

We have $A^{-1}X = \frac{1}{\lambda}X$

If we use this equation, then the above method yields the smallest eigenvalue.

Example 5.13 Determine the largest eigenvalue and the corresponding eigenvector of the matrix $\begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix}$.

Solution: Let the initial approximation to the eigenvector corresponding to the largest eigenvalue of A be $X = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

Then $AX = \begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 5 \\ 1 \end{bmatrix} = 5\begin{bmatrix} 1 \\ 0.2 \end{bmatrix} = \lambda^{(1)}X^{(1)}$

So the first approximation to the eigenvalue is $\lambda^{(1)} = 5$ and the corresponding eigenvector is $\mathrm{X}^{(1)} = \begin{bmatrix} 1 \\ 0.2 \end{bmatrix}$

Now $AX^{(1)} = \begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0.2 \end{bmatrix} = \begin{bmatrix} 5.8 \\ 14 \end{bmatrix} = 5.8\begin{bmatrix} 1 \\ 0.241 \end{bmatrix} = \lambda^{(2)}X^{(2)}$

Thus the second approximation to the eigenvalue is $\lambda^{(2)} = 5.8$ and the corresponding eigenvector is $X^{(2)} = \begin{bmatrix} 1 \\ 0.241 \end{bmatrix}$, repeating the above process, we get

$$
\begin{aligned}
AX^{(2)} &= \begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0.241 \end{bmatrix} = 5.966\begin{bmatrix} 1 \\ 0.248 \end{bmatrix} = \lambda^{(3)}X^{(3)} \\
AX^{(3)} &= \begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0.249 \end{bmatrix} = 5.966\begin{bmatrix} 1 \\ 0.250 \end{bmatrix} = \lambda^{(4)}X^{(4)} \\
AX^{(4)} &= \begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0.250 \end{bmatrix} = 5.999\begin{bmatrix} 1 \\ 0.25 \end{bmatrix} = \lambda^{(5)}X^{(5)} \\
AX^{(5)} &= \begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0.25 \end{bmatrix} = 6\begin{bmatrix} 1 \\ 0.25 \end{bmatrix} = \lambda^{(6)}X^{(6)}
\end{aligned}
$$

Clearly $\lambda^{(5)} = \lambda^{(6)}$ and $X^{(5)} = X^{(6)}$ upto 3 decimal places. Hence the largest eigenvalue is 6 and the corresponding eigenvector is $\begin{bmatrix} 1 \\ 0.25 \end{bmatrix}$

Example 5.14 Find the largest eigenvalue and the corresponding eigenvector of the Matrix $\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$ using the power method. Take $[1,0,0]^T$ as the initial eigenvector.

Solution: Let the initial approximation to the required eigenvector be $X = [1,0,0]'$.

Then $AX = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ -1 \\ 0 \end{bmatrix} = 2\begin{bmatrix} 1 \\ -0.5 \\ 0 \end{bmatrix} = \lambda^{(1)}X^{(1)}$

So the first approximation to the eigenvalue is 2 and the corresponding eigenvector

$X^{(1)} = [1, -0.5, 0]'$.

$$\text{Hence } AX^{(1)} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ -0.5 \\ 0 \end{bmatrix} = \begin{bmatrix} 2.5 \\ -2 \\ 0.5 \end{bmatrix} = \begin{bmatrix} 1 \\ -0.8 \\ 0.2 \end{bmatrix} = \lambda^{(2)} X^{(2)}$$

Repeating the above process, we get

$$AX^{(2)} = 2.8 \begin{bmatrix} 1 \\ -1 \\ 0.43 \end{bmatrix} = \lambda^{(3)} X^{(3)};\; AX^{(3)} = 3.43 \begin{bmatrix} 0.87 \\ -1 \\ 0.54 \end{bmatrix} = \lambda^{(4)} X^{(4)}$$

$$AX^{(4)} = 3.41 \begin{bmatrix} 0.80 \\ -1 \\ 0.61 \end{bmatrix} = \lambda^{(5)} X^{(5)};\; AX^{(5)} = 3.41 \begin{bmatrix} 0.76 \\ -1 \\ 0.65 \end{bmatrix} = \lambda^{(6)} X^{(6)}$$

$$AX^{(6)} = 3.41 \begin{bmatrix} 0.74 \\ -1 \\ 0.67 \end{bmatrix} = \lambda^{(7)} X^{(7)}$$

Clearly $\lambda^{(6)} = \lambda^{(7)}$ and $X^{(6)} = X^{(7)}$ approximately. Hence the largest eigenvalue is 3.41 and the corresponding eigenvector is $[0.74, -1, 0.67]'$

Example 5.15 Obtain by the power method, the numerically dominant eigenvalue and eigenvector of the matrix

$$A = \begin{bmatrix} 15 & -4 & -3 \\ -10 & 12 & -6 \\ -20 & 4 & -2 \end{bmatrix}.$$

Solution: Let the initial approximation to the eigenvector be $X = [1,1,1]'$. Then

$$AX = \begin{bmatrix} 15 & -4 & -3 \\ -10 & 12 & -6 \\ -20 & 4 & -2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 8 \\ -4 \\ -18 \end{bmatrix} = -18 \begin{bmatrix} -0.444 \\ 0.222 \\ 1 \end{bmatrix} = \lambda^{(1)} X^{(1)}$$

So the first approximation to eigenvalue is -18 and the corresponding eigenvector is $[-0.444, 0.222, 1]'$.

$$\text{Now } AX^{(1)} = \begin{bmatrix} 15 & -4 & -3 \\ -10 & 12 & -6 \\ -20 & 4 & -2 \end{bmatrix} \begin{bmatrix} -0.444 \\ 0.222 \\ 1 \end{bmatrix} = -10.548 \begin{bmatrix} 1 \\ -0.105 \\ -0.736 \end{bmatrix} = \lambda^{(1)} X^{(2)}$$

$\therefore$ The second approximation to the eigenvalue is -10.548 and the eigenvector is $[1, -0.105, -0.736]'$.

Repeating the above process

$$AX^{(2)} = -18.948\begin{bmatrix}-0.930\\0.361\\1\end{bmatrix} = \lambda^3 X^{(3)}; AX^{(3)} = -18.394\begin{bmatrix}1\\-0.415\\-0.981\end{bmatrix} = \lambda^4 X^{(4)}$$
$$AX^{(4)} = -19.698\begin{bmatrix}-0.995\\0.462\\1\end{bmatrix} = \lambda^{(5)} X^{(5)}; AX^{(5)} = -19.773\begin{bmatrix}1\\-480\\-0.999\end{bmatrix} = \lambda^{(6)} X^{(6)}$$
$$AX^{(6)} = -19.922\begin{bmatrix}-0.997\\0.490\\1\end{bmatrix} = \lambda^{(7)} X^{(7)}; AX^{(7)} = -19.956\begin{bmatrix}1\\-495\\-0.999\end{bmatrix} = \lambda^{(8)} X^{(8)}$$

Since $\lambda^{(7)} = \lambda^{(8)}$ and $X^{(7)} = X^{(8)}$ approximately, therefore the dominant eigenvalue and the corresponding eigenvector are given by

$$\lambda^{(8)} X^{(8)} = 19.956\begin{bmatrix}-1\\0.495\\0.999\end{bmatrix} \text{ i.e., } 20\begin{bmatrix}-1\\0.5\\1\end{bmatrix}$$

Hence the dominant eigenvalue is 20 and eigenvector is $[-1,0.5,1]'$.

RELAXATION METHOD

Consider the equations

$a_1x + b_1y + c_1z = d_1$
$a_2x + b_2y + c_2z = d_2$ We define the residuals R_x, R_y, R_z by the relations
$a_3x + b_3y + c_3z = d_3$

$$\left.\begin{aligned}R_x &= d_1 - a_1x - b_1y - c_1z\\R_y &= d_2 - a_2x - b_2y - c_2z\\R_z &= d_3 - a_3x - b_3y - c_3z\end{aligned}\right\} \quad \ldots (5.22)$$

To start with we assume $x = y = z = 0$ and calculate the initial residuals. Then the residuals are reduced step by step, by giving increments to the variables. For this purpose, we construct the following operation table:

	δR_x	δR_y	$\delta \mathrm{R}_z$
$\delta x = 1$	$-a_1$	$-a_2$	$-a_3$
$\delta y = 1$	$-b_1$	$-b_2$	$-b_3$
$\delta z = 1$	$-c_1$	$-c_2$	$-c_3$

We note from the equations (5.22) that if x is increased by 1 (keeping y and z constant), $R_{x^2}, R_{y'}$, and R_z decrease by a_1, a_2, a_3, respectively. This is shown in the above table along with the effects on the residuals when y and z are given unit increments. (The table is the transpose of the coefficient matrix).

At each step, the numerically largest residual is reduced to almost zero. To reduce a particular residual, the value of the corresponding variable is changed; e.g., to reduce R_x by p, x should be increased by p/a_1. When all the residuals have been reduced to almost zero, the increments in x, y, z are added separately to give the desired solution.

Relaxation method can be applied successfully only if the diagonal elements of the coefficient matrix dominate the other coefficients in the corresponding row, i.e., if in the equations (5.22)

$$|a_1| \geq |b_1| + |c_1|$$
$$|b_2| \geq |a2| + |c_2|$$
$$|c_3| \geq |a_3| + |b_3|$$

where $>$ sign should be valid for at least one row.

Example 5.16 Solve the equations:

$10x - 2y - 3z = 205; -2x + 10y - 2z = 154; -2x - y + 10z = 120$ by Relaxation method.

The residuals are given by

$$R_x = 205 - 10x + 2y + 3z$$
$$R_y = 154 + 2x - 10y + 2z$$
$$R_z = 120 + 2x + y - 10z$$

The operations table is

	δR_x	δR_y	δR_z
$\delta x = 1$	-10	2	2
$\delta y = 1$	2	-10	1
$\delta z = 1$	3	2	-10

The relaxation table is

	R_x	R_y	R_z
$x = y = z = 0$	205	154	120
$\delta x = 20$	5	194	160
$\delta y = 19$	43	4	179
$\delta z = 18$	97	40	-1
$\delta x = 10$	-3	60	19
$\delta y = 6$	9	0	25
$\delta z = 2$	15	4	5
$\delta x = 2$	-5	8	9
$\delta z = 1$	-2	10	-1
$\delta y = 1$	0	0	0
$\Sigma\delta x = 32, \Sigma\delta y = 26, \Sigma\delta z = 21$			

Hence $x = 32, y = 26, z = 21$.

5.5 CHECK YOUR PROGRESS

1. Use Jacobi and Gauss-Seidal methods to solve the following equations correct up to three decimal places.

   (i) $10x + 2y + z = 9, 2x + 20y - 2z = -44, -2x + 3y + 10z = 22$

   (ii) $83x + 11y - 4z = 95, 7x + 52y + 13z = 104, 3x + 8y + 29z = 71$

2. Use relaxation method to solve

   (i) $3x + 9y - 2z = 11, 4x + 2y + 13z = 24, 4x - 4y + 3z = -8$

   (ii) $10x - 2y - 2z = 6, -x + 10y - 2z = 7, -x - y + 10z = 8.$

3. Find the largest eigenvalue and corresponding eigenvectors of the matrix by power method

$$\begin{bmatrix} 10 & -2 & 1 \\ -2 & 10 & -2 \\ 1 & -2 & 10 \end{bmatrix}.$$

5.6 SUMMARY

The students are made familiar with some preliminary definitions and fundamental results of various iterative solution of system of linear equation.

5.7 KEYWORDS

Linear Systems, Jacobi's method, Gauss-Seidel method, SOR, Relaxation method, Power method, Ill-conditioned Systems.

5.8 SELF-ASSESSMENT TEST

1. Solve by Jacobi's method, the equations: $5x - y + z = 10; 2x + 4y = 12; x + y + 5z = -1$; starting with the solution $(2,3,0)$.
2. Solve by Jacobi's method the equations:

   $13x + 5y - 3z + u = 18; 2x + 12y + z - 4u = 13; x - 4y + 10z + u = 29;$

   $2x + y - 3z + 9u = 31.$
3. Solve the equations $27x + 6y - z = 85; x + y + 54z = 40; 6x + 15y + 2z = 72$ by (i) Jacobi's method (ii) Gauss-Seidal method.
4. Solve, by the Relaxation method, the following equations:

   $3x + 9y - 2z = 11; 4x + 2y + 13z = 24; 4x - 4y + 3z = -8.$

5.9 ANSWERS TO CHECK YOUR PROGRESS

1. (i) x=1.013, y= -1.996, z= 3.001

(ii) x=1.052, y= -1.369, z= 1.962

2. (i) x=1.35, y= 2.103, z= 2.845

(ii) x= y= z= 1

3. 9, $[1 \;\; 0 \;\; -1]^T$

5.10 REFERENCES/ SUGGESTED READINGS

1. JAMES F. EPPERSON; An Introduction to Numerical Methods and analysis. Second Edition Mathematical Reviews, John Wiley & Sons, Inc., Hoboken, New Jersey.
2. S S Shastry; Introductory Methods of Numerical Analysis, Fifth Edition ISBN-978-81-203-4592-8, Asoke K. Ghosh, PHI Learning Pvt. Ltd, M-97, Connaught Circus, New Delhi
3. C.F. Gerald and P.O. Wheatley : Applied Numerical Methods, Low- priced edition, Pearson Education Asia (2002), Sixth Edition.
4. D. Kincaid and W. Cheney, Numerical Analysis: Mathematics of Scientific Computing, 3rd Edn., AMS (2002).
5. D.V. Griffiths and I.M. Smith, Numerical Methods for Engineers, Blackwell Scientific Publications (1991).
6. John H Mathews, Numerical Methods for Mathematics, Science and Engineering, Prentice Hall of India (1994).
7. K. E. Atkinson, Introduction to Numerical Analysis, 2nd Edn., John Wiley (1989).
8. M.K. Jain: Numerical Solution of Differential Equations, 4th Edition, New Age (2018).

MAL-526: M. Sc. Mathematics (Advanced Numerical Methods)

LESSON No. 6 Written by- Dr. Joginder Singh

SYSTEM OF NONLINEAR EQUATIONS

STRUCTURE

6.0 LEARNING OBJECTIVES

Students are able to

- Solve nonlinear equations using various iterative methods : Newton Raphson method, General iterative method.
- Find complex roots.

6.1 INTRODUCTION

In this chapter we shall consider some numerical methods for the solution of nonlinear systems which can well be manipulated and managed on digital computers and microprocessors. We consider a system of two nonlinear equations in two unknowns as

$$\begin{aligned} f(x,y) &= 0 \\ g(x,y) &= 0 \end{aligned} \qquad \ldots (6.1)$$

6.2 SOLUTION OF NONLINEAR EQUATIONS

Let (x_k, y_k) be a suitable approximation to the root (ξ, η) of the system (6.1). Let Δx be an increment in x_k and Δy be an increment in y_k such that $(x_k + \Delta x, y_k + \Delta y)$ is the exact solution, that is

$$
\begin{aligned}
f(x_k + \Delta x, y_k + \Delta y) &\equiv 0 \\
g(x_k + \Delta x, y_k + \Delta y) &\equiv 0.
\end{aligned}
$$

Expanding in Taylor series about the point (x_k, y_k), we get

$$
\begin{aligned}
f(x_k, y_k) + \left[\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y}\right] f(x_k, y_k) + \frac{1}{2!}\left[\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y}\right]^2 f(x_k, y_k) + \cdots &= 0 \\
g(x_k, y_k) + \left[\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y}\right] g(x_k, y_k) + \frac{1}{2!}\left[\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y}\right]^2 g(x_k, y_k) + \cdots &= 0.
\end{aligned}
$$

Neglecting second and higher powers of Δx and Δy, we obtain

$$
\begin{aligned}
f(x_k, y_k) + \Delta x f_x(x_k, y_k) + \Delta y f_y(x_k, y_k) &= 0 \\
g(x_k, y_k) + \Delta x g_x(x_k, y_k) + \Delta y g_y(x_k, y_k) &= 0
\end{aligned}
\qquad \text{... (6.2)}
$$

where suffixes with respect to x and y represent partial differentiation.

