# *Numerical Analysis*

MAT327

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# Preface

This is a compilation of lecture notes with some books and my own thoughts. If there are any mistake/typing error or, for any query mail me at mehedi12@student.sust.edu. I didn't include "Solution of Linear System using Excel" and "Curve Fitting using Excel" sections from documents "Num methods 3(H)" and "Num methods(5H)". Partly because it wasn't in syllabus but mostly, I was too lazy to type these sections. For numerical analysis lab code written in ForTran visit here.

# Contents

# Part I

# Syllabus

# Syllabus

Errors in numerical calculations:

- Errors definitions, sources, examples;
- propagation error;
- a general error formula.

Root finding:

- The bisection method;
- the iteration method;
- the method of false position;
- Newton-Raphson method.

Methods of interpolation theory:

- Polynomial interpolation;
- error in polynomial interpolation;
- interpolation using Newton's forward and backward formulas and Newton's divided difference formula and central difference formula;
- Starling's interpolating polynomial;
- Lagrange's interpolating polynomial;
- quadratic, cubic spline and B -spline interpolation methods;
- idea of extrapolation.

Numerical differentiation.
Numerical integration:

- Trapezoidal method;
- Simpson's method;
- Weddle's method;
- Romberg's method;
- error analysis;
- Gaussian quadrature rule.

Solutions 0f system of linear equations:

- Gaussian elimination with and without pivoting;
- iteration method;
- solution of tri-diagonal system of equations.

# Part II

# Class Note/Sheet

# Chapter 1

# Errors In Numerical Analysis

## 1.1 Rounding Off

We come across numbers with a large number of digits, and it will be necessary to cut them to a measurable number of figures. This process is called rounding off.

To round off a number to $n$ significant digits, discard all digits to the right of the $n$th digit and if this discarded number is

(a) less than half a unit then in the $n$th place, leave the $n$th digit unaltered.

(b) greater than half a unit then in the $n$th place, increase the $n$th digit by unity.

(c) exactly half a unit then in the $n$th place, increase the $n$th digit by unity, if it is odd, otherwise leave it unchanged.

The number thus rounded off is said to be exact to $n$ significant figures.

**Example.** The numbers given below are rounded off to four significant figures.
1.658 3 to 1.658
30.056 7 to 30.06
0.859 378 to 0.859 4
3.141 59 to 3.142

## 1.2 Significant

The digits that are used to express numbers are called significant digits or significant figures.

Thus, the number $3.141\,6, 0.666\,67$ and $5.068\,7$ contain five significant digits. The number 0.00023 has, however, only two significant digits viz. 2 and 3. Since, the zeros serve only to fix the position of the decimal points.

Any real number is represented as $y = 0.d_1d_2 \ldots d_kd_{k+1} \cdots \times 10^n$ $\rightarrow$ floating point number.
FLOAT($y$) is obtained by terminating the mantissa of $y$ at $k$ decimal digits by,

1. chopping off the digits $d_{k+1} \ldots$ to get $\text{FLOAT}(y) = 0.d_1d_2 \ldots d_k \times 10^n$

2. Adding $10^{n-(k+1)}$ to $y$ and the $n$ chop off to get $\text{FLOAT}(y) = 0.d_1d_2 \ldots d_k \times 10^n \rightarrow$ rounding off.

**Example.** We have $\pi = 3.141\,592\,65\ldots$
$= 0.314\,159\,265 \times 10^1$
Let $k = 5$, here $n = 1$
So

(i) by chopping, $\text{FLOAT}(\pi) = 0.314\,15 \times 10^1$
$= 3.141\,5$

(ii) by rounding $\text{FLOAT}(\pi) = 0.314\,159\,265 \times 10^1 + 10^{1-(5+1)}$
$= (0.314\,159\,265 + 10^{-5}) \times 10^1$
$= (0.314\,15 + 0.000\,01) \times 10^1$
$= 3.141\,6$

Here rounding error is $0.000\,1$.

## 1.3 Errors and Their Analysis

In numerical analysis, we usually come across two types of errors:

1. Inherent errors:

   Most numerical computation are inexact, either due to the given data being approximate or due to the limitations of the computing aids: mathematical tables, disk calculators or the digital computer. Due to this limitation, numbers have to be rounded off, causing what are called rounding errors. In computations inherent errors can be minimized by obtaining better data, by correcting obvious errors in the data and by using computation aids of higher precision. In hand computations, the round off error can be reduced by carrying the computations to more significant figures at each step of the computation. A useful rule is:
   At each step of the computation, retain at least one more significant figure than that given in the data, perform the last operation and then round off.

2. Truncation errors:

   These are errors caused by using approximate formulae in computations such as the one that arises when a function $f(x)$ is evaluated from an infinite series for $x$ after 'truncating' it at a certain stage. The study of this type of error is usually associated with the problem of convergence.

   Truncation error in a problem can be evaluated, and it is desirable to make it as small as possible.

## 1.4 Absolute Error, Relative Error and Percentage Error

### 1.4.1 Absolute Error

The numerical difference between the true value of a quantity and its approximate value is called absolute error. Thus, the absolute error $E_A$ is given by
$E_A = X - X_1 = \delta_x$
Where,
$X$ = True value of a quantity
$X_1$ = The approximate value

### 1.4.2 Relative Error

Relative Error $E_R$ is defined by

$$E_R = \frac{E_A}{X} = \frac{\delta_X}{X}$$

### 1.4.3 Percentage Error

Percentage error $E_P$ is defined by

$$E_P = 100E_R$$

Let $\Delta x$ be a number such that $|X_1 - X| \leq \Delta X$. Then $\Delta X$ is an upper limit on the magnitude of the absolute error and is said to measure absolute accuracy. Similarly, the quantity $\frac{\Delta X}{|X|} \approx \frac{\Delta X}{|X_1|}$ measures the relative accuracy.

# Chapter 2

# Root Finding

## 2.1 Iteration

Iteration is a numerical method used to find approximation to solutions of equations of the following type, when the exact solution can not be obtained by algebraic methods.
Let,

$N_0(t) =$ Initial Population
$N(t) =$ Population at any time
$\lambda =$ Constant birth rate

Then we find the differential equations as

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\left(N(t)\right) = \lambda N(t) \tag{2.1}$$

Solutions of (2.1) is

$$N(t) = N_0 e^{\lambda t}$$

Suppose immigration is allowed at a constant rate $V$. Then the differential equation becomes

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\left(N(t)\right) = \lambda N(t) + V \tag{2.2}$$

Solution of (2.2) is

$$N(t) = N_0 e^{\lambda t} + \frac{V}{\lambda}(e^{\lambda t} - 1)$$

If any three are given then the other value can not easily find.

### 2.1.1 Solution of $f(x) = 0$ by Iteration

We start with an approximate $x_0$ to the solution and apply to it a procedure which gives another approximation $x_1$. This new approximation normally a better one, is now used as a new value of $x_0$, and the process is repeated.

This iteration is said to converge if we can reach a stage, where $x_1 = x_0$.

## 2.2 Bisection Method

### 2.2.1 Bisection Method

To discuss bisection method we study the following theorem:

*Theorem* 2.2.1. Let $f(x)$ be continuous on $[a, b]$ and $f(a)$ and $f(b)$ are of opposite signs, then there exists at least one $c \in (a, b)$ such that $f(c) = 0$.

Let $f(a)$ be negative and $f(b)$ be positive. Then the root lies between $a$ and $b$ and let its approximate value be given by $x_0 = \frac{a+b}{2}$. If $f(x_0) = 0$, we conclude that $x_0$ is a root of the equation $f(x) = 0$. Otherwise, the root lies either between $x_0$ and $b$ or between $x_0$ and $a$ depending on whether $f(x_0)$ is negative or positive. Again, choose the second approximation either $x_1 = \frac{a+x_0}{2}$ if $f(x_0)$ is +ve or $x_1 = \frac{b+x_0}{2}$ if $f(x_0)$ is −ve. If $f(x_1) = 0$ then we conclude that $x_1$ is the root of $f(x) = 0$. Otherwise, again choose a new approximation. Repeat the process until the root is known to the desired accuracy. This method is shown graphically in the following figure:

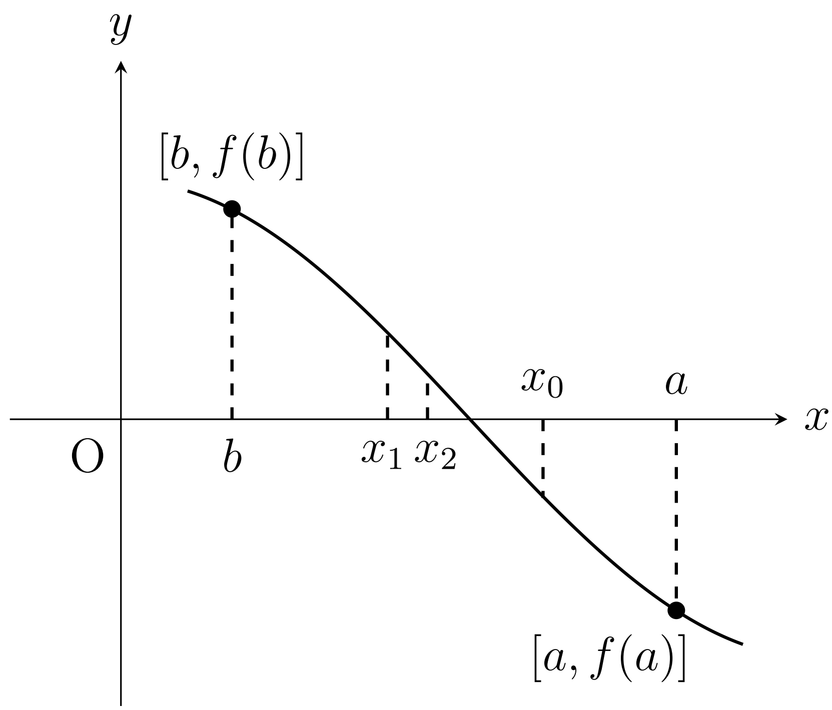



Figure 2.1: Bisection Method

**Problem 2.2.1.** Find a real root of the equation

$$f(x) = x^3 - x - 1 = 0$$

**Solution.** Here, $f(1) = -1$ and $f(2) = 2^3 - 2 - 1 = 5$
Thus $f(1) = -1 < 0 < 5 = f(2)$
By the above theorem (2.2.1) $f(x)$ has at least one root in the interval $[1, 2]$.
Here $f'(x) = 3x - 1, f'(1) = 2, f'(2) = 11$ If $f(x)$ vanishes at one or more points in the interval $[1, 2]$, then by Rolle's theorem $f'(x)$ should vanish somewhere in $[1, 2]$.

Since $f'(x)$ is positive on $[1,2]$, $f(x)$ has exactly one root in $[1,2]$, say $P$.

Take $P = \frac{1+2}{2} = 1.5$

Here $|\text{error}| \leq 0.5$

Evaluate $f(P) = f(1.5) = 0.875 > 0 > -1 = f(1)$

The root lies in the smaller interval $[1, 1.5]$

Now, take $P_1 = \frac{1+1.5}{2} = \frac{2.5}{2} = 1.25$

Here $|\text{error}| \leq 0.25$

Again,

$$f(1.25) = (1.25)^3 - 1.25 - 1$$
$$= -0.296\,875 < 0 < 0.875 = f(1.25)$$

So the new interval is $[1.25, 1.5]$, i.e. the root lies in the smaller interval $[1.25, 1.5]$.