Solving above equations for Δx and Δy, we get

$$
\begin{aligned}
\Delta x &= -\frac{1}{D_k}\left[f(x_k, y_k) g_y(x_k, y_k) - g(x_k, y_k) f_y(x_k, y_k)\right] \\
\Delta y &= -\frac{1}{D_k}\left[g(x_k, y_k) f_x(x_k, y_k) - f(x_k, y_k) g_x(x_k, y_k)\right]
\end{aligned}
$$

where

$$D_k = f_x(x_k, y_k) g_y(x_k, y_k) - g_x(x_k, y_k) f_y(x_k, y_k).$$

We obtain

$$x_{k+1} = x_k + \Delta x, \text{ and } y_{k+1} = y_k + \Delta y.$$

Writing the equations (6.2) in matrix form, we get

$$\begin{bmatrix} f_x(x_k, y_k) & f_y(x_k, y_k) \\ g_x(x_k, y_k) & g_y(x_k, y_k) \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = -\begin{bmatrix} f(x_k, y_x) \\ g(x_k, y_k) \end{bmatrix}$$

or

$$\boldsymbol{J}_k \Delta \boldsymbol{x} = -\boldsymbol{F}(x_k, y_k) \qquad \ldots (6.3)$$

where

$$\boldsymbol{J}_k = \begin{bmatrix} f_x & f_y \\ g_x & g_y \end{bmatrix}_{(x_k, y_k)}, \boldsymbol{F} = \begin{bmatrix} f \\ g \end{bmatrix}_{(x_k, y_k)}, \Delta x = \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix}$$

The solution of the system (6.3) is

$$\begin{aligned} \Delta \boldsymbol{x} &= -\boldsymbol{J}_k^{-1} \boldsymbol{F}(x_k, y_k) \\ \boldsymbol{J}_k^{-1} &= \begin{bmatrix} f_x & f_y \\ g_x & g_y \end{bmatrix}_{(x_k, y_k)}^{-1} = \frac{1}{D_k} \begin{bmatrix} g_y & -f_y \\ -g_x & f_x \end{bmatrix}_{(x_k, y_k)} \end{aligned}$$

Therefore, we can write

$$\begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = -J_k^{-1} \begin{bmatrix} f(x_k, y_k) \\ g(x_k, y_k) \end{bmatrix}$$

and $\begin{bmatrix} x_{k+1} \\ y_{k+1} \end{bmatrix} = \begin{bmatrix} x_k \\ y_k \end{bmatrix} + \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} x_k \\ y_k \end{bmatrix} - J_k^{-1} \begin{bmatrix} f(x_k, y_k) \\ g(x_k, y_k) \end{bmatrix}, k = 0, 1, \cdots$

or

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - \boldsymbol{J}_k^{-1} \boldsymbol{F}\left(x^{(k)}\right)$$

where

$$\boldsymbol{x}^{(k)} = \left[x^{(k)}, y^{(k)}\right]^T, F\left(\boldsymbol{x}^{(k)}\right) = [f(x_k, y_k), g(x_k, y_k)]^T.$$

This is known as **Newton-Raphson's** method. This method can be easily generalized for solving a system of n equations in n unknowns

$$f_1(x_1, x_2, \cdots, x_n) = 0$$

$$f_2(x_1, x_2, \cdots, x_n) = 0$$
$$\cdots \;\; \cdots$$
$$f_n(x_1, x_2, \cdots, x_n) = 0$$

or

$$\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{0}$$

where $\boldsymbol{x} = [x_1, x_2, \cdots, x_n]^T, \boldsymbol{F} = [f_1, f_2, \cdots, f_n]^T$.

If $\boldsymbol{x}^{(0)} = \left[x_1^{(0)}, x_2^{(0)}, \cdots, x_n{}^{(0)}\right]^T$ is an initial approximation to the solution vector $\boldsymbol{x}$, then we can write , the method as

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - \boldsymbol{J}_k^{-1}\boldsymbol{F}\left(\boldsymbol{x}^{(k)}\right), k = 0,1, \cdots$$

where

$$\boldsymbol{J}_k = \begin{bmatrix} \partial f_1/\,\partial x_1 & \partial f_1/\,\partial x_2 & \cdots & \partial f_1/\,\partial x_n \\ \partial f_2/\,\partial x_1 & \partial f_2/\,\partial x_2 & \cdots & \partial f_2/\,\partial x_n \\ \vdots & & \cdots & \\ \partial f_n/\,\partial x_1 & \partial f_n/\,\partial x_2 & \cdots & \partial f_n/\,\partial x_n \end{bmatrix}_{\left(x^{(k)}\right)}$$

is the Jacobian matrix of the functions $f_1, f_2, \cdots, f_n$ evaluated at $\boldsymbol{x}^{(k)}$.

Note that the matrix J_k^{-1} is to be evaluated for each iteration. We can also write the method as

$$J_k\left(\boldsymbol{x}^{(k+1)} - \boldsymbol{x}^{(k)}\right) = -\boldsymbol{F}\left(\boldsymbol{x}^{(k)}\right)$$

or

$$J_k\boldsymbol{\varepsilon}^{(k)} = -\boldsymbol{F}\left(\boldsymbol{x}^{(k)}\right)$$

where

$\boldsymbol{\varepsilon}^{(k)} = \boldsymbol{x}^{(k+1)} - \boldsymbol{x}^{(k)}$ is the error vector.

We solve it as a linear system of equations (by a direct method if the system is small and by an iterative method if the system is large) for each iteration.

The convergence of the method depends on the initial approximate vector $\boldsymbol{x}^{(0)}$. A sufficient condition for convergence is that for each k

$$\|\boldsymbol{J}_k^{-1}\| < 1$$

whereas a necessary and sufficient condition for convergence is

$$\rho(J_k^{-1}) < 1.$$

where $\|\cdot\|$ is a suitable norm and $\rho(\boldsymbol{J}_k^{-1})$ is the spectral radius (largest eigen value in magnitude) of the matrix J_k^{-1}.

If the method converges, then its rate of convergence is two. The iterations are stopped when

$$\|x^{(k+1)} - x^{(k)}\| < \varepsilon$$

where ε is the given error tolerance. We may use either the L_2 norm or the maximum norm.

Example 6.1   Perform three iterations of the Newton-Raphson method to solve the system of equations

$$\begin{aligned} x^2 + xy + y^2 &= 7 \\ x^3 + y^3 &= 9. \end{aligned}$$

Solution: Take the initial approximation as $x_0 = 1.5, y_0 = 0.5$. The exact solution is $x = 2, y = 1$. We have

$$\begin{aligned} f(x,y) &= x^2 + xy + y^2 - 7 \\ g(x,y) &= x^3 + y^3 - 9 \\ J_k &= \begin{bmatrix} f_x(x_k,y_k) & f_y(x_k,y_k) \\ g_x(x_k,y_k) & g_y(x_k,y_k) \end{bmatrix} = \begin{bmatrix} 2x_k + y_k & x_k + 2y_k \\ 3x_k^2 & 3y_k^2 \end{bmatrix} \\ J_k^{-1} &= \frac{1}{D_k}\begin{bmatrix} 3y_k^2 & -(x_k + 2y_k) \\ -3x_k^2 & 2x_k + y_k \end{bmatrix} \end{aligned}$$

where

$$D_k = |J_k| = 3y_k^2(2x_k + y_k) - 3x_k^2(x_k + 2y_k).$$

We can now write the method as

$$\begin{bmatrix} x_{k+1} \\ y_{k+1} \end{bmatrix} = \begin{bmatrix} x_k \\ y_k \end{bmatrix} - \frac{1}{D_k}\begin{bmatrix} 3y_k^2 & -(x_k + 2y_k) \\ -3x_k^2 & 2x_k + y_k \end{bmatrix}\begin{bmatrix} x_k^2 + x_k y_k + y_k^2 - 7 \\ x_k^3 + y_k^3 - 9 \end{bmatrix}$$
$$k = 0,1,\cdots$$

Using $(x_0, y_0) = (1.5, 0.5)$, we get

$$\begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 0.5 \end{bmatrix} - \frac{1}{-14.25}\begin{bmatrix} 0.75 & -2.5 \\ -6.75 & 3.5 \end{bmatrix}\begin{bmatrix} -3.75 \\ -5.50 \end{bmatrix} = \begin{bmatrix} 2.2675 \\ 0.9254 \end{bmatrix}$$
$$\begin{bmatrix} x_2 \\ y_2 \end{bmatrix} = \begin{bmatrix} 2.2675 \\ 0.9254 \end{bmatrix} - \frac{1}{-49.4951}\begin{bmatrix} 2.5691 & -4.1183 \\ -15.4247 & 5.4604 \end{bmatrix}\begin{bmatrix} 1.0963 \\ 3.4510 \end{bmatrix} = \begin{bmatrix} 2.0373 \\ 0.9645 \end{bmatrix}$$
$$\begin{bmatrix} x_3 \\ y_3 \end{bmatrix} = \begin{bmatrix} 2.0373 \\ 2.9645 \end{bmatrix} - \frac{1}{-35.3244}\begin{bmatrix} 2.7908 & -3.9663 \\ -12.4518 & 5.0391 \end{bmatrix}\begin{bmatrix} 0.0458 \\ 0.3532 \end{bmatrix} = \begin{bmatrix} 2.0013 \\ 0.9987 \end{bmatrix}$$

GENERAL ITERATION METHOD

Consider the solution of the following system of equations

$$f(x, y) = 0$$
$$g(x, y) = 0.$$

We may write this system in an equivalent form as

$$x = F(x, y)$$
$$y = G(x, y) \qquad \text{... (6.4)}$$

Let (ξ, η) be a solution of this system. Therefore, (ξ, η) satisfies the equations

$$\xi = F(\xi, \eta)$$

$$\eta = G(\xi, \eta) \qquad \ldots (6.5)$$

Let (x_0, y_0) be a suitable approximation to (ξ, η). Then, we write a general iteration method for the solution of (6.4) as

$$x_{k+1} = F(x_k, y_k)$$
$$y_{k+1} = G(x_k, y_k), k = 0,1,2,\cdots \qquad \text{... (6.6)}$$

If the method converges, then

$$\lim_{x\to\infty} x_k = \xi \text{ and } \lim_{x\to\infty} y_k = \eta.$$

The functions F and G are called the iteration functions. Not all forms of F and G can lead to convergence. Subtracting (6.6) from (6.5), we get

$$\begin{aligned}\xi - x_{k+1} &= F(\xi,\eta) - F(x_k, y_k)\\ \eta - y_{k+1} &= G(\xi,\eta) - G(x_k, y_k).\end{aligned}$$

Let $\varepsilon_k = \xi - x_k$ and $\delta_k = \eta - y_k$ be the errors in the k th iterate. Then, we obtain

$$\begin{aligned}\varepsilon_{k+1} &= F(x_k + \varepsilon_k, y_k + \delta_k) - F(x_k, y_k)\\ \delta_{k+1} &= G(x_k + \varepsilon_k, y_k + \delta_k) - G(x_k, y_k).\end{aligned}$$

Expanding in Taylor series about (x_k, y_k) and neglecting the second and higher powers of ε_k, δ_k, we obtain

$$\begin{aligned}\varepsilon_{k+1} &= \varepsilon_k F_x(x_k, y_k) + \delta_k F_y(x_k, y_k)\\ \delta_{k+1} &= \varepsilon_k G_x(x_k, y_k) + \delta_k G_y(x_k, y_k)\\ \begin{bmatrix}\varepsilon_{k+1}\\ \delta_{k+1}\end{bmatrix} &= \begin{bmatrix}F_x(x_k, y_k) & F_y(x_k, y_k)\\ G_x(x_k, y_k) & G_y(x_k, y_k)\end{bmatrix}\begin{bmatrix}\varepsilon_k\\ \delta_k\end{bmatrix}\\ \boldsymbol{\varepsilon}^{(k+1)} &= \boldsymbol{A}_k \boldsymbol{\varepsilon}^{(k)}\end{aligned}$$

where $\boldsymbol{\varepsilon}^{(k)} = [\varepsilon_k, \delta_k]^T$ and $\boldsymbol{A}_k = \begin{bmatrix}F_x(x_k, y_k) & F_y(x_k, y_k)\\ G_x(x_k, y_k) & G_y(x_k, y_x)\end{bmatrix}$

is the Jacobian matrix of the iteration functions F and G evaluated at (x_k, y_k).

A sufficient condition for convergence is that for each $k, \|A_k\| < 1$, where $\| . \|$ is a suitable norm.

If we use the maximum absolute row sum norm, we get the conditions

$$\begin{aligned}|F_x(x_k, y_k)| + |F_y(x_k, y_k)| &< 1\\ |G_x(x_k, y_k)| + |G_y(x_k, y_k)| &< 1.\end{aligned} \qquad \text{... (6.7)}$$

The necessary and sufficient condition for convergence is that for each k

$$\rho(\mathbf{A}_k) < 1$$

where $\rho(\mathbf{A}_k)$ is the spectral radius of the matrix $\mathbf{A}_k$.

If (x_0, y_0) is a close approximation to the root (ξ, η), then we usually test the conditions (6.7) at the initial approximation (x_0, y_0).

The method can be easily generalized to a system of n equations in n unknowns.

Example 6.2 The system of equations

$$\begin{aligned} f(x,y) &= x^2 + 3x + y - 5 = 0 \\ g(x,y) &= x^2 + 3y^2 - 4 = 0 \end{aligned}$$

has a solution $(1,1)$. Determine the iteration functions $F(x,y)$ and $G(x,y)$ so that the sequence of iterates obtained from

$$\begin{aligned} x_{k+1} &= F(x_k, y_k) \\ y_{k+1} &= G(x_k, y_k), k = 0,1,\cdots \end{aligned}$$

$(x_0, y_0) = (0.5,0.5)$ converges to the root. Perform five iterations.

Solution: We write the given system of equations in an equivalent form as

$$\begin{aligned} x &= x + \alpha(x^2 + 3x + y - 5) = F(x,y) \\ y &= y + \beta(x^2 + 3y^2 - 4) = G(x,y) \end{aligned}$$

where α and β are arbitrary parameters, which are to be determined. If we use the maximum absolute row sum norm, we require that

and

$$\begin{aligned} |F_x(x_0, y_0)| + |F_y(x_0, y_0)| &< 1 \\ |G_x(x_0, y_0)| + |G_y(x_0, y_0)| &< 1. \end{aligned}$$

Differentiating F and G partially with respect to x and y and evaluating at $(x_0, y_0) = (0.5,0.5)$, we get

$$\begin{aligned} &F_x(x,y) = 1 + (2x+3)\alpha, && F_x(0.5,0.5) = 1 + 4\alpha \\ &F_y(x,y) = \alpha, && F_y(0.5,0.5) = \alpha \\ &G_x(x,y) = 2\beta x, && G_x(0.5,0.5) = \beta \\ &G_y(x,y) = 1 + 6\beta y, && G_y(0.5,0.5) = 1 + 3\beta. \end{aligned}$$

Therefore, the conditions of convergence become

$$\begin{gathered} |1+4\alpha| + |\alpha| < 1 \\ |\beta| + |1+3\beta| < 1 \end{gathered} \qquad \dots (6.8)$$

Any values of α, β which satisfy (6.8) can be used. Obviously, both α and β are negative.

Taking $\alpha = -1/4$ and $\beta = -1/6$, we obtain the iteration method

$$\begin{aligned} x_{k+1} &= x_k - \frac{1}{4}(x_k^2 + 3x_k + y_k - 5) = -\frac{1}{4}(x_k^2 - x_k + y_k - 5) = F(x_k, y_k) \\ y_{k+1} &= y_k - \frac{1}{6}(x_k^2 + 3y_k^2 - 4) = -\frac{1}{6}(x_k^2 + 3y_k^2 - 6y_k - 4) = G(x_k, y_k). \end{aligned}$$

Starting with $(x_0, y_0) = (0.5,0.5)$, we get

$$\begin{aligned} &(x_1, y_1) = (1.1875,1.0),\ (x_2, y_2) = (0.944336,0.931641), \\ &(x_3, y_3) = (1.030231,1.015702), (x_4, y_4) = (0.988288,0.989647), \\ &(x_5, y_5) = (1.005482,1.003828). \end{aligned}$$

Example 6.3 Take one step from a suitable starting point with Newton-Raphson's method applied to the system

$$\begin{aligned} 10x + \sin(x+y) &= 1 \\ 8y - \cos^2(z-y) &= 1 \\ 12z + \sin z &= 1. \end{aligned}$$

Suggest some explicit method of the form $\mathbf{x}^{(k+1)} = \mathbf{F}(\mathbf{x}^{(k)})$ where no inversion is needed for $\mathbf{F}$, and estimate how many iterations are required to obtain a solution correct to six decimal points from the starting point.

Solution: We have the system of equations

$$f_1(x,y,z) = 10x + \sin(x+y) - 1 = 0$$
$$f_2(x,y,z) = 8y - \cos^2(z-y) - 1 = 0$$
$$f_3(x,y,z) = 12z + \sin z - 1 = 0.$$

To obtain a suitable starting point, we use the approximations

$$\begin{aligned} \sin(x+y) &\approx 0 \\ \cos(z-y) &\approx 1 \\ \sin(z) &\approx 0 \end{aligned}$$

and obtain from the given equations

$$x_0 = 1/10, y = 1/4, z_0 = 1/12.$$

We have

$$\begin{aligned} \boldsymbol{J}_k &= \begin{bmatrix} (f_1)_x & (f_1)_y & (f_1)_z \\ (f_2)_x & (f_2)_y & (f_2)_z \\ (f_3)_x & (f_3)_y & (f_3)_z \end{bmatrix}_k \\ &= \begin{bmatrix} 10 + \cos(x+y) & \cos(x+y) & 0 \\ 0 & 8 - \sin(2(z-y)) & \sin(2(z-y)) \\ 0 & 0 & 12 + \cos z \end{bmatrix}_k \end{aligned}$$

$$\begin{aligned} J_0 = J\left(\frac{1}{10}, \frac{1}{4}, \frac{1}{12}\right) &= \begin{bmatrix} 10.939373 & 0.939373 & 0 \\ 0 & 8.327195 & -0.327195 \\ 0 & 0 & 12.996530 \end{bmatrix} \\ J_0^{-1} &= \begin{bmatrix} 0.091413 & -0.010312 & -0.000260 \\ 0 & 0.120089 & 0.003023 \\ 0 & 0 & 0.076944 \end{bmatrix} \\ \boldsymbol{F}_0 &= \begin{bmatrix} f_1(1/10, 1/4, 1/12) \\ f_2(1/10, 1/4, 1/12) \\ f_3(1/10, 1/4, 1/12) \end{bmatrix} = \begin{bmatrix} 0.342898 \\ 0.027522 \\ 0.083237 \end{bmatrix} \end{aligned}$$

Using the Newton-Raphson method

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mathbf{J}_k^{-1}\mathbf{F}_k$$

we obtain, for $k = 0$

$$\begin{aligned} \mathbf{x}^{(1)} &= \mathbf{x}^{(0)} - \mathbf{J}_0^{-1}\mathbf{F}_0. \\ x_1 &= 0.0689, y_1 = 0.246443, z_1 = 0.076929. \end{aligned}$$

We can write an explicit method in the form

$$
\begin{aligned}
x_{k+1} &= \frac{1}{10}[1 - \sin(x_k + y_k)] = f_1(x_k, y_k, z_k) \\
y_{k+1} &= \frac{1}{8}[1 + \cos^2(z_k - y_k)] = f_2(x_k, y_k, z_k) \\
z_{k+1} &= \frac{1}{12}[1 - \sin(z_k)] = f_3(x_k, y_k, z_k).
\end{aligned}
$$

We note that the conditions (6.7) are satisfied at the initial approximation (x_0, y_0, z_0). Starting with the initial approximation $\mathbf{x}^{(0)} = [1/10, 1/4, 1/12]^T$, we obtain the sequence of iterates

$$
\begin{aligned}
\mathbf{x}^{(1)} &= [0.065710, 0.246560, 0.076397]^T \\
\mathbf{x}^{(2)} &= [0.069278, 0.246415, 0.076973]^T \\
\mathbf{x}^{(3)} &= [0.068952, 0.246445, 0.076925]^T \\
\mathbf{x}^{(4)} &= [0.068978, 0.246442, 0.076929]^T \\
\mathbf{x}^{(5)} &= [0.068978, 0.246442, 0.076929]^T
\end{aligned}
$$

Hence, the solution correct to six decimal places is obtained after five iterations.

6.3 METHODS FOR COMPLEX ROOTS

The root of an equation $f(z) = 0$, in which z is a complex variable can be obtained by using the methods discussed earlier provided we use complex arithmetic and complex initial approximation.

We can also obtain a root of the equation

$$f(z) = 0 \qquad \text{... (6.9)}$$

by using real arithmetic. Substituting $z = x + iy$ in equation (6.9), we get

$$f(z) = f(x + iy) = u(x, y) + iv(x, y) = 0$$

where $u(x, y)$ and $v(x, y)$ are the real and the imaginary parts of $f(z)$ respectively. Comparing the real and the imaginary parts, we get

$$u(x, y) = 0, v(x, y) = 0 \qquad \text{... (6.10)}$$

Thus, the problem of finding a complex root of (6.9) reduces to solving a system of two nonlinear equations (6.10).

The system of equations (6.10) can be solved using the methods discussed earlier.

Example 6.4 Obtain the complex roots of the equation

$$f(z) = z^3 + 1 = 0$$

correct to eight decimal places. Use the initial approximation to a root as $(x_0; y_0) = (0.25, 0.25)$. Compare with the exact values of the roots $(1 \pm i\sqrt{3})/2$.

Solution: Substituting $z = x + iy$ in the given equation, we get

$$\begin{aligned} f(x+iy) &= u(x,y) + iv(x,y) = (x+iy)^3 + 1 \\ &= (x^3 - 3xy^2 + 1) + i(3x^2y - y^3) = 0. \end{aligned}$$

Therefore,

$$\begin{aligned} u(x,y) &= x^3 - 3xy^2 + 1 = 0,\ v(x,y) = 3x^2y - y^3 = 0 \\ \mathbf{J} &= \begin{bmatrix} u_x & u_y \\ v_x & v_y \end{bmatrix} = \begin{bmatrix} 3x^2 - 3y^2 & -6xy \\ 6xy & 3x^2 - 3y^2 \end{bmatrix} \\ D &= |\mathbf{J}| = 9(x^2 - y^2)^2 + 36x^2y^2 = 9(x^2 + y^2)^2 \\ \mathbf{J}^{-1} &= \frac{1}{D}\begin{bmatrix} 3(x^2 - y^2) & 6xy \\ -6xy & 3(x^2 - y^2) \end{bmatrix} \end{aligned}$$

Using the Newton method, we obtain

$$\begin{bmatrix} x_{k+1} \\ y_{k+1} \end{bmatrix} = \begin{bmatrix} x_k \\ y_k \end{bmatrix} - \frac{1}{D_k}\begin{bmatrix} 3(x_k^2 - y_k^2) & 6x_ky_k \\ -6x_ky_k & 3(x_k^2 - y_k^2) \end{bmatrix}\begin{bmatrix} x_k^3 - 3x_ky_k^2 + 1 \\ 3x_k^2y_k - y_k^3 \end{bmatrix}$$

Using $(x_0, y_0) = (0.25, 0.25)$, we get

$$\begin{aligned} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} &= \begin{bmatrix} 0.25 \\ 0.25 \end{bmatrix} = -\frac{1}{0.140625}\begin{bmatrix} 0 & 0.375 \\ -0.375 & 0 \end{bmatrix}\begin{bmatrix} 0.96875 \\ 0.03125 \end{bmatrix} \\ &= \begin{bmatrix} 0.1666667 \\ 2.8333333 \end{bmatrix} \end{aligned}$$

The successive iterates are given in Table 6.1.

Table 6.1 Approximations to the Complex Root by the Newton-Raphson Method

k	z_k	$f(z_k)$	z_{k+1}
0	$(0.25,0.25)$	$(0.9687,0.3125(-1))$	$(0.16666667,2.83333333)$
1	$(0.16666667,2.83333333)$	$(-0.3009(1),-0.2251(2))$	$(0.15220505,1.89374026)$
2	$(0.15220505,1.89374026)$	$(-0.6340,-0.6660(1))$	$(0.19263553,1.27724322)$
3	$(0.19263553,1.27724322)$	$(0.6438(-1),-0.1941(1))$	$(0.31932197,0.91041889)$
4	$(0.31932197,0.91041889)$	$(0.2385,-0.4761)$	$(0.49252896,0.83063199)$
5	$(0.49252896,0.83063199)$	$(0.1000,03140(-1))$	$(0.49983161,0.86738607)$
6	$(0.49983161,0.86738607)$	$(-0.3284(-2),-0.2484(-2))$	$(0.49999870,0.86602675)$
7	$(0.49999870,0.86602675)$	$(-0.1548(-5),0.5414(-5))$	$(0.50000000,0.86602540)$

Obviously, the approximation to the second root is $(0.5,-0.8660254)$.

6.4 CHECK YOUR PROGRESS

1. Find a root of the equations $x^2 = 3\text{xy} - 7,\ \text{y} = 2(x+1)$..

2. Solve the non-linear equations $x^2 - y^2 = 4, x^2 + y^2 = 16$ numerically with $x_0 = y_0 = 2.828$ using the Newton-Raphson method. Carry out two iterations.

6.5 SUMMARY

The students are made familiar with fundamental results of various iterative solution of system of nonlinear equation.

6.6 KEYWORDS

Nonlinear systems, Complex roots, Newton Raphson method.

6.7 SELF-ASSESSMENT TEST

1. Find a root of the equations $xy = x + 9, y^2 = x^2 + 7$.
2. Use the Newton-Raphson method to solve the equations $x = x^2 + y^2, y = x^2 - y^2$ correct to two decimals, starting with the approximation (0.8,0.4).
3. Solve the non-linear equations $x^3 = \mathrm{y} + 100$, $y^3 = x + 100$ numerically using the Newton-Raphson method. Carry out two iterations.

6.8 ANSWERS TO CHECK YOUR PROGRESS

1. -1.9266, -1.8533
2. 3.162, 2.45

6.9 REFERENCES/ SUGGESTED READINGS

1. JAMES F. EPPERSON; An Introduction to Numerical Methods and analysis. Second Edition Mathematical Reviews, John Wiley & Sons, Inc., Hoboken, New Jersey.
2. S S Shastry; Introductory Methods of Numerical Analysis, Fifth Edition ISBN-978-81-203-4592-8, Asoke K. Ghosh, PHI Learning Pvt. Ltd, M-97, Connaught Circus, New Delhi
3. C.F. Gerald and P.O. Wheatley : Applied Numerical Methods, Low- priced edition, Pearson Education Asia (2002), Sixth Edition.
4. D. Kincaid and W. Cheney, Numerical Analysis: Mathematics of Scientific Computing, 3rd Edn., AMS (2002).
5. D.V. Griffiths and I.M. Smith, Numerical Methods for Engineers, Blackwell Scientific Publications (1991).
6. John H Mathews, Numerical Methods for Mathematics, Science and Engineering, Prentice Hall of India (1994).
7. K. E. Atkinson, Introduction to Numerical Analysis, 2nd Edn., John Wiley (1989).
8. M.K. Jain: Numerical Solution of Differential Equations, 4th Edition, New Age (2018).

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LESSON No. 6 Written by- Dr. Joginder Singh

INITIAL VALUE PROBLEM

STRUCTURE

7.0 LEARNING OBJECTIVES

- In this chapter we will be able to explaining the Runge-Kutta methods of order four, Multistep methods.
- It also brief about the Milan’s methods, simultaneous and higher order equations.

7.1 INTRODUCTION

An ordinary differential equation is a relation between a function, its derivatives and the variable upon which they depend. The general form of an ordinary differential equation is given by

$$f(x, y, y', y'', \dots \dots, y^m) = 0$$

where y and its derivatives $y', y'', \dots \dots .., y^m$ are functions of x.

Its general solution contains n arbitrary constants and is of the form $\phi(x, y, c_1, c_2, \dots \dots ., c_n) = 0$. For finding the particular solution, n conditions must be given and the values of constants $c_1, c_2, \dots \dots, c_n$ are to be determined. If these n conditions are prescribed at one point only, then the differential equation together with the conditions is called initial value problem of the nth order. In other cases, when the n conditions are prescribed at two or more points, then the problem is boundary value problem. In case of ordinary differential equations of first order, one arbitrary constant comes in the solution and this will be determined by the condition given to us. The ordinary differential equations can be solved using various methods which are categorized under single step method and multiple step methods.

7.2 SINGLE STEP METHODS

The method of solving an ordinary differential equation is called a single step method if it uses information available at one previous point only. The most common single step methods are Taylor series method, Runge-Kutta method, Picard's method and Euler's method.

7.3 MULTIPLE STEP METHODS

The method of solving an ordinary differentiable equation is called a multiple step method if it uses information available at more than one previous points. The most common multiple step methods are Euler's modified method, Predictor-Corrector method, Milne-Simpson's method and Adams-Bashforth method.

We shall now discuss important methods of solving ordinary differential equations of first order by using single and multiple step methods.

TAYLOR'S SERIES METHOD

Consider the first order equation

$$\frac{dy}{dx} = f(x, y), \text{ where } y = y_0 \text{ at } x = x_0 \qquad \dots (7.1)$$

Let $y = F(x)$ be the solution of the above equation such that $F(x_0) \neq 0$. Expanding $y = F[x_0 + (x - x_0)]$ by Taylor's series about point x_0, we get or

$$y = \mathrm{F}(x_0) + (x - x_0)\mathrm{F}'(x_0) + \frac{(x - x_0)^2}{2!}\mathrm{F}''(x_0) + \cdots$$

$$y = y_0 + (x - x_0)'y_0' + \frac{(x - x_0)^2}{2!}y_0'' + \cdots \qquad \text{... (7.2)}$$

This gives the value of y for every value of x for which equation (7.2) converges.

Putting $x = x_1 = x_0 + h$ and $y = y_1$ in (7.2), we get

$$y_1 = y_0 + hy_0' + \frac{h^2}{2!}y_0'' + \frac{h^3}{3!}y_0''' + \cdots$$

Similarly, we can obtain

$$y_{m+1} = y_m + hy_m' + \frac{h^2}{2!}y_m'' + \frac{h^3}{3!}y_m''' + \cdots$$

where $y_m{}^r$ denotes the r th derivative of y w.r.t. x at the point (x_m, y_m)

Putting the values of $y_m, y_m{}', y_m{}'', \dots \dots \dots$, we can find y_{m+1} which is the solution of (7.1) numerically.

Note. This method works well as long as the successive derivatives can be calculated easily. If the calculation of higher order derivatives become tedious, then Taylor's method is not useful. This is the main drawback of this method and is not of much importance. However, it is useful for finding starting values for the application of methods like Runge-Kutta method and Milne Simpson's method.

RUNGE-KUTTA METHOD

The Taylor's series method for solving differential equations numerically involves lot of labour in finding out the higher order derivatives. In Runge-Kutta method, the calculations of higher order derivatives is not required. Also this method gives greater accuracy. The method requires the functional values at some selected points and agrees with the Taylor's series solution up to the term containing h^r, where r differs from method to method and is called the order of that method. In these methods the accuracy increases at the cost of calculations. The most widely used method is Runge-Kutta of fourth order.

RUNGE-KUTTA METHOD OF FOURTH ORDER This method is most commonly used and is often referred to as Runge-Kutta method only.

To find the increment k of y corresponding to an increment h in x by R-K method from $\frac{dy}{dx} = f(x, y), y(x_0) = y_0$; we proceed as follows:

Calculate $k_1 = hf(x_0, y_0)$

$$k_2 = hf\left[x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right]$$

$$k_3 = hf\left[x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}\right],\ k_4 = hf[x_0 + h, y_0 + k_3]$$

and

$$k = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

After obtaining values of k_1, k_2, k_3, k_4 and k finally compute

$$y_1 = y_0 + k$$

or

$$y_1 = y_0 + \frac{1}{6}[k_1 + 2k_2 + 2k_3 + k_4]$$

Example 7.1 Using Taylor's method, obtain the approximate value of y at $x = 0.2$ for the differential equation $\frac{dy}{dx} = 2y + 3e^x, y(0) = 0$ and compare the numericalsolution obtained with the exact solution.

Solution: The given differential equation is

$$\frac{dy}{dx} = 2y + 3e^x = f(x, y)$$

The initial conditions are $y_0 = 0$ at $x_0 = 0$

We have

$$\begin{aligned} y' &= 2y + 3e^x & y'(0) &= 2y(0) + 3 = 3 \\ y'' &= 2y' + 3e^x & y''(0) &= 2y'(0) + 3 = 9 \\ y''' &= 2y'' + 3e^x & y'''(0) &= 2y''(0) + 3 = 21 \\ y^{(iv)} &= 2y''' + 3e^x & y^{(iv)}(0) &= 2y'''(0) + 3 = 45 \end{aligned}$$

By Taylor's series, we have

$$\begin{aligned} y(x) \quad &= y(0) + xy'(0) + \frac{x^2}{2!}y''(0) + \frac{x^3}{3!}y'''(0) + \frac{x^4}{4!}y^{(iv)}(0) + \cdots \ldots .. \\ &= 0 + 3x + \frac{9}{2}x^2 + \frac{21}{6}x^3 + \frac{45}{24}x^4 + \cdots \ldots \ldots \\ &= 3x + \frac{9}{2}x^2 + \frac{7}{2}x^3 + \frac{15}{8}x^4 + \cdots \ldots \ldots \end{aligned}$$

Putting $x = 0.2$, we get

$$
\begin{aligned}
y(0.2) \quad &= 3(0.2) + \frac{9}{2}(0.2)^2 + \frac{7}{2}(0.2)^3 + \frac{15}{8}(0.2)^4 + \cdots \\
&= -5.6 + \frac{9}{2}(0.04) + \frac{7}{2}(0.008) + \frac{15}{8}(0.0016) + \cdots \\
&= 0.6 + 0.18 + 0.028 + 0.0030 + \cdots \\
&= 0.8110
\end{aligned}
$$

To find exact value of y at $x = 0.2$:

Now, we have $\frac{dy}{dx} = 2y + 3e^x$

$$\frac{dy}{dx} - 2y = 3e^x$$

which is a linear differential equation of the form $\frac{dy}{dx} + \mathrm{P}y = \mathrm{Q}$, where $\mathrm{P} = -2, \mathrm{Q} = 3e^x$

$$\text{I.F.} \ = e^{\int \mathrm{P}dx} = e^{\int -2dx} = e^{-2x}.$$

Thus the solution is y (I.F.) $= \int$ Q(I.F.) $dx + c$

$$ye^{-2x} = 3\int \ e^{-x}dx + c$$

or

$$ye^{-2x} = -3e^{-x} + c$$

Multiplying both sides by e^{2x}, we get

$$y = -3e^x + ce^{2x}$$

Putting $x = 0, y = 0$, we have

$$0 = -3 + c \Rightarrow c = 3$$

Putting this value of c, we have

$$y = -3e^x + 3e^{2x}$$

Hence, exact solution of given equation is

$$y = 3(e^{2x} - e^x)$$

Putting $x = 0.2$, we have

$$y(0.2) = 3[e^{0.4} - e^{0.2}] = 0.8113$$

We can see that numerical solution approximates to the exact value upto 3 decimal places.

Example 7.2 Apply Runge-Kutta fourth order method to find an approximate value of y when $x = 0.2$, given that $\frac{dy}{dx} = x + y$ and $y = 1$ when $x = 0$.

Solution: The given differential equation is

$$\frac{dy}{dx} = x + y = f(x, y)$$

The initial conditions are $y(0) = 1$ when $x = 0$ i.e., $x_0 = 0$ and $y_0 = 1$

Taking $h = 0.2$, we have

$$\begin{aligned}
k_1 &= hf(x_0, y_0) = 0.2[x_0 + y_0] = 0.2 \\
k_2 &= hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right) = 0.2\left[\left(x_0 + \frac{h}{2}\right) + \left(y_0 + \frac{k_1}{2}\right)\right] \\
&= 0.2[0.1 + 1.1] = 0.24 \\
k_3 &= hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}\right) = 0.2\left[\left(x_0 + \frac{h}{2}\right) + \left(y_0 + \frac{k_2}{2}\right)\right] \\
&= 0.2[0.1 + 1.12] = 0.2440
\end{aligned}$$

$$\begin{aligned}
k_4 &= hf(x_0 + h, y_0 + k_3) = 0.2[(x_0 + h) + (y_0 + k_3)] \\
&= 0.2[0.2 + 1.244] = 0.2888 \\
k &= \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = \frac{1}{6}(0.2 + 0.48 + 0.488 + 0.2888) \\
&= 0.2428
\end{aligned}$$

Also

$$y_1 = y_0 + k = 1 + 0.2428 = 1.2428$$

$\therefore$ Required approximate value of y at $x = 0.2$ is $y_1 = 1.2428$.