Take the new approximation $P_2 = \frac{1.25+1.5}{2} = 1.375$

Here $|\text{error}| \leq 0.125$

The procedure is repeated and the successive approximations are $P_3 = 1.312\,5$, $P_4 = 1.343\,75$, $P_5 = 1.328\,125$, etc.

After 20 times $1.324\,171\,75 \leq P_{20} \leq 1.324\,471\,85$

### 2.2.2 Definition of Bisection Method

The process of locating a solution of an equation $f(x) = 0$ in a sequence of intervals of decreasing size and increasing accuracy is known as the *Bisection method.*

Each step of the above algorithm is of the bisection method produces one more correct digit of the root of $f(x) = 0$.

So one can always locate a root to any desired accuracy with this algorithm. But Bisection method converges to the required accuracy very slowly.

The bisection method calls for a repeated halving of a subintervals $[a, b]$ and at each step locating the 'half' containing the root $P$.

### 2.2.3 Bisection Method

Suppose $f(x)$ is a continuous function defined on $[a, b]$ with $f(a)$ and $f(b)$ of opposite signs.

Then by the theorem (2.2.1) there exists $P \in [a, b]$ such that $f(P) = 0$.

<u>Process:</u>

1. To start, set $a_1 = a$, $b_1 = b$, $P_1 = \frac{a+b}{2}$
2. If $f(P_1) = 0$, then $P = P_1$ and the process is complete
3. If $f(P_1) \neq 0$, then $f(P_1)$ has same sign as either $f(a_1)$ or $f(b_1)$
4. If $f(P_1)$ and $f(a_1)$ have the same sign then $P \in [P_1, b_1]$ and set $a_2 = P_1$, $b_2 = b_1$
5. If $f(P_1)$ and $f(b_1)$ have the same sign then $P \in [a_1, P_1]$ and set $a_2 = a_1$, $b_2 = P_1$

Repeat the process to the new interval $[a_2, b_2]$

### 2.2.4 Algorithm For Bisection Method

**Data Table**

Input Variables:

$$a, b, N = \text{no of iterations}$$
$$ERR = \text{maximum error allowed}$$
$$f(x) = 0$$

Output Variables:

$$P = \text{Approximate solution}$$
$$\text{or, } m = \text{Number of steps and message showing iteration failed in } m \text{ steps.}$$

**Algorithm**

Step 1 : Set $I = 1$ (initialized counter)

Step 2 : If $I \leq N$, Do steps 3-6

Step 3 : set $P = a + (b - a)/2.0$

Step 4 : If $f(P) = 0$ or $(b - a)/2.0 < ERR$, THEN
Output $P$(procedure compiled successfully)
STOP

Step 5 : ELSE set $I = I + 1$

Step 6 : If $f(a)f(P) > 0$ THEN
set $a = P$
ELSE set $b = P$

Step 7 : Output (Method failed after $m = N$ iterations, procedure computed unsuccessfully)
STOP

### 2.2.5 Sample Code

```fortran
program bisection
    !equation::x^3+x^2+x+7=0
    implicit none
    real a, b, p
    real, external :: f
    real, parameter :: error = 0.00001
    integer i, n

    print *, "Enter a(start interval) and b(end interval) and n(iterations)"
    read *, a, b, n

    do while (f(a)*f(b) > 0)
        print *, "No root contains in the given interval. Try again"
        print *, "Enter a(start interval) and b(end interval)"
        read *, a, b
    end do

    write (*, "(2x,'N',11x,'P',10x,'f(P)')")
    do i = 1, n
        p = (a + b)/2.0
        write (*, "(1x,i3,3x,1x,f9.5,3x,1x,f9.5)") i, p, f(p)
        if (f(p) == 0.0 .or. (abs((b - a)/2.0)) < error) then
            write (*, "('The root is P=',1x,f8.4)") p
            stop
        end if
        if (f(p) > 0) then
            a = p
        else
            b = p
        end if
    end do

    write (*, "('NO ROOT FOUND AFTER',1x,i3,1x,'ITERATIONS')") n

end program bisection

real function f(x)
    implicit none
    real, intent(in) :: x

    f = x**3 + x**2 + x + 7

end function f
```

Listing 2.1: A sample program to solve $x^3 + x^2 + x + 7 = 0$ by using bisection method

## 2.3 Newton-Raphson Method

### 2.3.1 Newton-Raphson Method

This is one of most powerful method general application for deriving an iteration formula for the solution of $f(x) = 0$.

### 2.3.2 Newton-Raphson Formula

Let,

$x_0$ = Initial approximation of root of $f(x) = 0$

$\xi$ = error, $\xi$ is sufficiently small

Now let $x_1 = x_0 + \xi$ then $f(x_1) = 0$

$\Rightarrow f(x_0 + \xi) = 0$

By Taylors expansion we get,

$$f(x_0) + \xi f'(x_0) + \frac{1}{2!}\xi^2 f''(x_0) + \cdots = 0$$

Now if $\xi$ is sufficiently small, we may neglect the terms containing second and higher powers of $\xi$ and we get

$$f(x_0) + \xi f'(x_0) = 0$$

This gives

$$\xi = \frac{f(x_0)}{f'(x_0)} \quad \text{provided } f'(x_0) \neq 0$$

A better approximation than $x_0$ is therefore given by $x_1$ where,

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

Successive approximations are given by $x_2, x_3, \ldots, x_{n+1}$ where

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

The above is known as Newton-Raphson formulae.

### 2.3.3 Graphical Interpretation of N-R Formulae

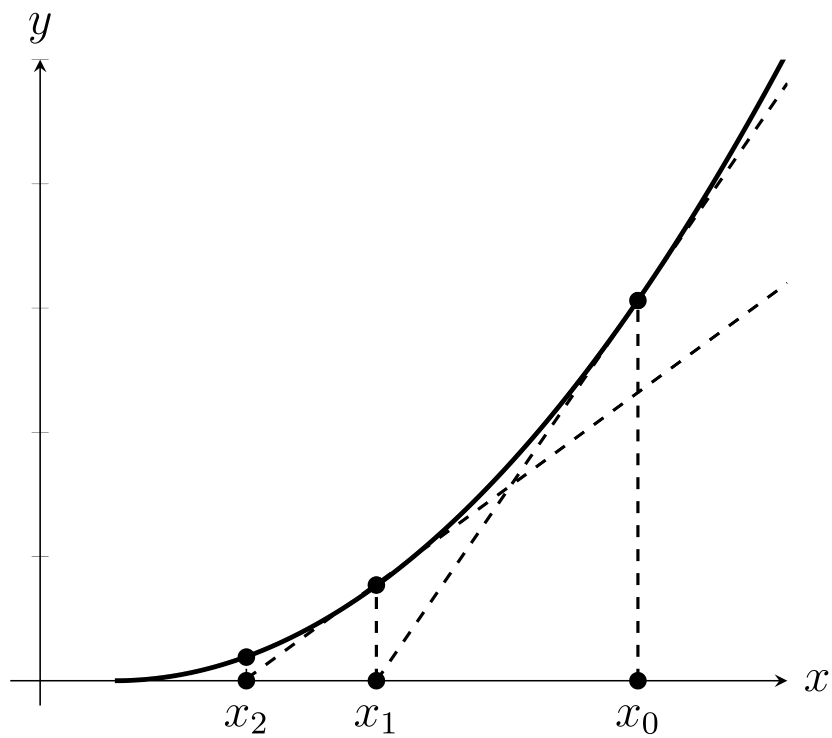



Figure 2.2: Graphical Interpretation of Newton-Raphson Method

Geometrically Newton-Raphson method consists in drawing a tangent to the curve $y = f(x)$ at $x = x_0$ and finding the point $x_1$, at which the tangent intersects the $x$-axis. This leads to,

$$\frac{f(x_0 - 0)}{x_0 - x_1} = f'(x_0)$$

gives the N-R iteration formula,

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

*Note.* If we need a root accurate to, say $k$ decimal places, then we have to need

$$\underbrace{|x_{n+1} - x_n| < 10^{-k}}_{\text{error tolerance}}$$

### 2.3.4 Disadvantages of Newton-Raphson Method

Newton-Raphson method is very good near the root, but has two disadvantages:

1. Initial estimate has to be close to the root, so we need a method for good estimate.
2. Newton-Raphson method required the derivative of $f(x)$, but this may be difficult.

### 2.3.5 Newton-Raphson's Method Converges Quadratically

Newton-Raphson's method gives a quadratic-convergence of the result, provided initial approximation is near to the root.

We know from Newton-Raphson formula,

$$\begin{aligned} x_{n+1} &= x_n - \frac{f(x_n)}{f'(x_n)} \\ \Rightarrow & f(x_n) + (x_{n+1} - x_n)f'(x_n) = 0 \end{aligned} \tag{2.3}$$

To find the root of $f(x) = 0$,

$$\begin{array}{r|r} \text{Suppose, } P = \text{root} & \xi = \text{error} \\ \therefore P = x_n + \xi & x_n = \text{approximate root} \\ & \therefore \xi = P - x_n \approx l_n \end{array}$$

By Taylor's expansion

$$0 = f(P) = f(x_n + \xi) = f(x_n) + \xi f'(x_n) + \frac{1}{2!}\xi^2 f''(x_n) + \dots \tag{2.4}$$

By subtracting (2.3) from (2.4)

$$\begin{aligned} &\Rightarrow (\xi - x_{n+1} + x_n)f'(x_n) + \frac{1}{2!}\xi^2 f''(x_n) = 0 \\ &\Rightarrow (P - x_{n+1})f'(x_n) + \frac{1}{2}\xi^2 f''(x_n) = 0 \end{aligned}$$

Now,

$$P - x_{n+1} = l_{n+1} = \text{ error after } (n+1) \text{ iteration}$$

Then,

$$\begin{aligned} & l_{n+1}f'(x_n) + \frac{1}{2}\xi^2 f''(x_n) = 0 \\ \Rightarrow & l_{n+1}f'(x_n) + \frac{1}{2}l_n^2 f''(x_n) = 0 \\ \Rightarrow & l_{n+1} = -\frac{1}{2}\frac{f''(x_n)}{f'(x_n)}l_n^2 \\ \Rightarrow & l_{n+1} = k \cdot l_n^2 \qquad \text{where } k = -\frac{1}{2}\frac{f''(x_n)}{f'(x_n)} \\ & \text{ie. } l_{n+1} \propto l_n^2 \end{aligned}$$

Hence each error is roughly proportional to the square of the previous error, i.e., the number of correct decimal places roughly doubles with each approximation. Hence, it is said that Newton-Raphson's method converges quadratically to the exact root.