Example 7.3 Given $\frac{dy}{dx} = 1 + y^2$, where $y = 0$ when $x = 0$; find $y(0.2), y(0.4)$ and $y(0.6)$.

Solution: The given differential equation is

$$\frac{dy}{dx} = 1 + y^2.$$

The initial conditions are $y = 0$ when $x = 0$ i.e., $x_0 = 0$ and $y_0 = 0$

Taking $h = 0.2$, we have

$$x_0 = 0, x_1 = 0.2, x_2 = 0.4, x_3 = 0.6$$

To compute y_1 we use $x_0 = 0, y_0 = 0$ and $h = 0.2$

$$\therefore\ k_1 = hf(x_0, y_0) = h(1 + y_0^2) = 0.2(1 + 0) = 0.2$$

$$k_2 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right) = 0.2\left[1 + \left(y_0 + \frac{k_1}{2}\right)^2\right] = 0.2[1 + (0.1)^2]$$

$$= 0.2(1 + .01) = 0.202$$

$$k_3 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}\right) = h\left[1 + \left(y_0 + \frac{k_2}{2}\right)^2\right] = 0.2[1 + (0.101)^2]$$

$$= 0.2(1 + 0.010201) = 0.20204.$$

$$k_4 = hf(x_0 + h, y_0 + k_3) = h[1 + (y_0 + k_3)^2] = 0.2[1 + (0.20204)^2]$$

$$= 0.2(1 + 0.040820) = 0.20816$$

$$y_1 = y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$= \frac{1}{6}[0.2 + 2(0.202 + 0.20204) + 0.20816] = 0.2027$$

To compute y_2, we use $x_1 = 0.2, y_1 = 0.2027$ and $h = 0.2$

$$k_1 = hf(x_1, y_1) = 0.2(1 + y_1^2) = 0.2[(1 + (0.2027)^2] = 0.2082$$

$$k_2 = hf\left(x_1 + \frac{h}{2}, y_1 + \frac{k_1}{2}\right) = 0.2\left[1 + \left(y_1 + \frac{k_1}{2}\right)^2\right]$$

$$= 0.2[1 + (0.2027 + 0.1041)^2]$$

$$= 0.2[1 + (0.3068)^2] = 0.2188$$

$$k_3 = hf\left(x_1 + \frac{h}{2}, y_1 + \frac{k_2}{2}\right) = 0.2\left[1 + \left(y_1 + \frac{k_2}{2}\right)^2\right]$$

$$= 0.2[1 + (0.2027 + 0.1094)^2] = 0.2[1 + (0.3121)^2] = 0.2195$$

$$k_4 = hf(x_1 + h, y_1 + k_3) = 0.2[1 + (y_1 + k_3)^2]$$

$$= 0.2[1 + (0.2027 + 0.2195)^2]$$

$$= 0.2[1 + (0.4222)^2] = 0.2356$$

$$y_2 = y_1 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$= 0.2027 + \frac{1}{6}[0.2082 + 0.4376 + 0.4390 + 0.2356]$$

$$= 0.2027 + 0.2201 = 0.4228.$$

To compute y_3, we use $x_2 = 0.4, y_2 = 0.4228$ and $h = 0.2.$

$$
\begin{aligned}
k_1 &= hf(x_2, y_2^*) = 0.2[1 + y_2^2] = 0.2[1 + (0.4228)^2] \\
&= 0.2[1 + 0.17876] \\
&= 0.2[1.17876] = 0.2358 \\
k_2 &= hf\left(x_2 + \frac{h}{2}, y_2 + \frac{k_1}{2}\right) = 0.2\left[1 + \left(y_2 + \frac{k_1}{2}\right)^2\right] \\
&= 0.2[1 + (0.4228 + 0.1179)^2] = 0.2[1 + (0.5407)^2] \\
&= 0.2[1 + 0.2924] = 0.2585 \\
k_3 &= hf\left(x_2 + \frac{h}{2}, y_2 + \frac{k_2}{2}\right) = 0.2\left[1 + \left(y_2 + \frac{k_2}{2}\right)^2\right] \\
&= 0.2[1 + (0.4228 + 0.12925)^2] \\
&= 0.2[1 + 0.3048] = 0.2609 \\
k_4 &= hf(x_2 + h, y_2 + k_3) \\
&= 0.2[1 + (0.4228 + 0.2609)^2] \\
&= 0.2[1 + 0.4674] = 0.2935 \\
y_3 &= y_2 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
&= 0.4228 + \frac{1}{6}[0.2358 + 2(0.2585 + 0.2609) + 0.2935] \\
&= 0.4228 + \frac{1}{6}(1.5681) \\
&= 0.4228 + 0.26135 = 0.68415.
\end{aligned}
$$

Thus we have $y(0.2) = 0.2027, y(0.4) = 0.4228$ and $y(0.6) = 0.68415$.

Milne-Simpson's method

Given $\frac{dy}{dx} = f(x, y)$ and $y = y_0$ at $x = x_0$. To find an approximate value of y for $x = x_0 + nh$ by Milne-Simpson's method.

The given differential equation is $\frac{dy}{dx} = f(x, y)$

The initial conditions are $y = y_0$ at $x = x_0$.

In this method, we first obtain the approximate value of y_{n+1} by predictor formula and then improve this value by means of corrector formula.

By Newton's formula for forward interpolation, we have

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

where $u = \frac{x - x_0}{h}$ i.e., $x = x_0 + uh$

In terms of y' and u, the formula is

$$y' = y_0' + u\Delta y_0' + \frac{u(u-1)}{2!}\Delta^2 y_0' + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0' + \frac{u(u-1)(u-2)(u-3)}{4!}\Delta^4 y_0' + \cdots \qquad \text{... (7.3)}$$

Integrating over the interval x_0 to $x_0 + 4h$ or $u = 0$ to 4, we have

$$\int_{x_0}^{x_0+4h} y'dx = \int_{x_0}^{x_0+4h} \left[y_0' + u\Delta y_0' + \frac{u(u-1)}{2}\Delta^2 y_0' + \frac{u(u-1)(u-2)}{6}\Delta^3 y_0' + \frac{u(u-1)(u-2)(u-3)}{24}\Delta^4 y_0' + \cdots\right] dx$$

or
$$y_4 - y_0 = h\int_0^4 \left[y_0' + u\Delta y_0' + \frac{u(u-1)}{2}\Delta^2 y_0' + \frac{u(u-1)(u-2)}{6}\Delta^3 y_0' + \frac{u(u-1)(u-2)(u-3)}{24}\Delta^4 y_0' + \cdots\right] du$$

$$= h\left[4y_0' + 8\Delta y_0' + \frac{20}{3}\Delta^2 y_0' + \frac{8}{3}\Delta^3 y_0' + \frac{28}{90}\Delta^4 y_0'\right]$$

Substituting $\Delta \equiv (E-1)$, we get

$$\begin{aligned}
y_4 - y_0 &= h\left[4y_0' + 8(\mathrm{E}-1)y_0' + \frac{20}{3}(\mathrm{E}-1)^2 y_0' + \frac{8}{3}(\mathrm{E}-1)^3 y_0'\right] + \frac{28}{90}h\Delta^4 y_0' + \cdots \\
&= h\left[4y_0' + 8(\mathrm{E}-1)y_0' + \frac{20}{3}(\mathrm{E}^2 - 2\mathrm{E} + 1)y_0' + \frac{8}{3}(\mathrm{E}^3 - 3\mathrm{E}^2 + 3\mathrm{E} - 1)y_0'\right] \\
&\quad + \frac{28}{90}h\Delta^4 y_0' + \cdots \\
&= h\left[4y_0' + 8y_1' - 8y_0' + \frac{20}{3}y_2' - \frac{40}{3}y_1' + \frac{20}{3}y_0' + \frac{8}{3}y_3' - 8y_2' + 8y_1' - \frac{8}{3}y_0'\right] \\
&\quad + \frac{28}{90}\Delta^4 y_0' + \cdots
\end{aligned}$$

$$\therefore\ y_4 = y_0 + \frac{4h}{3}(2y_1' - y_2' + 2y_3') + \frac{28}{90}h\Delta^4 y_0' + \cdots \qquad \text{... (7.4)}$$

This is Milne's predictor formula.

To obtain the corrector formula, we integrate (7.3) over the interval x_0 to $x_0 + 2h$ or $u = 0$ to 2 . Thus we have

$$\int_0^2 y'dx = h\int_0^2 \left[y_0' + u\Delta y_0' + \frac{u(u-1)}{2!}\Delta^2 y_0' + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0' + \frac{u(u-1)(u-2)(u-3)}{4!}\Delta^4 y_0' + \cdots \ldots\right] du$$

or

$$y_2 - y_0 = h\left[2y_0' + 2\Delta y_0' + \frac{1}{3}\Delta^2 y_0' - \frac{1}{90}\Delta^4 y_0'\right]$$

Substituting $\Delta \equiv (E-1)$, we get

$$y_2 = y_0 + h\left[2y_0' + 2(\mathrm{E}-1)y_0' + \frac{1}{3}(\mathrm{E}-1)^2 y_0'\right] - \frac{h}{90}\Delta^4 y_0' + \cdots$$

$$= y_0 + h\left[2y_0' + 2(\mathrm{E}-1)y_0' + \frac{1}{3}(\mathrm{E}^2 - 2\mathrm{E} + 1)y_0'\right] - \frac{h}{90}\Delta^4 y_0' + \cdots$$

$$= y_0 + h\left[2y_0' + 2y_1' - 2y_0' + \frac{1}{3}(y_2' - 2y_1' + y_0')\right] - \frac{h}{90}\Delta^4 y_0' + \cdots$$

$$y_2 = y_0 + \frac{h}{3}(y_0' + 4y_1' + y_2') - \frac{h}{90}\Delta^4 y_0' + \cdots \quad \text{... (7.5)}$$

This is Milne's corrector formula.

Since x_0, x_1, x_2, x_3, x_4 are any five consecutive values of x, so in general equations (7.4) and (7.5) can be written as

$$y_{n+1} = y_{n-3} + \frac{4h}{3}[2y_{n-2}' - y_{n-1}' + 2y_n'] \quad \text{... (7.6)}$$

and $$y_{n+1}^{(1)} = y_{n-1} + \frac{h}{3}[y_{n-1}' + 4y_n' + y_{n+1}'] \quad \text{... (7.7)}$$

Thus Milne-Simpson's method uses the formulae

$$x_{i+1} = x_i + h$$

and the predictor $y_{i+1} = y_{i-3} + \frac{4h}{3}[2f_{i-2} - f_{i-1} + 2f_i]$

and the corrector $y_{i+1}^{(1)} = y_{i-1} + \frac{h}{3}[f_{i-1} + 4f_i + f(x_{i+1}, y_{i+1})]$ for $i = 3,4,5, \dots \dots \dots, (m-1)$

as an approximate solution to the differential equation $\frac{dy}{dx} = f(x, y)$

Remarks:

1. As we fit up a polynomial of degree four, therefore we have considered the differences upto the third order. The terms containing $\Delta^4 y_0'$ are not used directly, but they give the principal parts of the errors in the two values of y_{n+1} computed from equations (7.4) and (7.5).
2. The Milne-Simpson's method is not a self starting method. Three additional starting values y_1, y_2, y_3 must be given. They are usually computed using the Runge-Kutta method.

Example 7.4 Find $y(2)$, if $y(x)$ is the solution of $\frac{dy}{dx} = \frac{1}{2}(x+y)$, assuming that

$$y(0) = 2, y(0.5) = 2.636, y(1.0) = 3.595 \text{ and } y(1.5) = 4.968.$$

Solution: The given equation is

$$\frac{dy}{dx} = \frac{1}{2}(x + y) = f(x, y)$$

Taking $h = 0.5$, we have $x_0 = 0, x_1 = 0.5, x_2 = 1.0, x_3 = 1.5$

$\therefore\ y_0 = 2, y_1 = 2.636, y_2 = 3.595$ and $y_3 = 4.968$

We have

$$y_0 = 2,\ y_1 = 2.636,\ y_2 = 3.595 \text{ and } y_3 = 4.968$$

$$f_0 = \frac{1}{2}(x_0 + y_0) = \frac{1}{2}(0 + 2) = 1$$

$$f_1 = \frac{1}{2}(x_1 + y_1) = \frac{1}{2}(0.5 + 2.636) = 1.568$$

$$f_2 = \frac{1}{2}(x_2 + y_2) = \frac{1}{2}(1.0 + 3.595) = 2.2975$$

$$f_3 = \frac{1}{2}(x_3 + y_3) = \frac{1}{2}(1.5 + 4.968) = 3.234$$

It is required to find y_4 corresponding to $x_4 = 2$

By Milne's predictor formula, we have

$$\begin{aligned} y_4 &= y_0 + \frac{4h}{3}[2f_1 - f_2 + 2f_3] \\ &= 2 + \frac{4(0.5)}{3}[2(1.568) - 2.2975 + 2(3.234)] \\ &= 2 + \frac{2}{3}[3.136 - 2.2975 + 6.468] = 6.8710 \\ f_4 &= \frac{1}{2}(x_4 + y_4) = \frac{1}{2}(2 + 6.8710) = 4.4355 \end{aligned}$$

Using corrector formula, we have

$$\begin{aligned} y_4^{(1)} &= y_2 + \frac{h}{3}[f_2 + 4f_3 + f_4] \\ &= 3.595 + \frac{0.5}{3}[2.2975 + 4(3.234) + 4.4355] \\ &= 3.595 + \frac{1}{6}[19.6690] = 3.595 + 3.27817 = 6.87317 \\ f_4^{(1)} &= \frac{1}{2}\left[x_4 + y_4^{(1)}\right] = \frac{1}{2}[2 + 6.87317] = 4.43659 \end{aligned}$$

Again applying the corrector formula, we get

$$
\begin{aligned}
y_4^{(2)} &= y_2 + \frac{h}{3}\left[f_2 + 4f_3 + f_4^{(1)}\right] \\
&= 3.595 + \frac{0.5}{3}[2.2975 + 4(3.234) + 4.43659] \\
&= 3.595 + \frac{1}{6}[19.67009] = 3.595 + 3.27835 = 6.87335
\end{aligned}
$$

Hence $y(2) = 6.873$.

Example 7.5 Use Milne-Simpson's method to obtain the solution of the equation $\frac{dy}{dx} = x - y^2$ at $x = 0.8$ given that $y(0) = 0, y(0.2) = 0.0200, y(0.4) = 0.0795, y(0.6) = 0.1762$.

Solution: The given equation is

$$\frac{dy}{dx} = x - y^2 = f(x, y)$$

The starting values with $h = 0.2$ are .

$$
\begin{array}{lll}
x_0 = 0 & y_0 = 0.0000 & f_0 = x_0 - y_0{}^2 = 0 \\
x_1 = 0.2 & y_1 = 0.0200 & f_1 = x_1 - y_1{}^2 = 0.1996 \\
x_2 = 0.4 & y_2 = 0.0795 & f_2 = x_2 - y_2{}^2 = 0.3937 \\
x_3 = 0.6 & y_3 = 0.1762 & f_3 = x_3 - y_3{}^2 = 0.5689
\end{array}
$$

By Milne's predictor formula, we get

$$
\begin{aligned}
y_4 &= y_0 + \frac{4h}{3}[2f_1 - f_2 + 2f_3] \\
&= 0 + \frac{0.8}{3}[2(0.1996) - 0.3937 + 2(0.5689)] = 0.3049 \qquad \text{... (7.8)}
\end{aligned}
$$

Thus, we have $x_4 = 0.8, y_4 = 0.3049$ and $f_4 = 0.8 - (0.3049)^2 = 0.7070$

By Milne's corrector formula, we get

$$
\begin{aligned}
y_4^{(1)} &= y_2 + \frac{h}{3}[f_2 + 4f_3 + f_4] \\
&= 0.0795 + \frac{0.2}{3}[0.3937 + 4(0.5689) + 0.7070] \\
&= 0.3046, \text{ which is nearly same as (7.8)}
\end{aligned}
$$

Thus, we have at $x = 0.8, y = 0.3046$

$$y(0.8) = 0.3046$$

Example 7.6 Use Milne-Simpson's method to find $y(0.3)$ from $y' = x^2 + y^2, y(0) = 1$. Find the initial values $y(-0.1), y(0.1)$ and $y(0.2)$ from the Taylor's series method.

Solution. The given equation is $y' = x^2 + y^2 = f(x, y)$

The initial conditions are $x_0 = 0$ and $y_0 = 1$.

We have

$$\begin{aligned} y'' &= 2x + 2yy' \\ y''' &= 2 + 2(y')^2 + 2yy'' \\ y^{iv} &= 4y'y'' + 2y'y'' + 2yy''' = 6y'y'' + 2yy''' \end{aligned}$$

Putting $x_0 = 0$ and $y_0 = 1$, we have

$$y'(0) = x_0^2 + y_0^2 = 0 + 1 = 1$$
$$y''(0) = 2x_0 + 2y_0y_0' = 0 + 2 = 2$$
$$y'''(0) = 2 + 2(y_0')^2 + 2y_0y_0'' = 2 + 2 + 4 = 8'$$
$$y^{iv}(0) = 6y_0'y_0'' + 2y_0y_0''' = 12 + 16 = 28$$

Using Taylor's series, we get

$$\begin{aligned} y(x) &= y(0) + xy'(0) + \frac{x^2}{2!}y''(0) + \frac{x^3}{3!}y'''(0) + \frac{x^4}{4!}y^{iv}(0) + \cdots \\ &= 1 + x(1) + \frac{x^2}{2!}(2) + \frac{x^3}{3!}(8) + \frac{x^4}{4!}(28) + \cdots \\ &= 1 + x + x^2 + \frac{4}{3}x^3 + \frac{7}{6}x^4 + \cdots \\ y(-0.1) &= 1 - 0.1 + 0.01 + \frac{4}{3}(-0.001) + \frac{7}{6}(0.0001) + \cdots \\ &= 1 - 0.1 + 0.01 - 0.00133 + 0.0001166 + \cdots \\ &= 0.9088 \\ y(0.1) &= 1 + 0.1 + 0.01 + \frac{4}{3}(0.001) + \frac{7}{6}(0.0001) + \cdots \\ &= 1 + 0.1 + 0.01 + 0.00133 + 0.00011 + \cdots \\ &= 1.11145 \\ y(0.2) &= 1 + 0.2 + 0.04 + \frac{4}{3}(0.008) + \frac{7}{6}(0.0016) + \cdots \\ &= 1 + 0.2 + 0.04 + 0.0106666 + 0.00186666 + \cdots \\ &= 1.2525 \end{aligned}$$

Taking $h = 0.1$, the starting values for Milne's method a

$$\begin{array}{lll} x_{-1} = -0.1 & y_{-1} = 0.9088 & f_{-1} = 0.8359 \\ x_0 = 0 & y_0 = 1 & f_0 = 1 \\ x_1 = 0.1 & y_1 = 1.11145 & f_1 = 1.2453 \\ x_2 = 0.2 & y_2 = 1.2525 & f_2 = 1.6088 \end{array}$$

By Milne's predictor formula, we have

$$\begin{aligned} y_3 &= y_{-1} + \frac{4h}{3}[2f_0 - f_1 + 2f_2] \\ &= 0.9088 + \frac{0.4}{3}[2 - 1.2453 + 3.2176] \\ &= 0.9088 + 0.5296 = 1.4384 \end{aligned}$$

$$f_3 = {x_3}^2 + {y_3}^2 = (0.3)^2 + (1.4384)^2 = 2.159$$

Using Milne's corrector formula, we have

$$\begin{aligned}
y_3^{(1)} &= y_1 + \frac{h}{3}[f_1 + 4f_2 + f_3] \\
&= 1.11145 + \frac{0.1}{3}[1.2453 + 4(1.6088) + 2.159] \\
&= 1.11145 + 0.328 = 1.43945 \\
f_3^{(1)} &= (0.3)^2 + (1.43945)^2 = 2.162
\end{aligned}$$

Again, using the corrector formula, we have

$$\begin{aligned}
y_3^{(2)} &= y_1 + \frac{h}{3}\left[i_1 + 4f_2 + f_3^{(1)}\right] \\
&= 1.11145 + \frac{0.1}{3}[1.2453 + 4(1.6088) + 2.162] \\
&= 1.11145 + 0.3281 = 1.4395
\end{aligned}$$

Thus, we have $y(0.3) = 1.4395$.

Example 7.7 Using Runge-Kutta method of order 4, find y for $x = 0.1, 0.2, 0.3$ given that $\frac{dy}{dx} = xy + y^2, y(0) = 1$. Continue the solution at $x = 0.4$ using Milne-Simpson's method .

Solution: The given differential equation is

$$\frac{dy}{dx} = xy + y^2 = f(x, y)$$

The initial conditions are $x_0 = 0$ and $y_0 = 1$.

Taking $h = 0.1$, we shall find y_1 corresponding to $x_1 = 0.1$ in the following way

$$\begin{aligned}
k_1 &= hf(x_0, y_0) = 0.1f(0,1) = 0.1[0 + 1] = 0.1 \\
k_2 &= hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1\right) = 0.1f(0.05,1.05) = 0.1(1.155) = 0.1155 \\
k_3 &= hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2\right) = 0.1f(0.05,1.0578) = 0.1(1.1718) = 0.1172 \\
k_4 &= hf(x_0 + h, y_0 + k_3) = 0.1f(0.1,1.1172) = 0.1(1.3598) = 0.13598
\end{aligned}$$

$$\begin{aligned}
k &= \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
&= \frac{1}{6}[(0.1 + 2(0.1155) + 2(0.1172) + 0.13598)] \\
&= \frac{1}{6}(0.70139) = 0.1169 \\
y_1 &= y_0 + k = 1 + 0.1169 = 1.1169
\end{aligned}$$

Now to compute y_2 corresponding to $x_2 = 0.2$ using $x_1 = 0.1, y_1 = 1.1169$ and $h = 0.1$

$$
\begin{aligned}
k_1 &= hf(x_1, y_1) = 0.1f(0.1, 1.1169) = 0.1(1.3592) = 0.1359 \\
k_2 &= hf\left(x_1 + \frac{1}{2}h, y_1 + \frac{1}{2}k_1\right) = 0.1f(0.15, 1.1849) = 0.1(1.5817) = 0.1582 \\
k_3 &= hf\left(x_1 + \frac{1}{2}h, y_1 + \frac{1}{2}k_2\right) = 0.1f(0.15, 1.196) = 0.1(1.6098) = 0.161 \\
k_4 &= hf(x_1 + h, y_1 + k_3) = 0.1f(0.2, 1.2779) = 0.1(1.8886) = 0.1889 \\
k &= \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
&= \frac{1}{6}[0.1359 + 2(0.1582 + 0.161) + 0.1889] \\
&= \frac{1}{6}[0.9632] = 0.1605 \\
y_2 &= y_1 + k = 1.1169 + 0.1605 = 1.2774
\end{aligned}
$$

To find y_3 corresponding to $x_3 = 0.3$ using $x_2 = 0.2, y_2 = 1.2774$ and $h = 0.1$.

$$
\begin{aligned}
k_1 &= hf(x_2, y_2) = 0.1f(0.2, 1.2774) = 0.1(1.8872) = 0.1887 \\
k_2 &= hf\left(x_2 + \frac{1}{2}h, y_2 + \frac{1}{2}k_1\right) = 0.1f(0.25, 1.3718) = 0.1(2.2248) = 0.2225 \\
k_3 &= hf\left(x_2 + \frac{1}{2}h, y_2 + \frac{1}{2}k_2\right) = 0.1f(0.25, 1.3887) = 0.1(2.2757) = 0.2276 \\
k_4 &= hf(x_2 + h, y_2 + k_3) = 0.1f(0.8, 1.5050) = 0.1(2.7165) = 0.2717 \\
k &= \frac{1}{6}[k_1 + 2(k_2 + k_3) + k_4] \\
&= \frac{1}{6}[0.1887 + 2(0.2225 + 0.2216) + 0.2717] = \frac{1}{6}[1.3606] = 0.2268
\end{aligned}
$$

$$
y_3 = y_2 + k = 1.2774 + 0.2268 = 1.5042
$$

Thus, the starting values for Milne's method are

$$
\begin{array}{lll}
x_0 = 0 & y_0 = 1 & f_0 = x_0 y_0 + y_0^2 = 1 \\
x_1 = 0.1 & y_1 = 1.1169 & f_1 = x_1 y_1 + y_1^2 = 1.3592 \\
x_2 = 0.2 & y_2 = 1.2774 & f_2 = x_2 y_2 + y_2^2 = 1.8872 \\
x_3 = 0.3 & y_3 = 1.5042 & f_3 = x_3 y_3 + y_3^2 = 2.7139
\end{array}
$$

Using Milne's predictor formula, we get

$$
\begin{aligned}
y_4 &= y_0 + \frac{4h}{3}[2f_1 - f_2 + 2f_3] \\
&= 1 + \frac{0.4}{3}[2(1.3592) - 1.8872 + 2(2.7139)] \\
&= 1 + 0.8345 = 1.8345 \\
\therefore\ x_4 &= 0.4, y_4 = 1.8345 \text{ and } f_4 = x_4 y_4 + y_4^2 = 4.0992
\end{aligned}
$$

Using Milne's corrector formula, we get

$$
\begin{aligned}
y_4^{(1)} &= y_2 + \frac{h}{3}[f_2 + 4f_3 + f_4] \\
&= 1.2774 + \frac{0.1}{3}[1.8872 + 4(2.7139) + 4.0992] \\
&= 1.2774 + 0.5614 \\
&= 1.8388. \\
f_4^{(1)} &= y_4^{(1)}\left[x_4 + y_4^{(1)}\right] = 1.8388[0.4 + 1.8388] = 4.1167.
\end{aligned}
$$

Again applying Milne's corrector formula, we have

$$
\begin{aligned}
y_4^{(2)} &= y_2 + \frac{h}{3}\left[f_2 + 4f_3 + f_4^{(1)}\right] \\
&= 1.2774 + \frac{0.1}{3}[1.8872 + 4(2.7139) + 4.1167] \\
&= 1.2774 + 0.56198 = 1.8394 \\
f_4^{(2)} &= y_4^{(2)}\left[x_4 + y_4^{(2)}\right] = 1.8394[0.4 + 1.8394] = 4.1192
\end{aligned}
$$

Again, by Milne's corrector formula, we have

$$
\begin{aligned}
y_4^{(3)} &= y_2 + \frac{h}{3}\left[f_2 + 4f_3 + f_4^{(2)}\right] \\
&= 1.2774 + \frac{0.1}{3}[1.8872 + 4(2.7139) + 4.1192] \\
&= 1.2774 + 0.5621 = 1.8395 \\
\therefore\ f_4^{(3)} &= y_4^{(3)}\left[x_4 + y_4^{(3)}\right] = 1.8395[0.4 + 1.8395] = 4.1196
\end{aligned}
$$

Hence $y(0.4) = 1.8395$.

ADAMS-BASHFORTH METHOD

We have

$$\frac{dy}{dx} = f(x, y), \text{ where } y_0 = y(x_0) \qquad \ldots (7.9)$$

In this method, we compute $y_{-1} = y(x_0 - h), y_{-2} = y(x_0 - 2h), y_{-3} = y(x_0 - 3h)$ by Taylor's series or Euler's method or Runge-Kutta method.

Using the given relation $y' = f(x, y)$, we have

$$
\begin{aligned}
&y'_{-1} = f(x_0 - h, y_{-1}), \\
&y'_{-2} = f(x_0 - 2h, y_{-2}) \text{ and } y'_{-3} = f(x_0 - 3h, y_{-3}),
\end{aligned}
$$

Integrating (7.9) from x_0 to $x_0 + h$, we get

$$y_1 = y_0 + \int_{x_0}^{x_0+h} f(x, y)dx \qquad \ldots (7.10)$$

The integral can be evaluated by replacing unknown function $f(x, y)$ by polynomial $p(x)$. Using Newton's backward interpolation formula, we have

$$f(x, y) \approx p(x) = f_0 + u\nabla f_0 + \frac{u(u+1)}{2!}\nabla^2 f_0 + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_0 + \cdots$$

where $u = \frac{x - x_0}{h}$ and $f_0 = f(x_0, y_0)$

∴ Equation (7.10) becomes

$$y_1 = y_0 + \int_{x_0}^{x_0+h} \left[f_0 + u\nabla f_0 + \frac{u(u+1)}{2!}\nabla^2 f_0 + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_0 + \cdots\right] dx$$

Since $x = x_0 + uh \therefore dx = hdu.$

At $x = x_0, u = 0$ and at $x = x_0 + h, u = 1$

$$\therefore\ y_1 = y_0 + h\int_0^1 \left[f_0 + u\nabla f_0 + \frac{u(u+1)}{2!}\nabla^2 f_0 + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_0 + \cdots\right] du$$

$$= y_0 + h\left[f_0 + \frac{1}{2}\nabla f_0 + \frac{1}{2!}\left(\frac{1}{3} + \frac{1}{2}\right)\nabla^2 f_0 + \frac{1}{3!}\left(\frac{9}{4}\right)\nabla^3 f_0 + \cdots.\right]$$

$$= y_0 + h\left[f_0 + \frac{\nabla f_0}{2} + \frac{5}{12}\nabla^2 f_0 + \frac{3}{8}\nabla^3 f_0 + \cdots..\right]$$

Substituting $\nabla = 1 - \mathrm{E}^{-1}$, we get

$$y_1 = y_0 + h\left[f_0 + \frac{1}{2}(1 - \mathrm{E}^{-1})f_0 + \frac{5}{12}(1 - \mathrm{E}^{-1})^2 f_0 + \frac{3}{8}(1 - \mathrm{E}^{-1})^3 f_0 + \cdots\right]$$

$$= y_0 + h\left[f_0 + \frac{1}{2}(1 - \mathrm{E}^{-1})f_0 + \frac{5}{12}(1 - 2\mathrm{E}^{-1} + \mathrm{E}^{-2})f_0 + \frac{3}{8}(1 - 3\mathrm{E}^{-1} + 3\mathrm{E}^{-2} - \mathrm{E}^{-3})f_0 + \cdots\right]$$

$$= y_0 + h\left[f_0 + \frac{1}{2}f_0 - \frac{1}{2}f_{-1} + \frac{5}{12}f_0 - \frac{5}{6}f_{-1} + \frac{5}{12}f_{-2} + \frac{3}{8}f_0 - \frac{9}{8}f_{-1} + \frac{9}{8}f_{-2} - \frac{3}{8}f_{-3} + \cdots\right]$$

$$= y_0 + h\left[\left(1 + \frac{1}{2} + \frac{5}{12} + \frac{3}{8}\right)f_0 - \left(\frac{1}{2} + \frac{5}{6} + \frac{9}{8}\right)f_{-1} + \left(\frac{5}{12} + \frac{9}{8}\right)f_{-2} - \frac{3}{8}f_{-3} + \cdots\right]$$

$$= y_0 + h\left[\frac{55}{24}f_0 - \frac{59}{24}f_{-1} + \frac{37}{24}f_{-2} - \frac{3}{8}f_{-3} + \cdots\right]$$

$$= y_0 + \frac{h}{24}[55f_0 - 59f_{-1} + 37f_{-2} - 9f_{-3} + \cdots] \qquad \text{... (7.11)}$$

This is called Adams-Bashforth Predictor Formula.

Now we shall obtain $f_1 = (x_0 + h, y_1)$

In order to obtain a better approximation for y_1, we shall derive a corrector formula by putting Newton's backward formula at f_1 i.e.,

$$f(x,y) = f_1 + u\nabla f_1 + \frac{u(u+1)}{2!}\nabla^2 f_1 + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_1 + \cdots \qquad \ldots (7.12)$$

where $x = x_1 + uh$ and $dx = hdu$.

Using (7.12) in (7.10), we get

$$y_1^{(1)} = y_0 + \int_{x_0}^{x_0+h} \left[-f_1 + u\nabla f_1 + \frac{u(u+1)}{2!}\nabla^2 f_1 + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_1 + \cdots\right] dx$$

Since $x = x_0 + h + uh$, so $x = x_0 \Rightarrow u = -1$ and $x = x_0 + h \Rightarrow u = 0$

$$\therefore y_1^{(1)} = y_0 + h\int_{-1}^{0} \left[f_1 + u\nabla f_1 + \frac{u(u+1)}{2!}\nabla^2 f_1 + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_1 + \cdots\right] du$$

$$= y_0 + h\left[f_1 - \frac{1}{2}\nabla f_1 - \frac{1}{12}\nabla^2 f_1 - \frac{1}{24}\nabla^3 f_1 + \cdots\right]$$

Taking $\nabla \equiv 1 - \mathrm{E}^{-1}$, we have

$$\begin{aligned}
y_1^{(1)} &= y_0 + h\left[f_1 - \frac{1}{2}(1-\mathrm{E}^{-1})f_1 - \frac{1}{12}(1-\mathrm{E}^{-1})^2 f_1 - \frac{1}{24}(1-\mathrm{E}^{-1})^3 f_1 + \cdots.\right] \\
&= y_0 + h\left[f_1 - \frac{1}{2}(f_1 - f_0) - \frac{1}{12}(1 - 2\mathrm{E}^{-1} + \mathrm{E}^{-2})f_1 - \frac{1}{24}(1 - 3\mathrm{E}^{-1} + 3\mathrm{E}^{-2} - \mathrm{E}^{-3})f_1 + \cdots\right] \\
&= y_0 + h\left[f_1 - \frac{1}{2}(f_1 - f_0) - \frac{1}{12}(f_1 - 2f_0 + f_{-1}) - \frac{1}{24}(f_1 - 3f_0 + 3f_{-1} - f_{-2}) + \cdots..\right] \\
&= y_0 + h\left[\left(1 - \frac{1}{2} - \frac{1}{12} - \frac{1}{24}\right)f_1 + \left(\frac{1}{2} + \frac{1}{6} + \frac{1}{8}\right)f_0 - \left(\frac{1}{12} + \frac{1}{8}\right)f_{-1} + \frac{1}{24}f_{-2} + \cdots..\right] \\
&= y_0 + \frac{h}{24}[9f_1 + 19f_0 - 5f_{-1} + f_{-2}] \qquad \ldots (7.13)
\end{aligned}$$

This is called Adams-Moulton Corrector Formula.

Note: For applying Adams-Bashforth method, we need four starting values of y which can be calculated by means of Taylor's series method or Euler's method or Runge-Kutta method. In practice fourth order RungeKutta formula together with Adams -Bashforth formula is most useful.

Example 7.8 Given

$$\frac{dy}{dx} = x^2(1+y) \text{ and } y(1) = 1, y(1.1) = 1.233, y(1.2) = 1.548, y(1.3) = 1.979$$

Evaluate $y(1.4)$ by Adams-Bashforth method.