### 2.3.6 Sample Code

```fortran
program newtonraphson
    !equation::x^3-3x+1
    implicit none
    real :: x, xold, error = 0.00001
    integer :: i, n
    real, external:: f, fprime

    print *, "Enter initial value(x nought) and number of iteration(n)"
    read *, xold,n

    do i = 0, n
        x = xold - (f(xold)/fprime(xold))
        write (*, "(1x,i3,2x,f10.6)") i, x
        if (f(x) == 0.0 .or. abs(x - xold) < error) then
            print *, "Root is ", x
            stop
        end if
        xold = x
    end do

    write (*, "('NO ROOT FOUND AFTER',1x,i3,1x,'ITERATIONS')") n

end program newtonraphson

real function f(x)
    implicit none
    real, intent(in) ::x

    f = x**3 - 3*x + 1

end function f

real function fprime(x)
    implicit none
    real, intent(in):: x

    fprime = 3*x**2 - 3

end function fprime
```

Listing 2.2: A sample program to solve $x^3 - 3x + 1 = 0$ by using Newton-Raphson method

### 2.3.7 Problems

**Problem 2.3.1.** Using Newton-Raphson's method, find the root of $x^3 - 3x = 3$ that lies near $x = 2$ correct upto 4D.

**Solution.** We know the Newton-Raphson's formula is

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{2.5}$$

We are given,
$f(x) = x^3 - 3x - 3 = 0$
$x_0 = 2$
Now, $f'(x) = 3x^2 - 3$
From (2.5),

$$\begin{aligned} x_{n+1} &= x_n - \frac{x_n^3 - 3x_n - 3}{3x_n^2 - 3} \\ &= \frac{3x_n^3 - 3x_n - x_n^3 + 3x_n + 3}{3x_n^2 - 3} \\ \therefore x_{n+1} &= \frac{2x_n^3 + 3}{3x_n^2 - 3} \end{aligned} \tag{2.6}$$

From (2.6), For $n = 0$,

$$x_1 = \frac{2x_0^3 + 3}{3x_0^2 - 3} = \frac{2 \cdot 2^3 + 3}{3 \cdot 2^2 - 3} = 2.111\,11$$

For $n = 1$,

$$x_2 = \frac{2x_1^3 + 3}{3x_1^2 - 3} = \frac{2 \cdot 2.111\,11^3 + 3}{3 \cdot 2.111\,11^2 - 3} = 2.103\,835$$

For $n = 2$,

$$x_3 = \frac{2x_2^3 + 3}{3x_2^2 - 3} = \frac{2 \cdot 2.103\,835^3 + 3}{3 \cdot 2.103\,835^2 - 3} = 2.103\,803\,4$$

So the required root $x \approx 2.103\,8$

**Problem 2.3.2.** Find a solution to the equation $x = \cos x$ correct upto 10D.

**Solution.** Here, we are given,
$f(x) = \cos x - x = 0$
$f'(x) = -\sin x - 1$
Here,

$$\begin{aligned} f(0) &= 1 - 0 = 1 \\ f(\frac{\pi}{2}) &= 0 - \frac{\pi}{2} = -\frac{\pi}{2} \\ \therefore f(\frac{\pi}{2}) &= -\frac{\pi}{2} < 0 < 1 = f(0) \end{aligned}$$

So we can choose the interval $[0, \frac{\pi}{2}]$ It is clear that $f(x)$ is continuous on $[0, \frac{\pi}{2}]$, so by theorem there exist a root of $f(x) = 0$ in the interval $[0, \frac{\pi}{2}]$.
We know,

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

Here,

$$\begin{aligned} x_{n+1} &= x_n - \frac{\cos x_n - x_n}{-\sin x_n - 1} \\ &= \frac{x_n \sin x_n + x_n + \cos x_n - x_n}{\sin x_n + 1} \\ \therefore x_{n+1} &= \frac{x_n \sin x_n + \cos x_n}{\sin x_n + 1} \end{aligned} \tag{2.7}$$

Suppose the first approximation is $x_0 = \frac{0+\frac{\pi}{2}}{2} = \frac{\pi}{4}$
Putting $n = 0, 1, 2, 3, \ldots$ in (2.7) we get,

| $n$ = iteration | $x_n$ (upto 10D) |
|---|---|
| | $x_0 = 0.785\,398\,163$ |
| 0 | $x_1 = 0.739\,536\,133$ |
| 1 | $x_2 = 0.739\,085\,178$ |
| 2 | $x_3 = 0.739\,085\,133$ |
| 3 | $x_4 = 0.739\,085\,133$ |

So the required root is $0.739\,085\,133$.

**Problem 2.3.3.** Obtain solution of $x^3 + 4x^2 - 10 = 0$ in the interval $[1, 2]$ by Newton-Raphson method correct upto 8D.

**Solution.** Here we are given,
$f(x) = x^3 + 4x^2 - 10 = 0$
$f'(x) = 3x^2 + 8x$
Here $f(1) = -5,\ f(2) = 14$
So $f(1) = -5 < 0 < 14 = f(2)$
So by theorem there exist a root of $f(x) = 0$ in the interval $[1, 2]$.
Suppose, an approximate root is $x_0 = \frac{1+2}{2} = 1.5$
We know, the Newton-Raphson formula is

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

Here,

$$\begin{aligned} x_{n+1} &= x_n - \frac{x_n^3 + 4x_n^2 - 10}{3x_n^2 + 8x_n} \\ \Rightarrow x_{n+1} &= \frac{2x_n^3 + 4x_n^2 + 10}{3x_n^2 + 8x_n} \end{aligned} \tag{2.8}$$

Putting $n = 0, 1, 2, 3, \ldots$ in (2.8) we get,

| $n =$ iteration | $x_n$ (upto 8D) |
|---|---|
| | $x_0 = 1.5$ |
| 0 | $x_1 = 1.373\,333\,333$ |
| 1 | $x_2 = 1.365\,262\,015$ |
| 2 | $x_3 = 1.365\,230\,014$ |
| 3 | $x_4 = 1.365\,230\,013$ |

$$x_1 = \frac{2x_0^3 + 4x_0^2 + 10}{3x_0^2 + 8x_0} = \frac{2(1.5)^3 + 4(1.5)^2 + 10}{3(1.5)^2 + 8(1.5)} = 1.373\,333\,333$$
$$x_2 = \frac{2x_1^3 + 4x_1^2 + 10}{3x_1^2 + 8x_1} = 1.365\,262\,015$$
$$x_3 = \frac{2x_2^3 + 4x_2^2 + 10}{3x_2^2 + 8x_2} = 1.365\,230\,014$$
$$x_4 = \frac{2x_3^3 + 4x_3^2 + 10}{3x_3^2 + 8x_3} = 1.365\,230\,013$$

So the required root is $1.365\,230\,01$.

**Problem 2.3.4.** Find the root of $x^3 - 3x + 1 = 0$ by Newton-Raphson Method, correct upto 5D.

**Solution.** Here we are given,
$f(x) = x^3 - 3x + 1 = 0$
$f'(x) = 3x^2 - 3$
Here $f(1) = -1,\ f(2) = 8 - 6 + 1 = 3$
So $\therefore f(1) = -1 < 0 < 3 = f(2)$
So by theorem there exist a root of $f(x) = 0$ in the interval $[1, 2]$.
Suppose, an approximate root is $x_0 = \frac{1+2}{2} = 1.5$
We know, the Newton-Raphson formula is

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

Here,

$$x_{n+1} = x_n - \frac{x_n^3 - 3x_n + 1}{3x_n^2 - 3}$$
$$\Rightarrow x_{n+1} = \frac{2x_n^3 - 1}{3x_n^2 - 3} \tag{2.9}$$

Putting $n = 0, 1, 2, 3, \ldots$ in (2.9) we get,

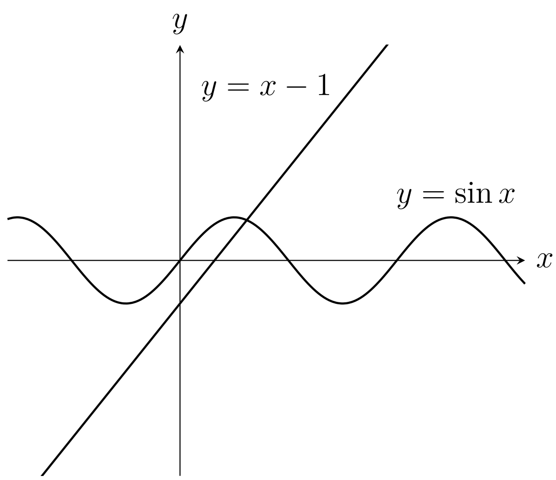
| $n =$ iteration | $x_n$ (upto 5D) |
|---|---|
| | $x_0 = 1.5$ |
| 0 | $x_1 = 1.533\,333\,333$ |
| 1 | $x_2 = 1.532\,090\,643$ |
| 2 | $x_3 = 1.532\,088\,886$ |
| 3 | $x_4 = 1.532\,088\,886$ |

So the required root is 1.532 08.

*Note.* Another interval $[0, 1]$
solution 0.347 29

**Problem 2.3.5.** Find the root of $x - \sin x - 1 = 0$ by Newton-Raphson method, correct upto 5D.

**Solution.** Here we are given,
$f(x) = x - \sin x - 1 = 0$
$f'(x) = 1 - \cos x$




Here $f(0) = -1$
$f(\pi) = \pi - 1$
$\therefore f(0) = -1 < 0 < \pi = f(\pi)$
So we can choose the interval $[0, \pi]$
Let us consider an approximate root, $x_0 = \frac{0+\pi}{2} = \frac{\pi}{2}$
We know, the Newton-Raphson formula is

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

$$\begin{aligned} x_{n+1} &= x_n - \frac{x_n - \sin x_n - 1}{1 - \cos x_n} \\ \Rightarrow x_{n+1} &= \frac{\sin x_n - x_n \cos x_n + 1}{1 - \cos x_n} \end{aligned}$$

When $n = 0$

$$\begin{aligned} x_1 &= \frac{\sin x_0 - x_0 \cos x_0 + 1}{1 - \cos x_0} \\ &= \frac{\sin \frac{\pi}{2} - \frac{\pi}{2} \cos \frac{\pi}{2} + 1}{1 - \cos \frac{\pi}{2}} \\ &= 2 \end{aligned}$$

When $n = 1$, then

$$x_2 = \frac{\sin 2 - 2\cos 2 + 1}{1 - \cos 2} = 1.935\,951\,152$$

When $n = 2$, then

$$x_3 = \frac{\sin x_2 - x_2 \cos x_2 + 1}{1 - \cos x_2} = 1.934\,563\,874$$

When $n = 3$, then

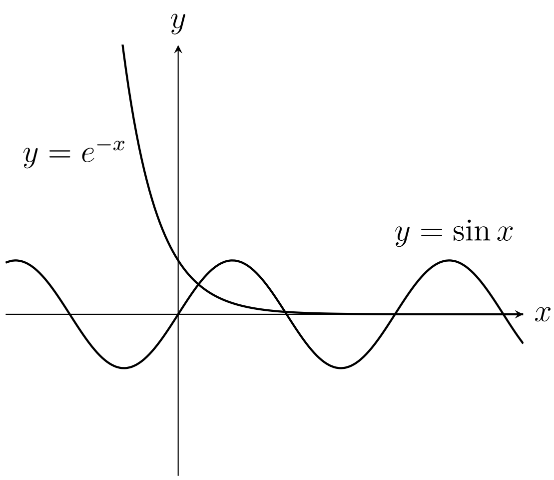
$$x_4 = \frac{\sin x_3 - x_3 \cos x_3 + 1}{1 - \cos x_3} = 1.934\,563\,211$$

So the required root is $1.934\,56$.