Solution: $f(x,y) = x^2(1+y)$

Taking $h = 0.1$, starting values are

$$x_{-3} = 1.00 \quad y_{-3} = 1$$
$$x_{-2} = 1.1 \quad y_{-2} = 1.233$$
$$x_{-1} = 1.2 \quad y_{-1} = 1.548$$
$$x_0 = 1.3 \quad y_0 = 1.979$$

$$f_{-3} = 1(1+1) = 2$$
$$f_{-2} = (1.1)^2[1 + 1.233] = 2.702$$
$$f_{-1} = (1.2)^2[1 + 1.548] = 3.669$$
$$f_0 = (1.3)^2[1 + 1.979] = 5.035$$

Using the predictor formula, we have

$$\begin{aligned} y_1 &= y_0 + \frac{h}{24}[55f_0 - 59f_{-1} + 37f_{-2} - 9f_{-3}] \\ &= 1.979 + \frac{0.1}{24}[55(5.035) - 59(3.669) + 37(2.702) - 9(2)] \\ &= 2.572 \end{aligned}$$

Thus we have $x_1 = 1.4, y_1 = 2.572$.

$$f_1 = x_1^2(1 + y_1) = (1.4)^2[1 + 2.572] = 7.003$$

Using the corrector formula, we have

$$\begin{aligned} y_1 &= y_0 + \frac{h}{24}[9f_1 + 19f_0 - 5f_{-1} + f_{-2}] \\ &= 1.979 + \frac{0.1}{24}[9(1.7003) + 19(5.035) - 5(3.669) + 2.702] \\ &= 2.376 \end{aligned}$$

Thus at $x = 1.4$, we have $y = 2.376$

Hence, $y(1.4) = 2.376$.

Example 7.9 Using Adams-Bashforth method, obtain the solution of $\frac{dy}{dx} = x - y^2$ at $x = 0.8$, given the values.

x:	0	0.2	0.4	0.6
y: −	0	0.0200	0.0795	0.1762

Solution: Here $\frac{dy}{dx} = x - y^2 = f(x, y)$

Taking $h = 0.2$, the starting values of Adams-Bashforth method are

$$\begin{aligned}
x_{-3} &= 0.0 & y_{-3} &= 0.0 & f_{-3} &= 0 - 0 = 0 \\
x_{-2} &= 0.2 & y_{-2} &= 0.02 & f_{-2} &= 0.2 - (0.02)^2 = 0.1996 \\
x_{-1} &= 0.4 & y_{-1} &= 0.0795 & f_{-1} &= 0.4 - (0.0795)^2 = 0.3937 \\
x_0 &= 0.6 & y_0 &= 0.1762 & f_0 &= 0.6 - (0.1762)^2 = 0.5689
\end{aligned}$$

Using the predictor formula, we have

$$y_1 = y_0 + \frac{h}{24}[55f_0 - 59f_{-1} + 37f_{-2} - 9f_{-3}]$$

$$= 0.1762 + \frac{0.2}{24}[55(0.5689) - 59(0.3937) + 37(0.1996) - 9(0)]$$
$$= 0.1762 + 0.1287 = 0.3049$$

Thus, we have $x_1 = 0.8, y_1 = 0.3049$

$$f_1 = 0.8 - (0.3049)^2 = 0.7070$$

Using the corrector formula, we have

$$\begin{aligned}
y_1^{(1)} &= y_0 + \frac{h}{24} \cdot [9f_1 + 19f_0 - 5f_{-1} + f_{-2}] \\
&= 0.1762 + \frac{0.2}{24}[9(0.7070) + 19(0.5689) - 5(0.3937) + 0.1996] \\
&= 0.1762 + 0.1284 = 0.3046
\end{aligned}$$

Thus, we have at $x = 0.8, y_1 = 0.3046$

$$y(0.8) = 0.3046.$$

Example 7.10 Given $y' = x^2 - y, y(0) = 1$ and the starting values $y(0.1) = 0.90516$, $y(0.2) = 0.82127, y(0.3) = 0.74918$. Evaluate $y(0.4)$ using Adams-Bashforth method .

Solution: Here $\frac{dy}{dx} = x^2 - y = f(x, y)$

Taking $h = 0.1$, the starting values of Adams-Bashforth formula are

$$\begin{aligned}
x_{-3} &= 0.0 & y_{-3} &= 1.0 & f_{-3} &= 0 - 1 = -1 \\
x_{-2} &= 0.1 & y_{-2} &= 0.90516 & f_{-2} &= (0.1)^2 - 0.90516 = -0.89516 \\
x_{-1} &= 0.2 & y_{-1} &= 0.82127 & f_{-1} &= (0.2)^2 - 0.82127 = -0.78127 \\
x_0 &= 0.3 & y_0 &= 0.74918 & f_0 &= (0.3)^2 - 0.74918 = -0.65918
\end{aligned}$$

Using the predictor formula, we have

$$\begin{aligned}
y_1 &= y_0 + \frac{h}{24}[55f_0 - 59f_{-1} + 37f_{-2} - 9f_{-3}] \\
&= 0.74918 + \frac{0.1}{24}[55(-0.65918) - 59(-0.78127) + 37(-0.89516) - 9(-1)] \\
&= 0.74918 - 0.0595 = 0.68968 \qquad \text{... (7.14)}
\end{aligned}$$

Thus, we have $x = 0.4, y_1 = 0.68968$

$$f_1 = (0.4)^2 - (0.68968) = -0.52968$$

Using the corrector formula, we have

$$
\begin{aligned}
y_1^{(1)} &= y_0 + \frac{h}{24}[9f_1 + 19f_0 - 5f_{-1} + f_{-2}] \\
&= 0.74918 + \frac{0.1}{24}[9(-0.52968) + 19(-0.65918) - 5(-0.78127) + (-0.89516) \\
&= 0.74918 = 0.0595 = 0.68968 \text{ which is same as (7.14)}
\end{aligned}
$$

Thus, we have at $x = 0.4, y = 0.68968$

$$y(0.4) = 0.68968.$$

7.4 SIMULTANEOUS FIRST ORDER DIFFERENTIAL EQUATIONS

The simultaneous differential equations of the type

$$\frac{dy}{dx} = f(x, y, z) \quad \text{... (7.15)}$$

$$\frac{dz}{dx} = \phi(x, y, z) \quad \text{... (7.16)}$$

with initial conditions $y(x_0) = y_0$ and $z(x_0) = z_0$ can be solved by the methods discussed in the preceding sections, especially Picard's or Runge-Kutta methods.

PICARD'S METHOD

This method is used as follows

$$
\begin{aligned}
y_1 &= y_0 + \int f(x, y_0, z_0)dx, z_1 = z_0 + \int \phi(x, y_0, z_0)dx \\
y_2 &= y_0 + \int f(x, y_1, z_1)dx, z_2 = z_0 + \int \phi(x, y_1, z_1)dx \\
y_3 &= y_0 + \int f(x, y_2, z_2)dx, z_3 = z_0 + \int \phi(x, y_2, z_2)dx
\end{aligned}
$$

and so on.

TAYLOR'S SERIES METHOD

This method is used as follows:

If h be the step-size, $y_1 = y(x_0 + h)$ and $z_1 = z(x_0 + h)$. Then Taylor's algorithm for (7.15) and (7.16) gives

$$y_1 = y_0 + hy_0' + \frac{h^2}{2!}y_0''' + \frac{h^3}{3!}y_0''' + \cdots \qquad \text{... (7.17)}$$

$$z_1 = z_0 + hz_0' + \frac{h^2}{2!}z_0'' + \frac{h^3}{3!}z_0''' + \cdots \qquad \text{... (7.18)}$$

Differentiating (7.15) and (7.16) successively, we get y'', z'', etc. So the values $y_0', y_0'', y_0''' \cdots$ and $z_0, z_0'', z_0''' \cdots$ are known. Substituting these in (7.17) and (7.18), we obtain y_1, z_1 for the next step.

Similarly, we have the algorithms

$$y_2 = y_1 + hy_1' + \frac{h^2}{2!}y_1'' + \frac{h^3}{3!}y_1'' + \cdots \qquad \text{… (7.19)}$$

$$z_2 = z_1 + hz_1' + \frac{h^2}{2!}z_1'' + \frac{h^3}{3!}z_1''' + \cdots \qquad \text{… (7.20)}$$

Since y_1 and z_1 are known, we can calculate $y_1', y_1'', \cdots$ and $z_1', z_1'', \cdots$. Substituting these in (7.19) and (7.20), we get y_2 and z_2.

Proceeding further, we can calculate the other values of y and z step by step.

RUNGE-KUTTA METHOD

Runge-Kutta method is applied as follows:

Starting at (x_0, y_0, z_0) and taking the step-sizes for x, y, z to be h, k, l respectively, the Runge-Kutta method gives,

$$k_1 = hf(x_0, y_0, z_0)$$
$$l_1 = h\phi(x_0, y_0, z_0)$$
$$k_2 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1, z_0 + \frac{1}{2}l_1\right)$$
$$l_2 = h\phi\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1, z_0 + \frac{1}{2}l_1\right)$$
$$k_3 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2, z_0 + \frac{1}{2}l_2\right)$$
$$l_3 = h\phi\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2, z_0 + \frac{1}{2}l_2\right)$$
$$k_4 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_3, z_0 + \frac{1}{2}l_3\right)$$
$$l_4 = h\phi\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_3, z_0 + \frac{1}{2}l_3\right)$$

Hence

$$y_1 = y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

and

$$z_1 = y_0 + \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4)$$

To compute y_2 and z_2, we simply replace x_0, y_0, z_0 by x_1, y_1, z_1 in the above formulae.

Example 7.11 Using Picard's method, find approximate values of y and z corresponding to $x = 0.1$, given that $y(0) = 2, z(0) = 1$ and $dy/dx = x + z, dz/dx = x - y^2$.

Solution: Here $x_0 = 0, y_0 = 2, z_0 = 1$,

and $\frac{dy}{dx} = f(x, y, z) = x + z$

$$\frac{dz}{dx} = \phi(x, y, z) = x - y^2$$

$\therefore\ y = y_0 + \int_{x_0}^{x} f(x, y, z)dx$ and $z = z_0 + \int_{x_0}^{x} \phi(x, y, z)dx$

First approximations

$$y_1 = y_0 + \int_{x_0}^{x} f(x, y_0, z_0)dx = 2 + \int_{x_0}^{x} (x + 1)dx = 2 + x + \frac{1}{2}x^2$$

$$z_1 = z_0 + \int_{x_0}^{x} \phi(x, y_0, z_0)dx = 1 + \int_{x_0}^{x} (x - 4)dx = 1 - 4x + \frac{1}{2}x^2$$

Second approximations

$$\begin{aligned} y_2 &= y_0 + \int_{x_0}^{x} f(x, y_1, z_1)dx = 2 + \int_{0}^{x} \left(1 - 4x + \frac{1}{2}x^2\right) dx \\ &= 2 + x - \frac{3}{2}x^2 + \frac{x^3}{6} \\ z_2 &= z_0 + \int_{x_0}^{x} \phi(x, y_1, z_1)dx = 1 + \int_{x_0}^{x} \left[x - \left(2 + x + \frac{1}{2}x^2\right)^2\right] dx \\ &= 1 - 4x + \frac{3}{2}x^2 - x^3 - \frac{x^4}{4} - \frac{x^5}{20} \end{aligned}$$

Third approximations

$$y_3 = y_0 + \int_{x_0}^{x} f(x, y_2, z_2)dx = 2 + x - \frac{3}{2}x^2 - \frac{1}{2}x^3 - \frac{1}{4}x^4 - \frac{1}{20}x^5 - \frac{1}{120}x^6$$

$$z_3 = z_0 + \int_{x_0}^{x} \phi(x, y_2, z_2)dx$$

$$= 1 - 4x + \frac{3}{2}x^2 + \frac{5}{3}x^3 + \frac{7}{12}x^4 - \frac{31}{60}x^5 + \frac{1}{12}x^6 - \frac{1}{252}x^7$$

and so on.

When $x = 0.1$

$$y_1 = 2.105, \quad y_2 = 2.08517, \quad y_3 = 2.08447$$
$$z_1 = 0.605, \quad z_2 = 0.58397, \quad z_3 = 0.58672.$$

Hence $y(0.1) = 2.0845,\ z(0.1) = 0.5867$

correct to four decimal places.

Example 7.12 Find an approximate series solution of the simultaneous equations $dx/\,dt = xy + 2t, dy/dt = 2ty + x$ subject to the initial conditions $x = 1, y = -1,\ t = 0.$

Solution: Since x and y both being functions of t, Taylor's series gives

$$\left.\begin{aligned} x(t) &= x_0 + tx_0' + \frac{t^2}{2!}x_0'' + \frac{t^3}{3!}x_0''' + \cdots \\ y(t) &= y_0 + ty_0' + \frac{t^2}{2!}y_0'' + \frac{t^3}{3!}y_0''' + \cdots \end{aligned}\right\}$$

Differentiating the given equations w.r.t. t, we get

$$x' = xy + 2t$$
$$y' = 2ty + x$$

and

$$x'' = xy' + x'y + 2$$
$$x''' = (xy'' + x'y') + x''y + x'y'$$
$$\left.\begin{aligned} y'' &= 2ty' + 2y + x' \\ y''' &= 2ty'' + 2y' + 2y' + x'' \end{aligned}\right\}$$

Putting $x_0 = 1, y_0 = -1, t_0 = 0$, we obtain

$$\begin{array}{lll} x_0 & = -1 + 2(0) = -1 & y_0' = 1 \\ x_0' & = x_0 y_0' + x_0' y_0 + 2 & y_0''' = 0 + 2y_0 + x_0' \\ & = 1.1 + (-1)(-1) + 2 = 4 & = 2(-1) + (-1) = -3 \\ x_0''' & = -3 + (-1)(1) + 4(-1) - 1 = -9 & y_0''' = 2 + 2 + 4 = 8 \text{ etc} \end{array}$$

Substituting these values in (i), we get

$$x(t) = 1 - t + 4\frac{t^2}{2!} + (-9)\frac{t^3}{3!} + \cdots = 1 - t + 2t^2 - \frac{3}{2}t^3 + \cdots$$

$$x(t) = 1 + t + 3\frac{t^2}{2!} + 8\frac{t^3}{3!} + \cdots = 1 + t - \frac{3}{2}t^2 + \frac{4}{3}t^3 + \cdots$$

Example 7.13 Solve the differential equations

$$\frac{dy}{dx} = 1 + xz, \frac{dz}{dx} = -xy \text{ for } x = 0.3$$

using the fourth order Runge-Kuta method. Intial values are $x = 0$, $y = 0, z = 1$.

Solution: Here

$$f(x,y,z) = 1 + xz, \phi(x,y,z) = -xy$$

$x_0 = 0, y_0 = 0, z_0 = 1$. Let us take $h = 0.3$.

$k_1 = hf(x_0, y_0, z_0) = 0.3f(0,0,1) = 0.3(1 + 0) = 0.3.$

$l_1 = h\phi(x_0, y_0, z_0) = 0.3(-0 \times 0) = 0$

$$k_2 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1, z_0 + \frac{1}{2}l_1\right)$$

$= (0.3)f(0.15,0.15,1) = 0.3(1 + 0.15) = 0.345$

$$l_2 = h\phi\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1, z_0 + \frac{1}{2}l_1\right)$$

$= (0.3)[-(0.15)(0.15)] = -0.00675$

$$k_3 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{k_2}{2}, z_0 + \frac{l_2}{2}\right)$$

$= (0.3)f(0.15,0.1725,0.996625)$

$= 0.3[1 + 0.996625 \times 0.15] = 0.34485$

$$l_3 = h\phi\left(x_0 + \frac{1}{2}h, y_0 + \frac{k_2}{2}, z_0 + \frac{l_2}{2}\right)$$

$= 0.3[-(0.15)(0.1725)] = -0.007762$

$k_4 = hf(x_0 + h, y_0 + k_3, z_0 + l_3)$

$= 0.3f(0.3,0.34485,0.99224) = 0.3893$

$l_4 = h\phi(x_0 + h, y_0 + k_3, z_0 + l_3)$

$= 0.3[-(0.3)(0.34485)] = -0.03104$

Hence $y(x_0+h)=y_0+\frac{1}{6}(k_1+2k_2+2k_3+k_4)$ i.e., $y(0.3)=0+\frac{1}{6}[0.3+2(0.345)+2(0.34485)+0.3893]=0.34483$

and $z(x+h)=y_0+\frac{1}{6}(l_1+2l_2+2l_3+l_4)$

i.e.

$$\begin{aligned} z(0.3) &= 1+\frac{1}{6}[0+2(-0.00675)+2(0.0077625)+(-0.03104)] \\ &= 0.98999 \end{aligned}$$

SECOND ORDER DIFFERENTIAL EQUATIONS

Consider the second order differential equation

$$\frac{d^2y}{dx_2}=f\left(x,y,\frac{dy}{dx}\right)$$

By writing $dy/dx=z$, it can be reduced to two first order simultaneous differential Equations

$$\frac{dy}{dx}=z,\frac{dz}{dx}f(x,y,z)$$

These equations can be solved as explained above.