**Problem 2.3.6.** Find the root of $e^{-x} = \sin x$ upto 5D.

**Solution.** Here we are given that,

$f(x) = e^{-x} - \sin x = 0$




| $x$ | $e^{-x}$ |
|---|---|
| 0 | 1 |
| 1 | 0.367 87 |
| 2 | 0.135 33 |
| 3 | 0.049 78 |
| $-1$ | 2.718 20 |
| $-2$ | 7.389 00 |

$$f(x) = \sin x - e^{-x}$$
$$f'(x) = \cos x + e^{-x}$$

Here, $\quad f(0) = -1$

$$f(\frac{\pi}{2}) = 1 - e^{-\frac{\pi}{2}} = 1 - 0.207\,879\,576 = 0.792\,120\,423$$

$$\therefore f(0) = -1 < 0 < 0.792\,1 = f(\frac{\pi}{2})$$

So we can choose the interval $[0, \frac{\pi}{2}]$

It is clear that $f(x)$ is continuous on $[0, \frac{\pi}{2}]$

So by theorem there exist a root of $f(x) = 0$ in the interval $[0, \frac{\pi}{2}]$.

We take the approximate root $x_0 = \frac{0+\frac{\pi}{2}}{2} = \frac{\pi}{4} = 0.785\,398\,163$

We know, the Newton-Raphson formula is

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

$$\begin{aligned}
x_{n+1} &= x_n - \frac{\sin x_n - e^{-x_n}}{\cos x_n + e^{-x_n}} \\
&= \frac{x_n \cos x_n + x_n e^{-x_n} - \sin x_n - e^{-x_n}}{\cos x_n + e^{-x_n}} \\
\Rightarrow x_{n+1} &= \frac{x_n \cos x_n - \sin x_n + (x_n + 1)e^{-x_n}}{\cos x_n + e^{-x_n}}
\end{aligned}$$

Put $n = 0$ then,

$$\begin{aligned}
x_1 &= \frac{x_0 \cos x_0 - \sin x_0 + (x_0 + 1)e^{-x_0}}{\cos x_0 + e^{-x_0}} \\
&= 0.569\,440\,334
\end{aligned}$$

Put $n = 1$ then,

$$\begin{aligned}
x_2 &= \frac{x_1 \cos x_1 - \sin x_1 + (x_1 + 1)e^{-x_1}}{\cos x_1 + e^{-x_1}} \\
&= 0.588\,389\,482
\end{aligned}$$

Put $n = 2$ then,

$$\begin{aligned}
x_3 &= \frac{x_2 \cos x_2 - \sin x_3 + (x_2 + 1)e^{-x_2}}{\cos x_2 + e^{-x_2}} \\
&= 0.588\,532\,735
\end{aligned}$$

Put $n = 3$ then,

$$\begin{aligned}
x_4 &= \frac{x_3 \cos x_3 - \sin x_3 + (x_3 + 1)e^{-x_3}}{\cos x_3 + e^{-x_3}} \\
&= 0.588\,532\,744
\end{aligned}$$

So the required root is $0.588\,53$.

**Problem 2.3.7.** Use Newton-Raphson's method to find approximate solutions of the following (within $10^{-5}$):

$$f(x) = x^3 - 2x^2 - 5 = 0 \;\text{ in }\; [1, 5] \;\text{ with }\; x_0 = 2.5$$

**Solution.** Here we are given,
$f(x) = x^3 - 2x^2 - 5 = 0$
$f'(x) = 3x^2 - 4x$
$f(1) = 1 - 2 - 5 = -6$
$f(4) = 4^3 - 2 \cdot 4^2 - 5 = 27$
So $f(1) = -6 < 0 < 27 = f(4)$

So by theorem there exist a root of $f(x) = 0$ in the interval $[1, 4]$.
Let the approximate solution be $x_0 = 2.5$ We know, the Newton-Raphson formula is

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

In this case,

$$\begin{aligned} x_{n+1} &= x_n - \frac{x_n^3 - 2x_n^2 - 5}{3x_n^2 - 4x_n} \\ \Rightarrow x_{n+1} &= \frac{3x_n^3 - 4x_n^2 - x_n^3 + 2x_n^2 + 5}{3x_n^2 - 4x_n} \\ \Rightarrow x_{n+1} &= \frac{2x_n^3 - 2x_n^2 + 5}{3x_n^2 - 4x_n} \end{aligned} \tag{2.10}$$

Put $n = 0$ in (2.10) we get,

$$x_1 = \frac{2x_0^3 - 2x_0^2 + 5}{3x_0^2 - 4x_0} = 2.714\,285\,714$$

Put $n = 1$ in (2.10) we get,

$$x_2 = \frac{2x_1^3 - 2x_1^2 + 5}{3x_1^2 - 4x_1} = 2.690\,951\,517$$

Put $n = 2$ in (2.10) we get,

$$x_3 = \frac{2x_2^3 - 2x_2^2 + 5}{3x_2^2 - 4x_2} = 2.690\,647\,499$$

Put $n = 3$ in (2.10) we get,

$$x_4 = \frac{2x_3^3 - 2x_3^2 + 5}{3x_3^2 - 4x_3} = 2.690\,647\,448$$

So the required root is $2.690\,647$.

**Problem 2.3.8.** Use Newton-Raphson's method to find approximate solutions of the following (within $10^{-5}$):

$$f(x) = x - \cos x = 0 \text{ in } \left[0, \frac{\pi}{2}\right] \text{ with } x_0 = 0.79$$

**Solution.** Here we are given,
$f(x) = x - \cos x = 0$
$f'(x) = 1 + \sin x$
Here $f(0) = -1,\ f\left(\frac{\pi}{2}\right) = 1.570\,796\,527$
So $\therefore f(0) = -1 < 0 < 1.57 = f\left(\frac{\pi}{2}\right)$
So by theorem there exist a root of $f(x) = 0$ in the interval $\left[0, \frac{\pi}{2}\right]$.
We are given the first approximate root $x_0 = 0.79$
We know, the Newton-Raphson formula is

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

In this case,

$$x_{n+1} = x_n - \frac{x_n - \cos x_n}{1 + \sin x_n}$$
$$\Rightarrow x_{n+1} = \frac{x_n \sin x_n + \cos x_n}{1 + \sin x_n}$$

Putting $n = 0, 1, 2, 3, \ldots$ we get,

| $n =$ iteration | $x_n$ (within $10^{-5}$) |
|---|---|
| | $x_0 = 0.79$ |
| 0 | $x_1 = 0.739\,627\,55$ |
| 1 | $x_2 = 0.739\,085\,198$ |
| 2 | $x_3 = 0.739\,085\,133$ |

So the required root is 0.739 085.

**Problem 2.3.9.** Use Newton-Raphson's method to find approximate solutions of the following (within $10^{-5}$):

$$f(x) = x - 0.8 - 0.2\sin x = 0 \;\text{ in }\; \left[0, \frac{\pi}{2}\right] \;\text{ with }\; x_0 = 0.7854$$

**Solution.** Here we are given,

$f(x) = x - 0.8 - 0.2\sin x = 0$
$f'(x) = 1 - 0.2\cos x$
$f(0) = -0.8$
$f\left(\frac{\pi}{2}\right) = \frac{\pi}{2} - 0.8 - 0.2 = 0.57796326$

So $f(0) = -0.8 < 0 < 0.570796326 = f\left(\frac{\pi}{2}\right)$
So by theorem there exist a root of $f(x) = 0$ in the interval $\left[0, \frac{\pi}{2}\right]$.
We are given the first approximate solution $x_0 = 0.7854$
We know, the Newton-Raphson formula is

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

In this case,

$$\begin{aligned} x_{n+1} &= x_n - \frac{x_n - 0.8 - 0.2\sin x_n}{1 - 0.2\cos x_n} \\ &= \frac{x_n - 0.2x_n\cos x_n - x_n + 0.8 + 0.2\sin x_n}{1 - 0.2\cos x_n} \\ \therefore x_{n+1} &= \frac{0.2\sin x_n - 0.2x_n\cos x_n + 0.8}{1 - 0.2\cos x_n} \end{aligned} \tag{2.11}$$

Put $n = 0$ in (2.11) we get,

$$x_1 = \frac{0.2\sin x_0 - 0.2x_0\cos x_0 + 0.8}{1 - 0.2\cos x_0} = 0.967\,120\,765$$

Put $n = 1$ in (2.11) we get,

$$x_2 = \frac{0.2 \sin x_1 - 0.2 x_1 \cos x_1 + 0.8}{1 - 0.2 \cos x_1} = 0.964\,334\,608$$

Put $n = 2$ in (2.11) we get,

$$x_3 = \frac{0.2 \sin x_2 - 0.2 x_2 \cos x_2 + 0.8}{1 - 0.2 \cos x_2} = 0.964\,333\,887$$

Put $n = 4$ in (2.11) we get,

$$x_4 = \frac{0.2 \sin x_3 - 0.2 x_3 \cos x_3 + 0.8}{1 - 0.2 \cos x_3} = 0.964\,333\,887$$

So the required root is 0.964 333.

**Problem 2.3.10.** Write down the algorithm for Newton-Raphson method and implement it into Fortran for the function $f(x) = x_2 - e^{-x}$

**Solution.** Data Table
Input Variables:

$$\begin{aligned} x_0 &= \text{Initial approximation} \\ ERR &= \text{Maximum error allowance} \\ N &= \text{Maximum number of iterations} \end{aligned}$$

Output Variables:

$$x = \text{Approximate solution or message of failure}$$

Algorithm

Step 1 : Define function $f(x)$ and $f'(x)$

Step 2 : When $I \leq N$, Do steps 3-5

Step 3 : set $x = x_0 - \frac{f(x_0)}{f'(x_0)}$

Step 4 : If $|x - x_0| < ERR$, then output $x$ and message compiled successfully
STOP

Step 5 : Otherwise (ELSE)
set $x_0 = x$(update value of $x_0$)
CONTINUE

Step 6 : Output Method failed after $N$ iterations,
procedure computed unsuccessfully
STOP

# Chapter 3

# Interpolation

## 3.1 Interpolation

This is the technique of obtaining the most likely estimate of a certain quantity under certain assumption.

Suppose the values if a function $f(x)$ are given for a discrete set of values of $x$ (independent variable). Interpolation is defined as the method of estimating the values of $f(x)$ for any intermediate value of the arguments $x_i (i = 0, 1, 2, \ldots, n)$.

Let us suppose we are given the census figures for the population of Bangladesh for four years $1931, 1941, 1951$ and 1961 and we want to estimate the figures for any intermediate year, e.g. for 1955 or 1958 etc. This can be done by applying the technique of interpolation.

## 3.2 Extrapolation

If we have to estimate the value of $f(x)$ for any value outside the given range then the technique is known as extrapolation.

## 3.3 Fundamental Assumptions

1. There are no sudden jumps or falls in the values of the data; i.e. data can be represented by a smooth continuous curve.

   Data can be represented by a polynomial of certain degree, which can be determined by,

   *Theorem* 3.3.1. One and only one polynomial (curve) of degree less than or equal to $n$ passes through a given set of $(n + 1)$ distinct points.

2. The data can be expressed as a polynomial function with fair degree of accuracy.

3. The rise or fall of data is uniform.

4. The method is not exact.

5. The method becomes complicated when the numbers of observations (data) is large.

6. This method gives closer approximation than the graphical method.

*Theorem* 3.3.2 (Existance and Uniqueness). If $x_0, x_1, x_2, \dots, x_n$ are $(n+1)$ distinct points and $f(x)$ is a function whose values are known at these points; then there exists a unique polynomial $P_n(x)$ of degree $\leq n$ which interpolates $f(x)$ such that $P_n(x_i) = f(x_i),\ i = 0, 1, 2, \dots, n$ and

$$P_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x)$$

*Proof (Existance).* Let $x_0, x_1, \dots, x_n$ be $(n+1)$ distinct points on the real axis and let $f(x)$ be a real values function defined on some interval $[a, b]$ containing these points. We need to construct a polynomial $P_n(x)$ of degree $\leq n$ which interpolates $f(x)$ at the $(n+1)$ points and satisfies $P_n(x_i) = f(x_i),\ i = 0, 1, 2, \dots, n$.

For this, we use the form, called Lagrange's form:

$$P_n(x) = \sum_{k=0}^{n} a_k l_k(x)$$

where

$$l_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i},\ k = 0, 1, 2, \dots, n$$

are called the Lagrange polynomials for the points $x_0, x_1, \dots, x_n$.

This function $l_k(x)$ is the product of $n$ linear factors, hence gives a polynomial of exact degree $n$. Hence, the Lagrange form given by

$$P_n(x) = \sum_{k=0}^{n} a_k l_k(x)$$

describes a polynomial of degree $\leq n$.

Also, $l_k(x)$ vanishes at $x_i$ for all $i \neq k$ and takes the value 1 at $x_k$, ie,

$$l_k(x_i) = \begin{cases} 1, & i = k \\ 0, & i \neq k \end{cases} \qquad i = 0, 1, 2, \dots, n$$

$$\begin{aligned}
\therefore P_n(x_i) &= \sum_{k=0}^{n} a_k l_k(x_i) \\
&= a_0 l_0(x_i) + a_1 l_1(x_i) + \dots + a_i l_i(x_i) + a_{i+1} l_{i+1}(x_i) + \dots + a_n l_n(x_i) \\
&= 0 + 0 + \dots + a_i \times 1 + 0 + \dots \\
P_n(x_i) &= a_i \quad (i = 0, 1, 2, \dots, n)
\end{aligned}$$

The co-efficient $a_0, a_1, \dots, a_n$ are simply the values of the polynomials $P_n(x)$ at the points $x_0, x_1, \dots, x_n$.

Consequently, for any function $f(x)$,

$$P_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x)$$

is a polynomial of degree $\leq n$ which interpolates $f(x)$ at $x_0, x_1, \dots, x_n$. □

*Proof (Uniqueness).* Let $P_n(x)$ and $q_n(x)$ are two Lagrange's interpolating polynomials of degree $\leq n$ which interpolates $f(x)$ at $x_0, x_1, \ldots, x_n$, then we have,

$$P_n(x_i) = f(x_i) \tag{3.1}$$

$$q_n(x_i) = f(x_i) \tag{3.2}$$

Consider the polynomial $p_n(x)$ given by

$$\phi_n(x) = P_n(x) - q_n(x)$$

Then $\phi_n(x)$ vanishes at the points $x_0, x_1, \ldots, x_n$.
Hence we have $\phi_n(x) \equiv 0$
$\Rightarrow P_n(x) = q_n(x)$
Thus Lagrange interpolating polynomial is unique. □

**Problem 3.3.1.** Find the linear form of Lagrange's interpolation polynomial.

**Solution.** We know, the Lagrange's polynomial is

$$P_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x)$$

where,

$$l_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i}$$

Put $n = 1$, then we have only two distinct points namely $x_0, x_1$.
Now

$$l_0(x) = \prod_{\substack{i=0 \\ i \neq 0}}^{1} \frac{x - x_i}{x_0 - x_i} = \frac{x - x_1}{x_0 - x_1}$$

and,

$$l_1(x) = \prod_{\substack{i=0 \\ i \neq 1}}^{1} \frac{x - x_i}{x_1 - x_i} = \frac{x - x_0}{x_1 - x_0}$$

Now,

$$\begin{aligned}
P_1(x) &= \sum_{k=0}^{1} f(x_k) l_k(x) \\
&= f(x_0) l_0(x) + f(x_1) l_1(x) \\
&= f(x_0) \frac{x - x_1}{x_0 - x_1} + f(x_1) \frac{x - x_0}{x_1 - x_0} \\
&= f(x_0) \frac{x_1 - x}{x_1 - x_0} + f(x_1) \frac{x - x_0}{x_1 - x_0} \\
&= f(x_0) \left( \frac{x_1 - x_0 + x_0 - x}{x_1 - x_0} \right) + f(x_1) \frac{x - x_0}{x_1 - x_0} \\
&= f(x_0) \left( 1 + \frac{x_0 - x}{x_1 - x_0} \right) + f(x_1) \frac{x - x_0}{x_1 - x_0} \\
&= f(x_0) + f(x_0) \frac{x - x_0}{x_1 - x_0} + f(x_1) \frac{x - x_0}{x_1 - x_0} \\
&= f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0} (x - x_0)
\end{aligned}$$

ie, $P_1(x) = f(x_0) + \frac{f(x_1)-f(x_0)}{x_1-x_0}(x - x_0)$

This is the linear form of Lagrange's interpolation polynomial.

**Problem 3.3.2.** Suppose $f(x) = \frac{1}{x}, x_0 = 2, x_1 = 2.5, x_2 = 4$. Find the second degree interpolating polynomial and determine the coefficients $l_0, l_1, l_2$ and hence find an approximate value of $f(3)$.

**Solution.** We know, the Lagrange's polynomial is

$$P_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x) \tag{3.3}$$

where

$$l_k(x) = \prod_{\substack{i=0 \\ i\neq k}}^{n} \frac{x - x_i}{x_k - x_i},\ k = 0, 1, \ldots, n \tag{3.4}$$

In this case we are given $x_0.x_1, x_2$
So that $n = 2$
Thus from 5.3 we have

$$l_k(x) = \prod_{\substack{i=0 \\ i\neq k}}^{2} \frac{x - x_i}{x_k - x_i},\ k = 0, 1, 2$$

$$\begin{aligned} l_0(x) &= \prod_{\substack{i=0 \\ i\neq 0}}^{2} \frac{x - x_i}{x_0 - x_i} \\ &= \frac{x - x_1}{x_0 - x_1} \cdot \frac{x - x_2}{x_0 - x_2} \\ &= \frac{x - 2.5}{2 - 2.5} \cdot \frac{x - 4}{2 - 4} \\ &= \frac{x - 2.5}{-0.5} \cdot \frac{x - 4}{-2} \\ &= x^2 - 6.5x + 10 \end{aligned}$$

$$\begin{aligned} l_1(x) &= \prod_{\substack{i=0 \\ i\neq 1}}^{2} \frac{x - x_i}{x_1 - x_i} \\ &= \frac{x - x_0}{x_1 - x_0} \cdot \frac{x - x_2}{x_1 - x_2} \\ &= \frac{x - 2}{2.5 - 2} \cdot \frac{x - 4}{2.5 - 4} \\ &= \frac{x - 2}{0.5} \cdot \frac{x - 4}{-1.5} \\ &= \frac{x^2 - 6x + 8}{-0.75} \\ &= -\frac{1}{3}(4x^2 - 24x + 32) \end{aligned}$$

$$
\begin{aligned}
l_2(x) &= \prod_{\substack{i=0\\ i\neq 2}}^{2} \frac{x - x_i}{x_2 - x_i} \\
&= \frac{x - x_0}{x_2 - x_0} \cdot \frac{x - x_1}{x_2 - x_1} \\
&= \frac{x - 2}{4 - 2} \cdot \frac{x - 2.5}{4 - 2.5} \\
&= \frac{x - 2}{2} \cdot \frac{x - 2.5}{1.5} \\
&= \frac{1}{3}(x^2 - 4.5x + 5)
\end{aligned}
$$

Now we are given that $f(x) = \frac{1}{x}$
So writing the following table we get

| $i$ | $x_i$ | $f(x) = \frac{1}{x}$ | |
|---|---|---|---|
| 0 | $x_0 = 2$ | $f(x_0) =$ | 0.5 |
| 1 | $x_1 = 2.5$ | $f(x_1) =$ | 0.4 |
| 2 | $x_2 = 4$ | $f(x_2) =$ | 0.25 |

Now, the Lagrange's polynomial is

$$
P_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x)
$$

Here

$$
\begin{aligned}
P_2(x) = P_n(x) &= \sum_{k=0}^{2} f(x_k) l_k(x) \\
&= f(x_0)l_0(x) + f(x_1)l_1(x) + f(x_2)l_2(x) \\
&= (0.5)(x^2 - 6.5x + 10) - (0.4)\frac{1}{3}(4x^2 - 24x + 32) + (0.25)\frac{1}{3}(x^2 - 4.5x + 5) \\
&= 0.05x^2 - 0.425x + 1.15
\end{aligned}
$$

$\therefore P_2(x) = 0.05x^2 - 0.425x + 1.15 \approx f(x)$
Which is the interpolating polynomial of 2nd degree.
$\therefore f(3) = (0.05)(3)^2 - (0.425)(3) + 1.15 = 0.325 \approx 0.33$

**Problem 3.3.3.** Use the following table for the function $f(x) = \log_{10}(\tan x)$, to find the interpolating polynomial to estimate the value of $f(1.09)$

| $x$ | $f(x)$ |
|---|---|
| 1.00 | 0.1924 |
| 1.05 | 0.2414 |
| 1.10 | 0.2933 |
| 1.15 | 0.3492 |

**Solution.** We know, the Lagrange's interpolation polynomial is

$$P_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x)$$

where

$$l_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i}, k = 0, 1, \ldots, n$$

Now,

$$\begin{aligned}
l_0(x) &= \prod_{\substack{i=0 \\ i \neq 0}}^{3} \frac{x - x_i}{x_0 - x_i} \\
&= \frac{x - x_1}{x_0 - x_1} \cdot \frac{x - x_2}{x_0 - x_2} \cdot \frac{x - x_3}{x_0 - x_3} \\
&= \frac{x - 1.05}{1 - 1.05} \cdot \frac{x - 1.10}{1 - 1.10} \cdot \frac{x - 1.15}{1 - 1.15} \\
&= \frac{(x^2 - 2.15x + 1.155)(x - 1.15)}{(-0.05)(-0.10)(-0.15)} \\
&= -\frac{x^3 - 3.30x^2 + 3.6275x - 1.328\,25}{0.000\,75} \\
&= -\frac{1}{0.000\,75}(x^3 - 3.3x^2 + 3.6275x - 1.328\,25)
\end{aligned}$$

$$\begin{aligned}
l_1(x) &= \frac{x - x_0}{x_1 - x_0} \cdot \frac{x - x_2}{x_1 - x_2} \cdot \frac{x - x_3}{x_1 - x_3} \\
&= \frac{x - 1}{1.05 - 1} \cdot \frac{x - 1.1}{1.05 - 1.1} \cdot \frac{x - 1.15}{1.05 - 1.15} \\
&= \frac{(x^2 - 2.1x + 1.1)(x - 1.15)}{(0.05)(-0.05)(-0.1)} \\
&= \frac{1}{0.000\,25}(x^3 - 3.25x^2 + 3.515x - 1.265)
\end{aligned}$$

$$\begin{aligned}
l_2(x) &= \frac{x - x_0}{x_2 - x_0} \cdot \frac{x - x_1}{x_2 - x_1} \cdot \frac{x - x_3}{x_2 - x_3} \\
&= \frac{x - 1}{1.1 - 1} \cdot \frac{x - 1.05}{1.1 - 1.05} \cdot \frac{x - 1.15}{1.1 - 1.15} \\
&= \frac{(x^2 - 2.05x + 1.05)(x - 1.15)}{(0.01)(0.05)(-0.05)} \\
&= -\frac{1}{0.000\,25}(x^3 - 3.20x^2 + 3.4075x - 1.2075)
\end{aligned}$$

$$
\begin{aligned}
l_3(x) &= \frac{x-x_0}{x_3-x_0}\cdot\frac{x-x_1}{x_3-x_1}\cdot\frac{x-x_2}{x_3-x_2}\\
&= \frac{x-1}{1.15-1}\cdot\frac{x-1.05}{1.15-1.05}\cdot\frac{x-1.1}{1.15-1.1}\\
&= \frac{(x^2-2.05x+1.05)(x-1.1)}{(0.15)(0.1)(0.05)}\\
&= \frac{1}{0.000\,75}(x^3-3.15x^2+3.305x-1.155)
\end{aligned}
$$