Example 7.14 Find the value of $y(1.1)$ and $y(1.2)$ from $y''+y^2y'=x3; y(1)=1, y'(1)=1,$ using the Taylor series method

Solution: Let $y'=z$ so that $y''=z'$

Then the given equation becomes $z'+y^2z=z^3$

$\therefore\ y'=z$

$$z'=x^3-y^2z$$

such that

$$y(1)=1, z(1)=1, h=0.1.$$

Now

$$\left.\begin{aligned} y' &= z, y''=z', y'''=z'' \\ z' &= x^3-y^2z, z''=3x^2-y^2z'-2yz^2(\because y'=z) \\ z''' &= 6x-(y^2z''+2yy'z')-2(y'z^2+y^2zz') \\ &= 6x-(y^2z''+2yz'^2)-2(z^3+2yzz') \end{aligned}\right\}$$

and Taylor's series for $y(1.1)$ is

$$y(1.1) = y(1) + hy'(1) + \frac{h^2}{2!}y''(1) + \frac{h^3}{3!}y'''(1) + \cdots$$

Also

$$y(1) = 1, y'(1) = 1, y''(1) = z'(1) = 0, y'''(1) = z''(1) = 1$$
$$y(1.1) = (1) + 0.1(1) + \frac{(0.1)^2}{2}(0) + \frac{(0.1)^3}{6}(0) = 1.1002.$$

Taylor's series for $z(1.1)$ is

$$z(1.1) = z(1) + hz'(1) + \frac{h^2}{2!}z''(1) + \frac{h^3}{3!}z'''(1) + \cdots$$

Here

$$z(1) = 1, z'(1) = 0, z''(1) = 1, z'''(1) = 3$$
$$z(1.1) = (1) + 0.1(0) + \frac{(0.1)^2}{2}(1) + \frac{(0.1)^3}{6}(3) = 1.0055$$

Hence $y(1.1) = 1.1002$ and $z(1.1) = 1.0055$.

Example 7.15 Using the Runge-Kutta method, solve $y'' = xy'^2 - y^2$ for $x = 0.2$ correct to 4 decimal places. Initial conditions are $x = 0, y = 1, y' = 0$.

Solution: Let $dy/dx = z = f(x, y, z)$

Then $\frac{dy}{dx} = xz^2 - y^2 = \phi(x, y, z)$

We have $x_0 = 0, y_0 = 1, z_0 = 0, h = 0.2$

∴ Runge-Kutta formulae become

$$k_1 = hf(x_0, y_0, z_0) = 0.2(0) = 0$$
$$k_2 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1, z_0 + \frac{1}{2}l_1\right)$$
$$= 0.2(-0.1) = -0.02$$
$$k_3 = hf\left(x_o + \frac{1}{2}h, y_0 + \frac{1}{2}k_2, z_0 + \frac{1}{2}l_2\right)$$
$$= 0.2(-0.0999) = -0.02$$
$$k_4 = hf(x_o + h, y_0 + k_3, z_0 + l_3)$$
$$= 0.2(-0.1958) = -0.0392$$

Hence at $x = 0.2$,

$$\therefore \ k = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.0199$$
$$l_1 = hf(x_0, y_0, z0) = 0.2(-1) = -0.2$$
$$l_2 = h\phi\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1, z_0 + \frac{1}{2}l_1\right)$$
$$= 0.2(-0.999) = -0.1998$$
$$l_3 = h\phi\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2, z_0 + \frac{1}{2}l_2\right)$$
$$= 0.2(-0.9791) = -0.1958$$
$$l_4 = h\phi(x_0 + h, y_0 + k_3, z_0 + l_3)$$
$$= 0.2(0.9527) = -0.1905$$
$$l = \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4) = -0.1970$$

and

$$y = y_0 + k = 1 - 0.0199 = 0.9801$$
$$y' = z = z0 + l = 0 - 0.1970 = -0.1970.$$

Example 7.16 Given $y'' + xy' + y = 0, y(0) = 1, y'(0) = 0$, obtain y for $x = 0(0.1)0.3$ by any method. Further, continue the solution by Milne's method to calculate $y(0.4)$.

Solution: Putting $y' = z$, the given equation reduces to the simultaneous equations

$$z' + xz + y = 0, y' = z$$

We employ Taylor's series method to find y.

Differentiating the given equation n times, we get

$$y_{n+2} + x_{n+1} + ny_n + y_n = 0$$

At

$$x = 0, (y_{n+2})_0 = -(n+1)(y_n)_0$$

$\therefore$ $y(0) = 1$, gives $y_2(0) = -1, y_4(0) = 3, y_6(0) = -5 \times 3, \ldots \ldots$

and $y_1(0) = 0$ yields $y_3(0) = y_5(0) = \cdots \ldots = 0$. Expanding $y(x)$ by Taylor's series, we have

$$y(x) = y(0) + xy_1(0) + \frac{x^2}{2!}y_2(0) + \frac{x^3}{3!}y_3(0) + \cdots$$
$$y(x) = 1 - \frac{x^2}{2!} + \frac{3}{4!}x^4 - \frac{5 \times 3}{6!}x^6 + \cdots$$

and

$$z(x) = y'(x) = -x + \frac{1}{2}x^3 - \frac{1}{8}x^5 + \cdots = -xy,$$

Now, we have

$$y(0.1) = 1 - \frac{(0.1)^2}{2} + \frac{1}{8}(0.1)^4 - \cdots = 0.995$$
$$y(0.2) = 1 - \frac{(0.2)^2}{2} + \frac{(0.2)^4}{8} - \cdots = 0.9802$$
$$y(0.3) = 1 - \frac{(0.3)^2}{2} + \frac{(0.3)^4}{8} - \frac{(0.3)^6}{48} \cdots = 0.956$$

Also, we have

$$z(0.1) = -0.0995, z(0.2) = -0.196, z(0.3) = -0.2863.$$

Also from (1), $z'(x) = -(xz + y)$

$\therefore\ z'(0.1) = 0.985, z'(0.2) = -0.941, z'(0.3) = -0.87.$

Applying Milne's predictor formula, first to z and then to y, we obtain

$$\begin{aligned} z(0.4) \quad &= z(0) + \frac{4}{3}(0.1)\{2z'(0.1) - z'(0.2) + 2z'(0.3)\} \\ &= 0 + \left(\frac{0.4}{3}\right)\{-1.79 + 0.941 - 1.74\} = -0.3692 \end{aligned}$$

and

$$\begin{aligned} y(0.4) \quad &= y(0) + \frac{4}{3}(0.1)\{2y'(0.1) - y'(0.2) + 2y'(0.3)\}\ [\because y' = z] \\ &= 0 + \left(\frac{0.4}{3}\right)\{-0.199 + 0.196 - 0.5736\} = 0.9231 \end{aligned}$$

Also $z'(0.4) = -\{x(0.4)z(0.4) + y(0.4)\}$

$$= -\{0.4(-0.3692) + 0.9231\} = -0.7754.$$

Now applying Milne's corrector formula, we get

$$\begin{aligned} z(0.4) \quad &= z(0.2) + \frac{h}{3}\{z'(0.2) + 4z'(0.3) + z'(0.4)\} \\ &= -0.196 + \left(\frac{0.1}{3}\right)\{-0.941 - 3.48 - 0.7754\} = -0.3692 \end{aligned}$$

and

$$\begin{aligned} y(0.4) \quad &= y(0.2) + \frac{h}{3}\{y'(0.2) + 4y'(0.3) + y'(0.4)\} \\ &= 0.9802 + \left(\frac{0.1}{3}\right)\{-0.196 - 1.1452 - 0.3692\} = 0.9232 \end{aligned}$$

Hence $y(0.4) = 0.9232$ and $z(0.4) = -0.3692$.

7.6 CHECK YOUR PROGRESS

1. Use the Runge-Kutta fourth order method to find the value of y when $x = 1$ given that $\frac{dy}{dx} = \frac{y-x}{y+x}, y(0) = 1$
2. Use the Runge-Kutta method to solve $10\frac{dy}{dx} = x^2 + y^2, y(0) = 1$ for the interval $0 < x \leq 0.4$ with $h = 0.1$
3. Use predictor-corrector method for tabulating a solution of $10\frac{dy}{dx} = x^2 + y^2, y(0) = 1$ for the range $0.5 \leq x \leq 1.0$
4. Tabulate the solution of $\frac{dy}{dx} = x + y, y(0) = 0$ for $0.4 < x \leq 1.0$ with $h = 0.1$, using predictor corrector formulae
5. Solve the system of differential equations $\frac{dx}{dt} = y - t, \frac{dy}{dt} = x + t$ with $x = 1, y = 1$ when $t = 0$ taking $\Delta t = h = 0.1$
6. Compute $y(1.1)$ and $z(1.1)$ given that $\frac{dy}{dx} = xyz, \frac{dz}{dx} = \frac{xy}{z}$ and $y(1) = \frac{1}{3}, z(1) = 1$.
7. Solve the equation $\frac{d^2y}{dx^2} + y = 0$ with the conditions $y(0) = 1$ and $y'(0) = 0$. Compute $y(0.2)$ and $y(0.4)$

7.7 SUMMARY

Students are made familiar with some preliminary definitions and the methods for finding the solution of initial value problems.

7.8 KEYWORDS

Initial value problem, Multi-Step methods, Simultaneous First Order Differential Equations.

7.9 SELF-ASSESSMENT TEST

1. Explain Runge-Kutta method carefully for solving a first order differential equation.
2. Using Runge-Kutta method of fourth order, compute $y(0.2)$ in steps of 0.1 if $\frac{dy}{dx} = x + y^2$ given that $y = 1$ when $x = 0$.

3 Solve numerically $\frac{dy}{dx} = 2e^x - y$, at $x = 0.4, 0.5$ by Milne-Simpson's method given their values at points $x = 0, 0.1, 0.2, 0.3$ are $y_0 = 2, y_1 = 2.010, y_2 = 2.040, y_3 = 2.090$.

4 Solve the initial value problem $\frac{dy}{dx} = 1 + xy^2, y(0) = 1$ for $x = 0.4; 0.5$ by using Milne-Simpson's method, given that

x:	0.1	0.2	0.3
y:	1.105	1.223	1.355

5 Use Milne-Simpson's method to solve $\frac{dy}{dx} = x + y$ with initial condition $y(0) = 1$ from $x = 0.20$ to $x = 0.30$.

6 Given $\frac{dy}{dx} = 1 + y^2$, where $y(0) = 0, y(0.2) = 0.2027, y(0.4) = 0.4228, y(0.6) = 0.6841$. Using Milne-Simpson's method compute $y(0.8)$.

7 Apply Milne-Simpson's method to find a solution of the differential equation $y' = x - y^2$ in the range $0 \leq x \leq 1$ for the boundary condition $y = 0$ at $x = 0$.

8 Use Milne-Simpson's method to solve $\frac{dy}{dx} = x + y$ with initial condition $y(0) = 0$ for $x = 0.4$ to $x = 1$

9 Solve by Milne-Simpson's method, the differential equation $\frac{dy}{dx} = y - x^2$ with the following starting values:

$$y(0) = 1,\ y(0.2) = 1.12186,\ y(0.4) = 1.4682,\ y(0.6) = 1.7379$$

and find the value of y when $x = 0.8$.

10 Find $y(0.1), z(0.1), y(0.2)$, and $z(0.2)$ from the system of equations: $y' = x + z, z' = x - y^2$ given $y(0) = 0, z(0) = 1$ using Runge-Kutta method of the fourth order.

11 Using Picard's method, obtain the second approximation to the solution of

$$\frac{d^2y}{dx^2} = x^3\frac{dy}{dx} + x^3 y \text{ so that } y(0) = 1.\, y'(0) = \frac{1}{2}.$$

7.10 ANSWERS TO CHECK YOUR PROGRESS

1 $y(1) = 1.4983$

2 1.0101, 1.0207, 1.0318, 1.0438

3 1.0569, 1.0713, 1.0871, 1.1048, 1.1244, 1.1464

4 0.0918, 0.1487, 0.2221, 0.3138, 0.4255, 0.5596, 0.7183

5 $(0.1) = 1.1003, y(0.1) = 1.1102$

6 $y(1.1) = 0.3707, z(1.1) = 1.0361$

7 $y(0.2) = 1.0204, y(0.4) = 1.0$

7.11 REFERENCES/ SUGGESTED READINGS

1. JAMES F. EPPERSON; An Introduction to Numerical Methods and analysis. Second Edition Mathematical Reviews, John Wiley & Sons, Inc., Hoboken, New Jersey.
2. S S Shastry; Introductory Methods of Numerical Analysis, Fifth Edition ISBN-978-81-203-4592-8, Asoke K. Ghosh, PHI Learning Pvt. Ltd, M-97, Connaught Circus, New Delhi
3. C.F. Gerald and P.O. Wheatley : Applied Numerical Methods, Low- priced edition, Pearson Education Asia (2002), Sixth Edition.
4. D. Kincaid and W. Cheney, Numerical Analysis: Mathematics of Scientific Computing, 3rd Edn., AMS (2002).
5. D.V. Griffiths and I.M. Smith, Numerical Methods for Engineers, Blackwell Scientific Publications (1991).
6. John H Mathews, Numerical Methods for Mathematics, Science and Engineering, Prentice Hall of India (1994).
7. K. E. Atkinson, Introduction to Numerical Analysis, 2nd Edn., John Wiley (1989).
8. M.K. Jain: Numerical Solution of Differential Equations, 4th Edition, New Age (2018).

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BOUNDARY VALUE PROBLEM

STRUCTURE

8.0 LEARNING OBJECTIVES

- In this chapter we will be able to explaining the solution of boundary value problems based on second order finite difference methods.
- It also brief about the Shooting method, cubic spline methods, and mixed boundary value problems.

8.1 INTRODUCTION

The boundary value problems require solution of a differential equation in a region R subject to the various conditions on the boundary of R. Practical applications give rise to many boundary value problems. Some simple examplés of two point linear boundary value problems are:

$$y''(x) + f(x)y'(x) + g(x)y(x) = r(x) \qquad \dots (8.1)$$

with the boundary conditions

$$y(x_0) = a, \mathrm{y}(\mathrm{x_n}) = b,\ y'(x) + p(x)y(x) = q(x) \qquad \dots (8.2)$$

Also with the conditions $y(x_0) = y'(x_0) = a,\ y(x_n) = y'(x_n) = b$

There exists many numerical methods of solving such boundary value problems, the method of finite-difference is a popular one and will be described here.

8.2 FINITE DIFFERENCE METHOD

The Finite-difference method for the solution of a two point boundary value problem consists in replacing the derivatives occurring in the differential equation and the boundary conditions by means of their finite-difference approximations and solving the resulting linear system of equations by a standard procedure. To obtain the appropriate finite-difference approximations to the derivatives, we proceed as follows: If $y(x)$ and its derivatives are single-valued continuous functions of x then Taylor's series expansion leads to

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2}y''(x) + \frac{h^3}{6}y''(x) + \cdots \qquad \dots (8.3)$$

which implies that

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

Thus we have

$$y'(x) = \frac{1}{h}[y(x+h) - y(x)] + o(h) \qquad \dots (8.4)$$

which is the forward difference approximation of $y'(x)$ with an error of order h.

Similarly, expansion of $y(x-h)$ in Taylor's series gives

$$y(x-h) = y(x) - hy'(x) + \frac{h^2}{2}y''(x) - \frac{h^3}{6}y''(x) + \cdots \qquad \dots (8.5)$$

from which we obtain

$$y'(x) = \frac{1}{h}[y(x) - y(x-h)] + o(h)$$

which is the backward difference approximation $y'(x)$ with an error of the order h. Subtracting (8.3) and (8.5), we obtain

$$y'(x) = \frac{1}{2h}[y(x+h) - y(x-h)] + o(h^2)$$

which is the central difference approximation of $y'(x)$ with an error of the order h^2. Clearly this central difference approximation to $y'(x)$ is better than the forward or backward difference approximations and hence should be preferred. Again adding (8.3) and (8.5), we get

$$y''(x) = \frac{1}{h^2}[y(x+h) - 2y(x) + y(x-h)] + o(h^2)$$

which is the central difference approximation to $y''(x)$. In a similar manner, it is possible to derive finite-difference approximations to higher order derivatives. To solve the boundary value problems defined by (8.1) and (8.2), we divide the range $[x_0, x_n]$ into n equal subintervals of width h so that

$$x_i = x_0 + ih, i = 1,2,3 \dots n.$$

The corresponding values of y at these points are denoted by

$$y(x_i) = y_i = y(x_0 + ih), i = 1,2,3 \dots$$

Hence the working expressions for the central difference approximations to the first four derivatives of y_i are as under:

$$y_i' = \frac{1}{2h}(y_{i+1} - y_{i-1})$$
$$y_i'' = \frac{1}{h^2}(y_{i+1} - 2y_i + y_{i-1})$$
$$y_i^m = \frac{1}{2h^3}(y_{i+2} - 2y_{i+1} - y_{i-2})$$
$$y_i^{iv} = \frac{1}{h^4}(y_{i+2} - 4y_{i+1} + 6y_i - 4y_{i-1} + y_{i-2})$$

The accuracy of this method depends on the size of the subinterval viz h and also on the order of approximations. As we reduce h, the accuracy improves although the number of equations to be solved increases.

Example 8.1 To solve the equation $y'' + y + 1 = 0$ with the boundary conditions $y(0) = 0$ and $y(1) = 0$.

Solution: The given equation is

$$y'' + y + 1 = 0$$

we divide the interval (0,1) into four sub intervals so that $h = 0.25$ and the pivot points are $x_0 = 0, x_1 = 0.25, x_2 = 0.5, x_3 = 0.75$ and $x_4 = 1.0$. Then the differential equation is approximated as

$$\frac{1}{h^2}[y_{i+1} - 2y_i + y_{i-1}] = -1 - y_i$$

or

$$16y_{i+1} - 31y_i + 16y_{i-1}, = -1, i = 1,2,3$$

Using $y_0 = y_4 = 0$, we get the system of equations

$$16y_2 - 31y_1 = -1$$

$$16y_3 - 31y_2 + 16y_1 = -1$$
$$-31y_3 + 16y_2 = -1$$

Their solutions are

$$y_1 = 0.1047, y_2 = 0.1403, y_3 = 0.1047$$

up to four decimal places. The exact solution of the given differential equation is

$$y(x) = \frac{1 - e^{-x}}{1 - e^{-1}} - x$$

The error at each nodal point is given in the table below:

X	Computed value of $y(x)$	Exact value of $y(x)$	Error
0.25	0.1047	0.099932	0.004768
0.5	0.1403	0.1224593	0.0178407
0.75	0.1047	0.0847038	0.0199961

Example 8.2 The deflection of a beam is governed by the equation $\frac{d^4y}{dx^4} + 81y = \phi(x)$, where $\phi(x)$ is given by

x	$\frac{1}{3}$	$\frac{2}{3}$	1
$\phi(x)$	81	162	243

and boundary conditions $y(0) = y'(0) = y''(1) = y''(1) = 0$. Evaluate the deflection at the pivot points of the beam using three subintervals.