So the required polynomial is

$$
\begin{aligned}
P_3(x) &= f(x_0)l_0(x)+f(x_1)l_1(x)+f(x_2)l_2(x)+f(x_3)l_3(x)\\
&= 0.1924\left\{-\frac{1}{0.000\,75}\left(x^3-3.3x^2+3.6275x-1.328\,25\right)\right\}\\
&+0.2414\left\{\frac{1}{0.000\,25}\left(x^3-3.25x^2+3.515x-1.265\right)\right\}\\
&+0.2933\left\{-\frac{1}{0.000\,25}\left(x^3-3.20x^2+3.4075x-1.2075\right)\right\}\\
&+0.3492\left\{\frac{1}{0.000\,75}\left(x^3-3.15x^2+3.305x-1.155\right)\right\}\\
\Rightarrow P_3(x) &= 1.466\,666\,667x^3-4.04x^2+4.638\,333\,33x-1.8726\approx f(x)
\end{aligned}
$$

$\therefore f(1.09) = 0.282\,635\,2$
Hence the required polynomial is $P_3(x) = 1.466\,66x^3 - 4.04x^2 + 4.638\,33x - 1.8726$ and $f(1.09) = 0.2826$

**Problem 3.3.4.** Use the following table, find an approximate value of $f(1.25)$ when $f(x) = e^{x^2} - 1$

| $x$ | $f(x)$ |
|---|---|
| 1.0 | 1.000 00 |
| 1.1 | 1.233 68 |
| 1.2 | 1.552 71 |
| 1.3 | 1.493 72 |
| 1.4 | 2.611 70 |

**Solution.** We know, the Lagrange's interpolation polynomial is

$$P_n(x) = \sum_{k=0}^{n} f(x_k)l_k(x)$$

where

$$l_k(x) = \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{x-x_i}{x_k-x_i}, k = 0, 1, \ldots, n$$

In this case we are given, $x_0, x_1, x_2,$ and $x_4$ so that $n = 4$ and we get

$$P_4(x) = \sum_{k=0}^{4} f(x_k)l_k(x)$$

where

$$l_k(x) = \prod_{\substack{i=0\\i\neq k}}^{4} \frac{x - x_i}{x_k - x_i}, k = 0, 1, 2, 3, 4$$

$$\begin{aligned}
\therefore l_0(x) &= \frac{x - x_1}{x_0 - x_1} \cdot \frac{x - x_2}{x_0 - x_2} \cdot \frac{x - x_3}{x_0 - x_3} \cdot \frac{x - x_4}{x_0 - x_4} \\
\Rightarrow l_0(1.25) &= \frac{1.25 - 1.1}{1.00 - 1.1} \cdot \frac{1.25 - 1.2}{1.00 - 1.2} \cdot \frac{1.25 - 1.3}{1.00 - 1.3} \cdot \frac{1.25 - 1.4}{1.00 - 1.4} \\
&= 0.023\,437\,5
\end{aligned}$$

$$\begin{aligned}
\therefore l_1(x) &= \frac{x - x_0}{x_1 - x_0} \cdot \frac{x - x_2}{x_1 - x_2} \cdot \frac{x - x_3}{x_1 - x_3} \cdot \frac{x - x_4}{x_1 - x_4} \\
\Rightarrow l_1(1.25) &= \frac{1.25 - 1.0}{1.1 - 1.0} \cdot \frac{1.25 - 1.2}{1.1 - 1.2} \cdot \frac{1.25 - 1.3}{1.1 - 1.3} \cdot \frac{1.25 - 1.4}{1.1 - 1.4} \\
&= \frac{0.25}{0.1} \cdot \frac{0.05}{-0.1} \cdot \frac{-0.05}{-0.2} \cdot \frac{-0.15}{-0.3} \\
&= -\frac{0.000\,093\,75}{0.000\,6} \\
&= -0.156\,25
\end{aligned}$$

$$\begin{aligned}
\therefore l_2(x) &= \frac{x - x_0}{x_2 - x_0} \cdot \frac{x - x_1}{x_2 - x_1} \cdot \frac{x - x_3}{x_2 - x_3} \cdot \frac{x - x_4}{x_2 - x_4} \\
\Rightarrow l_2(1.25) &= \frac{1.25 - 1.0}{1.2 - 1.0} \cdot \frac{1.25 - 1.1}{1.2 - 1.1} \cdot \frac{1.25 - 1.3}{1.2 - 1.3} \cdot \frac{1.25 - 1.4}{1.2 - 1.4} \\
&= \frac{0.25}{0.2} \cdot \frac{0.15}{0.1} \cdot \frac{-0.05}{-0.1} \cdot \frac{-0.15}{-0.2} \\
&= \frac{0.000\,281\,25}{0.0004} \\
&= 0.703\,125
\end{aligned}$$

$$\begin{aligned}
\therefore l_3(x) &= \frac{x - x_0}{x_3 - x_0} \cdot \frac{x - x_1}{x_3 - x_1} \cdot \frac{x - x_2}{x_3 - x_2} \cdot \frac{x - x_4}{x_3 - x_4} \\
\Rightarrow l_3(1.25) &= \frac{1.25 - 1.0}{1.3 - 1.0} \cdot \frac{1.25 - 1.1}{1.3 - 1.1} \cdot \frac{1.25 - 1.2}{1.3 - 1.2} \cdot \frac{1.25 - 1.4}{1.3 - 1.4} \\
&= \frac{0.25}{0.3} \cdot \frac{0.15}{0.2} \cdot \frac{0.05}{0.1} \cdot \frac{-0.15}{-0.1} \\
&= \frac{0.000\,281\,25}{0.0006} \\
&= 0.468\,75
\end{aligned}$$

$$
\begin{aligned}
\therefore l_4(x) &= \frac{x-x_0}{x_4-x_0}\cdot\frac{x-x_1}{x_4-x_1}\cdot\frac{x-x_2}{x_4-x_2}\cdot\frac{x-x_3}{x_4-x_3}\\
\Rightarrow l_4(1.25) &= \frac{1.25-1.0}{1.4-1.0}\cdot\frac{1.25-1.1}{1.4-1.1}\cdot\frac{1.25-1.2}{1.4-1.2}\cdot\frac{1.25-1.3}{1.4-1.3}\\
&= \frac{0.25}{0.4}\cdot\frac{0.15}{0.3}\cdot\frac{0.05}{0.2}\cdot\frac{-0.05}{0.1}\\
&= -\frac{0.000\,093\,75}{0.0024}\\
&= -0.039\,062\,5
\end{aligned}
$$

So writing Lagrange's interpolating polynomial, we get

$$
\begin{aligned}
P_4 &= f(x_0)l_0(x) + f(x_1)l_1(x) + f(x_2)l_2(x) + f(x_3)l_3(x) + f(x_4)l_4(x) \equiv f(x)\\
\Rightarrow f(x) &= (1.00)l_0(x) + (1.233\,68)l_1(x) + (1.552\,75)l_2(x) + (1.993\,72)l_3(x) + (2.611\,70)l_4(x)
\end{aligned}
$$

$$
\begin{aligned}
\therefore f(1.25) = {} & (1.00)(0.023\,437\,5) + (1.233\,68)(-0.156\,25) + (1.552\,75)(0.468\,75)\\
& + (1.993\,72)(0.468\,75) + (2.611\,70)(-0.039\,062\,5)\\
= {} & 1.754\,96
\end{aligned}
$$

**Problem 3.3.5.** If $f(x) = e^x$, using the following table

| $x$ | $f(x)$ |
|---|---|
| 0.0 | 1.0 |
| 0.5 | 1.648 72 |
| 1.0 | 2.718 58 |
| 2.0 | 7.389 06 |

1. Find the approximate value $f(0.25)$ using linear interpolation with $x_0 = 0$, $x_1 = 0.5$
2. Find the approximate value $f(0.75)$ using linear interpolation with $x_0 = 0.5$, $x_1 = 1.0$
3. Approximate value of $f(0.25)$, $f(0.75)$ using second degree interpolating polynomial with $x_0 = 0, x_1 = 1.0, x_2 = 2.0$

Which approximation is better and why?

**Solution.** We know, the Lagrange's interpolation polynomial is

$$P_n(x) = \sum_{k=0}^{n} f(x_k)l_k(x)$$

where

$$l_k(x) = \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{x-x_i}{x_k-x_i}, k = 0, 1, \ldots, n$$

*Part i*
Here, we are given $x_0 = 0$, $x_1 = 0.5$
So that $n = 1$ We know, the Lagrange's interpolation polynomial is

$$P_1(x) = \sum_{k=0}^{1} f(x_k)l_k(x)$$

where

$$l_k(x) = \prod_{\substack{i=0\\i\neq k}}^{1} \frac{x - x_i}{x_k - x_i}, k = 0, 1$$

$$\begin{aligned}
\therefore l_0(x) &= \frac{x - x_1}{x_0 - x_1} \\
\Rightarrow l_0(0.25) &= \frac{0.25 - 0.25}{0 - 0.5} \\
&= \frac{-0.25}{-0.5} \\
&= 0.5
\end{aligned}$$

$$\begin{aligned}
\therefore l_1(x) &= \frac{x - x_0}{x_1 - x_0} \\
\Rightarrow l_1(0.25) &= \frac{0.25 - 0}{0.5 - 0} \\
&= 0.5
\end{aligned}$$

$$\begin{aligned}
P_1(x) \approx f(x) &= f(x_0)l_0(x) + f(x_1)l_1(x) \\
\Rightarrow f(0.25) &= (1.0)(0.5) + (1.648\,72)(0.5) \\
&= 1.324\,36
\end{aligned}$$

*Part ii*
Here, we are given $x_0 = 0.5$, $x_1 = 1.0$
So that $n = 1$ We know, the Lagrange's interpolation polynomial is

$$P_1(x) = \sum_{k=0}^{1} f(x_k) l_k(x)$$

where

$$l_k(x) = \prod_{\substack{i=0\\i\neq k}}^{1} \frac{x - x_i}{x_k - x_i}, k = 0, 1$$

$$\begin{aligned}
\therefore l_0(x) &= \frac{x - x_1}{x_0 - x_1} \\
&= \frac{x - 1.0}{0.5 - 1.0} \\
&= -\frac{1}{5(x - 1)} \\
&= -2(x - 1)
\end{aligned}$$

$$\begin{aligned}
\therefore l_1(x) &= \frac{x - x_0}{x_1 - x_0} \\
&= \frac{x - 0.5}{1 - 0.5} \\
&= 2(x - .5)
\end{aligned}$$

So the linear interpolating polynomial is

$$
\begin{aligned}
P_1(x) &= f(x_0)l_0(x) + f(x_1)l_1(x) \\
&= (1.648\,72)\,\{-2(x-1)\} + (2.718\,28)\,\{-2(x-1)\} \\
&= 2.113\,912x + 0.579\,16 \\
&\approx f(x)
\end{aligned}
$$

$$
\begin{aligned}
\therefore f(0.75) &= (2.139\,12)(0.75) + 0.579\,16 \\
&= 2.183\,50
\end{aligned}
$$

*Part iii*
Here, we are given $x_0 = 0$, $x_1 = 1.0$ & $x_2 = 2.0$
So that $n = 2$ We know, the Lagrange's interpolation polynomial is

$$P_2(x) = \sum_{k=0}^{2} f(x_k)l_k(x)$$

where

$$l_k(x) = \prod_{\substack{i=0 \\ i\neq k}}^{2} \frac{x - x_i}{x_k - x_i}, k = 0, 1, 2$$

$$
\begin{aligned}
\therefore l_0(x) &= \frac{x - x_1}{x_0 - x_1} \cdot \frac{x - x_2}{x_0 - x_2} \\
&= \frac{x - 1.0}{0 - 1.0} \cdot \frac{x - 2.0}{1.0 - 2.0} \\
&= \frac{1}{2}(x^2 - 3.0x + 2.0)
\end{aligned}
$$

$$
\begin{aligned}
\therefore l_1(x) &= \frac{x - x_0}{x_1 - x_0} \cdot \frac{x - x_2}{x_1 - x_2} \\
&= \frac{x - 0.0}{1.0 - 0.0} \cdot \frac{x - 2.0}{1.0 - 2.0} \\
&= -(x^2 - 2.0x) \\
&= 2.0x - x^2
\end{aligned}
$$

$$
\begin{aligned}
\therefore l_2(x) &= \frac{x - x_0}{x_2 - x_0} \cdot \frac{x - x_1}{x_2 - x_1} \\
&= \frac{x - 0.0}{2.0 - 0.0} \cdot \frac{x - 1.0}{2.0 - 1.0} \\
&= \frac{1}{2}(x^2 - 1.0x)
\end{aligned}
$$

So the second degree interpolating polynomial is

$$
\begin{aligned}
P_2(x) &= f(x_0)l_0(x) + f(x_1)l_1(x) + f(x_2)l_2(x) \\
&= (1.0)\left\{\frac{1}{2}(x^2 - 3.0x + 2.0)\right\} + (2.718\,28)(2.0x - x^2) + (7.389\,06)\left\{\frac{1}{2}(x^2 - 1.0x)\right\} \\
&= 1.476\,25x^2 + 0.242\,03x + 1 \\
&\approx f(x)
\end{aligned}
$$

$$\begin{aligned}\therefore f(0.25) &= (1.476\,25)(0.25)^2 + (0.242\,03)(0.25) + 1\\ &= 1.152\,77\end{aligned}$$

$$\begin{aligned}\therefore f(0.75) &= (1.476\,25)(0.75)^2 + (0.242\,03)(0.75) + 1\\ &= 2.011\,91\end{aligned}$$

*Comment:*
We see that,
from part i, $f(0.25) = 1.324\,36$
from part iii, $f(0.25) = 1.152\,77$
But exactly $f(0.25) = 1.284\,02$
So the approximate value of $f(0.25) = 1.324\,36$ is better because in part i the interval is closer than in part iii.
Similarly, $f(0.75) = 2.183\,50$ is better.

**Problem 3.3.6.** Consider the curve $y = x^3$. Five points on this curve are $(0, 0), (1, 1)(, 2, 8), (3, 27), (4, 68)$. Compute $\sqrt[3]{20}$ by inverse Lagrange's interpolating polynomial. Find the result by

1. cubic polynomial (using first 4 points)
2. quadratic polynomial (using all the points)
3. linear polynomial (using $y_0 = 8,\ y_1 = 27$)

**Solution.** *Part i*
We have the (inverse) Lagrange's polynomial is

$$P_n(y) = \sum_{k=0}^{n} f(y_k) l_k(y)$$

where

$$l_k(y) = \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{y - y_i}{y_k - y_i}, k = 0, 1, 2, \ldots, n$$

In this case, we are given
$y_0 = 1, y_1 = 1, y_2 = 8, y_3 = 27$ so that $n = 3$
Thus

$$P_3(y) = \sum_{k=0}^{3} f(y_k) l_k(y)$$

where

$$l_k(y) = \prod_{\substack{i=0\\ i\neq k}}^{3} \frac{y - y_i}{y_k - y_i}, k = 0, 1, 2, 3$$

$$
\begin{aligned}
\therefore l_0(y) &= \frac{y-y_1}{y_0-y_1}\cdot\frac{y-y_2}{y_0-y_2}\cdot\frac{y-y_3}{y_0-y_3}\\
\Rightarrow l_0(20) &= \frac{20-1}{0-1}\cdot\frac{20-8}{0-8}\cdot\frac{20-27}{0-27}\\
&= \frac{19\cdot 12\cdot(-7)}{(-1)(-8)(-27)}\\
&= \frac{1596}{216}\\
&= 7.388\,88
\end{aligned}
$$

$$
\begin{aligned}
\therefore l_1(y) &= \frac{y-y_0}{y_1-y_0}\cdot\frac{y-y_2}{y_1-y_2}\cdot\frac{y-y_3}{y_1-y_3}\\
\Rightarrow l_1(20) &= \frac{20-0}{1-0}\cdot\frac{20-8}{1-8}\cdot\frac{20-27}{1-27}\\
&= \frac{20\cdot 12\cdot(-7)}{1(-7)(-26)}\\
&= -\frac{1680}{182}\\
&= -9.230\,76
\end{aligned}
$$

$$
\begin{aligned}
\therefore l_2(y) &= \frac{y-y_0}{y_2-y_0}\cdot\frac{y-y_1}{y_2-y_1}\cdot\frac{y-y_3}{y_2-y_3}\\
\Rightarrow l_2(20) &= \frac{20-0}{8-0}\cdot\frac{20-1}{8-1}\cdot\frac{20-27}{8-27}\\
&= \frac{20\cdot 19\cdot(-7)}{8\cdot 7(-19)}\\
&= \frac{2660}{1064}\\
&= 2.5
\end{aligned}
$$

$$
\begin{aligned}
\therefore l_3(y) &= \frac{y-y_0}{y_3-y_0}\cdot\frac{y-y_1}{y_3-y_1}\cdot\frac{y-y_2}{y_3-y_2}\\
\Rightarrow l_3(20) &= \frac{20-0}{27-0}\cdot\frac{20-1}{27-1}\cdot\frac{20-8}{27-8}\\
&= \frac{20\cdot 19\cdot 12}{27\cdot 26\cdot 19}\\
&= 0.341\,88
\end{aligned}
$$

So,

$$
\begin{aligned}
P_3(y) &= f(y_0)l_0(y)+f(y_1)l_1(y)+f(y_2)l_2(y)+f(y_3)l_3(y)\approx f(y)\\
\Rightarrow f(20) &= 0\cdot 7.388\,88+1\cdot(-923\,076)+2\cdot(2.5)+\cdot(0.341\,88)\\
&= -3.205\,12
\end{aligned}
$$

i.e. $\sqrt[3]{20}=-3.2$

*Note.* In this case we first have to find polynomial.

*Part iii*

Here, we are given,

$y_0 = 8, y_1 = 27$ so that $n = 1$

Thus

$$P_1(y) = \sum_{k=0}^{1} f(y_k) l_k(y)$$

where

$$l_k(y) = \prod_{\substack{i=0\\ i\neq k}}^{1} \frac{y - y_i}{y_k - y_i}, k = 0, 1$$

$$\therefore l_0(y) = \frac{y - y_1}{y_0 - y_1} = \frac{y - 28}{8 - 27} = -\frac{1}{19}(y - 27)$$

$$\therefore l_1(y) = \frac{y - y_0}{y_1 - y_0} = \frac{y - 8}{27 - 8} = \frac{1}{19}(y - 8)$$

So the (inverse) linear interpolating polynomial is

$$\begin{aligned} P_1(y) &= f(y_0) l_0(y) + f(y_1) l_1(y) \\ &= 2\left\{-\frac{1}{19}(y - 27)\right\} + 3\left\{\frac{1}{19}(y - 8)\right\} \\ &= 0.052\,63y + 1.578\,94 \approx f(y) \end{aligned}$$

$$\begin{aligned} \therefore f(20) &= 0.052\,63(20) + 1.578\,94 \\ &= 2.631\,54 \end{aligned}$$

i.e. $\sqrt[3]{20} = 2.63$

## 3.4 Power form of the polynomial

A polynomial of degree $\leq n$ is $P(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$ if $a_n \neq 0$; $\deg(P(x)) = n$

*Remark.* The power form sometimes leads to loss of significance (in digits).

**Problem 3.4.1.** Find equation of the straight line passing through $(6000, \frac{1}{3}), (6001, -\frac{2}{3})$

**Solution.** We know, the equation of the straight line passing through $(x_1, y_1)$ and $(x_2, y_2)$ is

$$\frac{x - x_1}{x_1 - x_2} = \frac{y - y_1}{y_1 - y_2}$$

In this case,

$$\begin{aligned} &\frac{y - \frac{1}{3}}{\frac{1}{3} + \frac{2}{3}} = \frac{x - 6000}{6000 - 6001} \\ \Rightarrow &\frac{3y - 1}{3} = \frac{x - 6000}{-1} \\ \Rightarrow &3y - 1 = 3(6000 - 3x) \\ \Rightarrow &y = 6000 + \frac{1}{3} - x \\ \Rightarrow &P(x) \equiv y = 6\,000.333\,33 - x \end{aligned}$$

Suppose a machine only allow upto 5 significant digit
Therefore, in five significant digits, it becomes,

$P(x) \approx 6000.3 - x$

Now,

$P(60000) = 6000.3 - 6000 = 0.3 \qquad P(60001) = 6000.3 - 6001 = -0.7$ On the other hand, $\frac{1}{3} = 0.333\,33 \qquad -\frac{2}{3} = -0.666\,67$

## 3.5 Shifted Power Form

The shifted power form of the polynomial

$$P(x) = a_0 + a_1(x-c) + a_2(x-c)^2 + \cdots + a_n(x-c)^n \text{ for some } c. \tag{3.5}$$

*Note.* $c$ is called the center.

[In the above example $c$ may be 6000]
Now, $P(x) = 6000.3 - x$ can be written as

$P(x) = 0.333\,33 - 1(x - 6000)$

So by comparing we get, $\quad a_0 = 0.333\,33$

$a_1 = -1$

$c = 6000$

Now,

$$\left.\begin{aligned} P(6000) &= 0.333\,33 \\ P(6001) &= -0.666\,67 \end{aligned}\right\} \text{ exact value}$$

*Remark.* Shifted form is better than power form.