Solution: Here $h = 1/3$ and the pivot points are $x_0 = 0, x_1 = 1/3, x_2 = 2/3$ and $x_3 = 1$.

The corresponding values of y are $y_0 = 0, y_1, y_2, y_3$. The given differential equation can be approximated to

$$\frac{1}{h^4}[y_{i+2} - 4y_{i+1} + 6y_i - 4y_i + y_{i-2}] + 81y_i = \phi(x_i), i = 1, 2, 3$$

This leads to system of equations

$$
\begin{aligned}
y_3 - 4y_2 + 7y_1 - 4y_0 + y_{-1} &= 1 \\
y_4 - 4y_3 + 7y_2 - 4y_1 + y_0 &= 2 \\
y_5 - 4y_4 + 7y_3 - 4y_2 + y_1 &= 3
\end{aligned} \qquad \ldots (8.6)
$$

where $y_0 = 0$. Since $y_i' = \frac{1}{2h}(y_{i+1} - y_{i-1})$, therefore for $i = 0$, we have

$$0 = y_0' = \frac{1}{2h}(y_1 - y_{-1}) \Rightarrow y_{-1} = y_1 \qquad \ldots (8.7)$$

Also $y_i'' = \frac{1}{h^2}(y_{i+1} - 2y_i + y_{i-1})$, for $i = 3$ gives us

$$0 = y_3'' = \frac{1}{h^2}(y_4 - 2y_3 + y_2) \Rightarrow y_4 = 2y_3 - y_2 \qquad \ldots (8.8)$$

Again $y_i''' = \frac{1}{2h^3}(y_{i+2} - 2y_{i+1} + 2y_{i-1} - y_{i-2})$, for $i = 3$ leads to

$$0 = y_3^{m\prime} = \frac{1}{2h^3}(y_5 - 2y_4 + 2y_2 - y_1) \Rightarrow y_5 = 2y_4 - 2y_2 + y_1 \qquad \ldots (8.9)$$

Using equations (8.7) to (8.9) in equation (8.6) we obtain

$$
\begin{aligned}
y_3 - 4y_2 + 8y_1 &= 1 \\
-y_3 + 3y_2 - 2y_1 &= 1 \\
3y_3 - 4y_2 + 2y_1 &= 3
\end{aligned}
$$

Solving this system of equations, we get

$$y_1 = 8/13, y_2 = 22/13, y_3 = 37/13$$

Hence the required solution is

$$y(1/3) = 0.6154, y(2/3) = 1.6923, y(1) = 2.8462$$

correct to four decimal places.

8.3 SHOOTING METHOD

This method can be applied to both linear and non-linear problems and required good initial guesser for the slope. It is easy and convenient to apply. The men steps involve in this method are:

(i) transformation of the boundary value problem into an initial value problem

(ii) solution of the initial value problem by Taylor' series method ,or Runge-Kutta method etc. and

(iii) solution of the given boundary value problem

Consider the second order boundary value problem

$$y''(x) = f(x), y(0) = 0, y(1) = 1$$

Let us assume that the true value of $y'(0)$ be m. We take two initial guesses for m as m_0 and m_1. Let $y(m_0, 1)$ and $y(m_1, 1)$ be the corresponding values of $y(1)$ obtained by initial value method. The by using liner interpolation, we option a better approximation m_2 for m, given by

$$\frac{m_2 - m_0}{y(1) - y(m_0, 1)} = \frac{m_1 - m_0}{y(m_1, 1) - y(m_0, 1)}$$

which implies that

$$m_2 = m_0 + (m_1 - m_0)\frac{y(1)-y(m_0,1)}{y(m_1,1)-y(m_0,1)} \qquad \dots (8.10)$$

We now solve that initial problem

$y''(x) = f(x), y(0) = 0$ and $y'(0) = m_2$ and obtain $y(m_2 1)$.we again apply interpolation with $\left(m_1, y(m_1, 1)\right)$ and $\left(m_1, y(m_2, 1)\right)$ to obtain a better approximation m_3 for m and so on. The process is repeated until the convergence and desisted level of accuracy is obtained i.e., until the value of $y(m_1, 1)$ agree with $y(1)$ of to the desired level of accuracy. The spaced of convergence depends, on how good the initial guesses are chosen. However, the method will be difficult to apply to higher order boundary value problem and in the case of now linear problems.

Example 8.3 Solve the boundary value problem $y''(x) = y(x), y(0) = 0$ and $y(1) = 1.1752$ by shooting method, taking $m_0 = 0$ and $\mathrm{y}(1) = 0.9$.

Solution: Appling Taylor's series method, we obtain

$$y(x) = y'(0) \cdot \left[x + \frac{x^3}{6} + \frac{x^5}{120} + \frac{x^7}{5040} + \frac{x^9}{362800} + \cdots\right]$$

Hence

$$y(1) = y'(0)\left[1 + \frac{1}{6} + \frac{1}{120} + \frac{1}{5040} + \frac{1}{362800} + \cdots\right] = 1.1752\mathrm{y}'(0)$$

With $m_0 = 0.8$ and $m_1 = 0.9$, we get

$$y(m_0, 1) = 0.9402 \text{ and } y(m_1, 1) = 1.578$$

Using liner interpolation formula (8.10), we get

$$m_2 = 0.8 + (0.1)\frac{1.1752 - 0.9402}{1.0578 - 0.9404} = 0.8 + 0.1998 = 0.9998$$

which is closer to the exact value of $y'(0) = 1$ We now solve the initial value problem $y''(x) = y(x), y(0) = 0$, m_2. Again using Taylor's series solution, we get $y(m_2, 1) = 1.174$ which is also closer to the exact value $y(1) = 1.175$. This problem can also be solve by using Runge Kutta fourth order method.

8.4 CUBIC SPLINE METHOD

Let $s(x)$ be the cubic spline approximating the function $y(x)$ and let $s''(x_i) = M_i$. Then, at $x = x_i$ the differential equation given in (8.1) gives

$$M_i + f_i s'(x_i) + g_i y_i = r_i \qquad \dots (8.11)$$

But

$$s'(x_i -) = \frac{h}{3!}(2M_i + M_{i-1}) + \frac{1}{h}(y_i - y_{i-1}) \qquad \dots (8.12)$$

and

$$s'(x_i +) = -\frac{h}{3!}(2M_i + M_{i+1}) + \frac{1}{h}(y_{i+1} - y_i) \qquad \dots (8.13)$$

Substituting (8.12) and (8.13) successively in (8.11), we obtain the equations

$$M_i + f_i\left[\frac{h}{6}(2M_i + M_{i-1}) + \frac{1}{h}(y_i - y_{i-1})\right] + g_i y_i = r_i \qquad \dots (8.14)$$

and

$$M_i + f_i\left[-\frac{h}{6}(2M_i + M_{i+1}) + \frac{1}{h}(y_{i+1} - y_i)\right] + g_i y_i = r_i. \qquad \dots (8.15)$$

Since y_0 and y_n are known, Eqs. (8.14) and (8.15) constitute a system of $2n$ equations in $2n$ unknowns, viz., $M_0, M_1, \dots, M_n, y_1, y_2, \dots, y_{n-1}$. It is, however, possible to eliminate the M_i and obtain a tridiagonal system for y_i. The following examples illustrate the use of the spline method.

Example 8.4 Solve the problem $y'' + y + 1 = 0,\ y(0) = y(1) = 0$

Solve: If we divide the interval [0,1] into two equal subintervals, then from given problem and the recurrence relations for M_i, we obtain

$$y(0.5) = \frac{3}{22} = 0.13636$$

and

$$M_0 = -1,\ M_1 = -\frac{25}{22},\ M_2 = -1$$

Hence we obtain

$$s'(0) = \frac{47}{88},\ s'(1) = -\frac{47}{88},\ s'(0.5) = 0.$$

From the analytical solution of the problem, we observe that $y(0.5) = 0.13949$ and hence the cubic spline solution of the boundary-value problem has an error of 2.24%.

Example 8.5 Given the boundary-value problem

$$x^2y'' + xy' - y = 0;\ y(1) = 1,\ y(2) = 0.5$$

apply the cubic spline method to determine the value of $y(1.5)$.

Solution: The given differential equation is

$$y'' = -\frac{1}{x}y' + \frac{1}{x^2}y$$

Setting $x = x_i$ and $y''(x_i) = M_i$, given problem gives

$$M_i = -\frac{1}{x_i}y_i' + \frac{1}{x_i^2}y_i$$

Using the expressions given in (8.12) and (8.13), we obtain

$$M_i = -\frac{1}{x_i}\left(-\frac{h}{3}M_i - \frac{h}{6}M_{i+1} + \frac{y_{i+1} - y_i}{h}\right) + \frac{1}{x_i^2}y_i,\ i = 0,1,2,\dots,n-1. \qquad \dots (8.16)$$

and

$$M_i = -\frac{1}{x_i}\left(\frac{h}{3}M_i + \frac{h}{6}M_{i-1} + \frac{y_i - y_{i-1}}{h}\right) + \frac{1}{x_i^2}y_i,\ i = 1,2,\dots,n \qquad \dots (8.17)$$

If we divide [1,2] into two subintervals, we have $h = 1/2$ and $n = 2$. Then Eqs. (8.16) and (8.17) give

$$\begin{aligned} 10M_0 - M_1 + 24y_1 &= 36 \\ 16M_1 - M_2 - 32y_1 &= -12 \\ M_0 + 20M_1 + 16y_1 &= 24 \\ M_1 + 26M_2 - 24y_1 &= -9 \end{aligned}$$

Eliminating M_0, M_1 and M_2 from these system of equation we obtain

$$y_1 = 0.65599.$$

Since the exact value of $y_1 = y(1.5) = 2/3$, the error in the computed value of y_1 is 0.01 , which is about 1.5% smaller.

8.5 MIXED BOUNDARY PROBLEMS

We now consider the boundary conditions

$$\begin{aligned} a_0 y(a) - a_1 y'(a) &= \gamma_1, \\ b_0 y(b) + b_1 y'(b) &= \gamma_2. \end{aligned}$$

We obtain the second order approximations for the boundary conditons as follows.

(i) At $x = x_0$: $a_0 y_0 - \frac{a_1}{2h}[y_1 - y_{-1}] = \gamma_1$

or

$$y_{-1} = -\frac{2ha_0}{a_1} y_0 + y_1 + \frac{2h}{a_1}\gamma_1$$

$$\text{At } x = x_{N+1}\text{: } b_0 y_{N+1} + \frac{b_1}{2h}[y_{N+2} - y_N] = \gamma_2$$

or

$$y_{N+2} = y_N - \frac{2hb_0}{b_1} y_{N+1} + \frac{2h}{b_1}\gamma_2$$

The values y_{-1} and y_{N+2} can be eliminated by assuming that the difference equation for given differential equation holds also for $j = 0$ and $N + 1$, that is, at the boundary points x_0 and x_{N+1}.

(ii) At $x = x_0$: $a_0 y_0 - \frac{a_1}{2h}(-3y_0 + 4y_1 - y_2) = \gamma_1$

or

$$(2ha_0 + 3a_1)y_0 - 4a_1 y_1 + a_1 y_2 = 2h\gamma_1.$$

At $x = x_{N+1}$: $b_0 y_{N+1} + \frac{b_1}{2h}(3y_{N+1} - 4y_N + y_{N-1}) = \gamma_2$

or

$$b_1 y_{N-1} - 4b_1 y_N + (2hb_0 + 3b_1) y_{N+1} = 2h\gamma_2$$

Example 8.6 Use a second order method for the solution of the boundary value problem

$$\begin{aligned} y'' &= xy + 1, x \in [0,1], \\ y'(0) + y(0) &= 1, y(1) = 1, \end{aligned}$$

with the step length $h = 0.25$.

Solution: The nodal points are $x_n = nh, n = 0(1)4, h = 1/4, Nh = 1$. The discretizations of the differential equation at $x = x_n$ and that of the boundary conditions at $x = 0$ and $x = x_N = 1$ lead to

$$\begin{aligned} &-\frac{1}{h^2}(y_{n-1} - 2y_n + y_{n+1}) + x_n y_n + 1 = 0, n = 0(1)3, \\ &\frac{y_1 - y_{-1}}{2h} + y_0 = 1, y_4 = 1. \end{aligned}$$

Simplifying we get

$$\begin{aligned} &-y_{n-1} + (2 + x_n h^2) y_n - y_{n+1} = -h^2, n = 0(1)3 \\ &y_{-1} = 2hy_0 + y_1 - 2h,\ y_4 = 1. \end{aligned}$$

We have the following results.

$$\begin{aligned} &n = 0, x_0 = 0:\ -y_{-1} + 2y_0 - y_1 = -\frac{1}{16} \\ &n = 1, x_1 = 0.25:\ -y_0 + \frac{129}{64} y_1 - y_2 = -\frac{1}{16} \\ &n = 2, x_2 = 0.5:\ -y_1 + \frac{65}{32} y_2 - y_3 = -\frac{1}{16} \\ &n = 3, x_3 = 0.75:\ -y_2 + \frac{131}{64} y_3 - y_4 = -\frac{1}{16} \\ &\text{and }\ y_{-1} = \frac{1}{2} y_0 + y_1 - \frac{1}{2}, y_4 = 1. \end{aligned}$$

x	4	5	6	7
y	0.15024	4 40.56563	3 1.54068	8 3.25434

	x	8	9	10
	y 5.	6.5		

Substituting for y_{-1} and y_4, we get the following system of equations

$$\begin{bmatrix} 3/2 & -2 & 0 & 0 \\ -1 & 129/64 & -1 & 0 \\ 0 & -1 & 65/32 & -1 \\ 0 & 0 & -1 & 131/64 \end{bmatrix} \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{bmatrix} = -\frac{1}{16} \begin{bmatrix} 9 \\ 1 \\ 1 \\ -15 \end{bmatrix}$$

Using the Gauss elimination method, we find

$$y_0 = -7.4615, y_1 = -5.3149, y_2 = -3.1888, y_3 = -1.0999.$$

8.6 CHECK YOUR PROGRESS

1. Solve the equation $\frac{d^2y}{dx^2} + y = 0$ with the conditions $y(0) = 1$ and $y'(0) = 0$. Compute $y(0.2)$ and $y(0.4)$

2. Solve the boundary value problem $y'' - 64y + 10 = 0$ with $y(0) = y(1) = 0$, by finite difference method. Compute $y(0.5)$ and compute it with the true value.

3. Solve the boundary value problem

$$y''(x) - y(x) = 0, y(0) = 0, y(1) = 1$$

by finite difference and cubic spline methods. In each case take h=0.5 and h=0.25.

4. Solve the boundary value problems

(a) $y''(x) = y(x), y(0) = 0, y(1) = 1$

(b) $y'' - 64y + 10 = 0, y(0) = y(1) = 0$

by shooting method.

8.7 SUMMARY

- The students are made familiar with some preliminary definitions and results of finite difference solution of boundary value problems.
- Lastly the solution of mixed boundary value problems has been explained in detail.

8.8 KEYWORDS

Boundary value problems, finite difference methods, shooting method, cubic spline method, mixed boundary value problems.

8.9 SELF-ASSESSMENT TEST

1. Solve the boundary value problem $y'' - 64y + 10 = 0$ with $y(0) = y(1) = 0$ by the finite difference method. Compute the value of $y(0.5)$ and compare with the true value.
2. Solve the boundary value problem
$$y'' + xy' + y = 3x^2 + 2, y(0) = 0, y(1) = 1.$$
3. Apply shooting method to solve the boundary value problem
$$\frac{d^2y}{dx2} = y, y(0) = 0 \text{ and } y(1) = 1.1752$$
4. Using shooting method, solve the boundary value problem
$$\frac{d^2y}{dx2} = 6y^2, y(0) = 1, y(0.5) = 0.44$$

8.10 ANSWERS TO CHECK YOUR PROGRESS

1. y(0.2)=1.0204, y(0.4)=1.0

2 y(0.5)=0.1389 for n=2, y(0.5)=0.1470 for n=4.

3 0.443674, 0.443140

8.11 REFERENCES/ SUGGESTED READINGS

1 JAMES F. EPPERSON; An Introduction to Numerical Methods and analysis. Second Edition Mathematical Reviews, John Wiley & Sons, Inc., Hoboken, New Jersey.

2 S S Shastry; Introductory Methods of Numerical Analysis, Fifth Edition ISBN-978-81-203-4592-8, Asoke K. Ghosh, PHI Learning Pvt. Ltd, M-97, Connaught Circus, New Delhi

3 C.F. Gerald and P.O. Wheatley : Applied Numerical Methods, Low- priced edition, Pearson Education Asia (2002), Sixth Edition.

4 D. Kincaid and W. Cheney, Numerical Analysis: Mathematics of Scientific Computing, 3rd Edn., AMS (2002).

5 D.V. Griffiths and I.M. Smith, Numerical Methods for Engineers, Blackwell Scientific Publications (1991).

6 John H Mathews, Numerical Methods for Mathematics, Science and Engineering, Prentice Hall of India (1994).

7 K. E. Atkinson, Introduction to Numerical Analysis, 2nd Edn., John Wiley (1989).

8 M.K. Jain: Numerical Solution of Differential Equations, 4th Edition, New Age (2018).