## 3.6 A Generalization of Shift Form

### 3.6.1 Newton's form

$$P(x) = a_0 + a_1(x-c_1) + a_2(x-c_1)(x-c_2) + a_3(x-c_1)(x-c_2)(x-c_3) + \cdots + a_n(x-c_1)(x-c_2)\ldots(x-c_n) \tag{3.6}$$

The above form is known as Newton's form.

*Remark.* If $c_1 = c_2 = \cdots = c_n = c$ then (3.6) is same as (3.5)

### 3.6.2 Evaluation of The Newton's form of interpolating polynomial

From (3.6) we can write,

$$\begin{aligned} P(x) &= a_0 + (x-c_1)(a_1 + a_2(x-c_2) + a_3(x-c_2)(x-c_3) + \cdots + a_n(x-c_2)(x-c_3)\ldots(x-c_n)) \\ &= a_0 + (x-c_1)(a_1 + (x-c_2)(a_2 + a_3(x-c_3) + \cdots + a_n(x-c_3)\ldots(x-c_n))) \end{aligned}$$

In this way we get, $\quad P(x)$ in nested form

$$P(x) = a_0 + (x-c_1)(a_1 + (x-c_2)(a_2 + (x-c_3)(a_3 + \cdots + (x-c_{n-1})(a_{n-1} + (x-c_n)a_n))\ldots))_{(n-1) \text{ bracket}}$$

**Example.**

$$
\begin{aligned}
P(x) &= 1 + 2(x-1) + 3(x-1)(x-2) + 4(x-1)(x-2)(x-3) \\
\Rightarrow P(x) &= 1 + (x-1)[2 + (x-2)\{3 + (x-3)\cdot 4\}]
\end{aligned}
$$

$$
\begin{aligned}
\therefore P(4) &= 1 + (4-1)[2 + (4-2)\{3 + (4-3)\cdot 4\}] \\
&= 1 + 3[2 + 2\{3 + 1\cdot 4\}] \\
&= 1 + 3[2 + 14] \\
&= 1 + 3\dot{1}6 \\
&= 49
\end{aligned}
$$

## 3.7 Newton's Interpolating Polynomial

### 3.7.1 Divided Difference

Writing the interpolating polynomial in shifted power form (3.6) using the points $x_0, x_1, \ldots, x_{n-1}$ as centers, then

$$P_n(x) = a_0 + a_1(x-x_0) + a_2(x-x_0)(x-x_1) + \cdots + a_n(x-x_0)(x-x_1)\ldots(x-x_{n-1}) \tag{3.7}$$

*Note.* Put $x = x_0$ then,
$P_n(x_0) = a_0 \approx f(x_0)$
Similarly, if we put $x = x_1$, then

$$
\begin{aligned}
P_n(x_1) &= a_0 + a_1(x_1 - x_0) \approx f(x_1) \\
&= f(x_0) + a_1(x_1 - x_0) = f(x_1) \\
\Rightarrow a_1 &= \frac{f(x_1) - f(x_0)}{x_1 - x_0}
\end{aligned}
$$

## 3.8 Divided Difference Notation for $f$

### 3.8.1 Zeroth divided difference

The zeroth divided difference of $f$ is
$a_0 = f(x_0) = f[x_0]$

In general, $f(x_i) = f[x_i]$

### 3.8.2 First Divided Difference

The first divided difference of $f$ is

$$\begin{aligned} a_1 &= \frac{f(x_1) - f(x_0)}{x_1 - x_0} \\ &= \frac{f[x_1] - f[x_0]}{x_1 - x_0} \\ &= f[x_1, x_0] \\ &= f[x_0, x_1] \end{aligned}$$

i.e. $f[x_0, x_1] = \frac{f[x_0]-f[x_1]}{x_0-x_1}$
In general, $f[x_i, x_{i+1}] = \frac{f[x_i]-f[x_{i+1}]}{x_i-x_{i+1}}$
Similarly the second divided difference is,

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

In general,

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_i, x_{i+1}] - f[x_{i+1}, x_{i+2}]}{x_i - x_{i+2}}$$

Inductively, we can define the $k$-th divided difference as,

$$f[x_0, x_1, \ldots, x_k] = \frac{f[x_0, x_1, \ldots, x_{k-1}] - f[x_1, x_2, \ldots, x_k]}{x_0 - x_k}$$

For any integer $k$ between 0 and $n$, let $q_k(x)$ be the sum of the first $(k+1)$ times, i.e.,

$$q_k(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots + a_k(x - x_0)\ldots(x - x_{k-1}) \quad (0 \le k \le n)$$

Then every one of the remaining terms in (3.7) has the factor $(x - x_0)\ldots(x - x_k)$ common.
Therefore, equation (3.7) can be written as

$$P_n(x) = q_k(x) + (x - x_0)\ldots(x - x_k)r(k)$$

for some polynomial $r(k)$.
The last term here vanishes at $x = x_0, x_1, \ldots, x_k$
$\therefore r(x)$ is of no further interest.
Hence, $q_k(x)$ interpolates $f(x)$ at $x_0, x_1, \ldots, x_k$, since $P_n(x)$ does.
Now $q_k(x)$ is of degree $\le k$
$\therefore q_k(x) = P_k(x)$ is unique and interpolates $f(x)$ at $x_0, x_1, \ldots, x_k$. This shows that Newton's form in (3.7) can be built up step by step from the sequence $P_0(x), P_1(x), \ldots$ with $P_k(x)$ obtained from $P_{k-1}(x)$ just by adding the next term in (3.7).
i.e. $P_k(x) = P_{k-1}(x) + a_k(x - x_0)\ldots(x_k - x_{k-1})$
The coefficient $a_k$ depends only on the values of $f(x)$.

$a_k = f[x_0, x_1, \ldots, x_k]$ the $k$th divided difference.

So we get the Newton's interpolating divided formula as

$$\begin{aligned} P_n(x) &= f[x_0] + f[x_0, x_1](x - x_0) + \cdots + f[x_0, x_1, \ldots, x_n](x - x_0)\ldots(x - x_{n-1}) \\ &= \sum_{i=0}^{n} f[x_0, x_1, \ldots, x_i] \prod_{j=0}^{i-1}(x - x_j) \end{aligned}$$

## 3.9 Newton's Divided Difference Formula

$$P_n(x) = \sum_{i=0}^{n} f[x_0, x_1, \ldots, x_i] \prod_{j=0}^{i-1} (x - x_j)$$

For $n = 1$

$$\begin{aligned} P_1(x) &= f[x_0] + f[x_0, x_1](x - x_0) \\ \Rightarrow P_1(x) &= f(x_0) + \frac{f(x_0) - f(x_1)}{(x_0 - x_1)}(x - x_0) \end{aligned} \quad \left| \quad \begin{aligned} \text{where, } f[x_0] &= f(x_0) \\ f[x_0, x_1] &= \frac{f(x_0) - f(x_1)}{(x_0 - x_1)} \end{aligned} \right.$$

**Problem 3.9.1.** Use a divided difference table and Newton's form of interpolating polynomial for $f(x) = \log_{10}(x)$ to estimate $\log_{10}(4.5)$

| $x_i$ | $f(x_i)$ | |
|---|---|---|
| $x_0 = 1.2$ | $f(x_0) =$ | $0.079\,181$ |
| $x_1 = 1.4$ | $f(x_1) =$ | $0.146\,128$ |
| $x_2 = 1.6$ | $f(x_2) =$ | $0.204\,120$ |
| $x_3 = 1.8$ | $f(x_3) =$ | $0.255\,273$ |

**Solution.** First we construct the following divided difference table We know, the Newton's interpolating

| $x_i$ | Zeroth divided difference $f(x_i) = f[x_i]$ | First divided difference $f[x_i, x_{i+1}] = \frac{f[x_i] - f[x_{i+1}]}{x_i - x_{i+1}}$ | Second divided difference $f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_i, x_{i+1}] - f[x_{i+1}, x_{i+2}]}{x_i - x_{i+2}}$ | Third divided difference $f[x_i, x_{i+1}, x_{i+2}, x_{i+3}] = \frac{f[x_i, x_{i+1}, x_{i+2}] - f[x_{i+1}, x_{i+2}, x_{i+3}]}{x_i - x_{i+3}}$ |
|---|---|---|---|---|
| $x_0 = 1.2$ | $f[x_0] = 0.079\,181$ | | | |
| | | $f[x_0, x_1] = \frac{f[x_0] - f[x_1]}{x_0 - x_1} = 0.334\,735$ | | |
| | | | $f[x_0, x_1, x_2] = \frac{f[x_0, x_1] - f[x_1, x_2]}{x_0 - x_2} = -0.111\,937\,5$ | |
| $x_1 = 1.4$ | $f[x_1] = 0.146\,128$ | | | |
| | | $f[x_1, x_2] = \frac{f[x_1] - f[x_2]}{x_1 - x_2} = 0.289\,96$ | | $f[x_0, x_1, x_2, x_3] = \frac{f[x_0, x_1, x_2] - f[x_1, x_2, x_3]}{x_0 - x_3} = 0.044\,083\,333$ |
| $x_2 = 1.6$ | $f[x_2] = 0.204\,120$ | | | |
| | | | $f[x_1, x_2, x_3] = \frac{f[x_1, x_2] - f[x_2, x_3]}{x_1 - x_3} = -0.085\,487\,5$ | |
| | | $f[x_2, x_3] = \frac{f[x_2] - f[x_3]}{x_2 - x_3} = 0.255\,765$ | | |
| $x_3 = 1.8$ | $f[x_3] = 0.255\,273$ | | | |

divided difference formula is

$$P_n(x) = \sum_{i=0}^{n} f[x_0, x_1, \ldots, x_i] \prod_{j=0}^{i-1} (x - x_j)$$

In this case, $n = 3$

$$\begin{aligned}
\therefore P_3(x) &= \sum_{i=0}^{3} f[x_0, x_1, \ldots, x_i] \prod_{j=0}^{i-1}(x - x_j) \\
&= f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) \\
&= 0.079\,181 + 0.334\,735(x - 1.2) + 0.111\,937\,5(x - 1.2)(x - 1.4) + 0.044\,083\,333(x - 1.2)(x - 1.4)(x - 1 \\
&= 0.079\,181 + (x - 1.2)[0.334\,735 - (x - 1.4)\{0.111\,937\,5 + (x - 1.6)(0.044\,083\,333)\}]
\end{aligned}$$

Since $\log_{10}(14.5) = 1 + \log_{10}(1.45)$

$$\begin{aligned}
\therefore P_3(1.45) &= 0.079\,181 + (1.45 - 1.2)[0.334\,735 - (1.45 - 1.4)\{0.111\,937\,5 + (1.45 - 1.6)(0.044\,083\,333)\}] \\
&= 0.161\,548\,187
\end{aligned}$$

$$\begin{aligned}
\therefore P_3(14.5) &= 1 + 0.161\,548\,187 \\
&= 1.161\,588
\end{aligned}$$

**Problem 3.9.2.** Construct the divided difference table to find the Newton's form of polynomial of deg$\leq 3$ and estimate $f(1.25)$. Also evaluate $f(1.25)$ in Lagrange's form and compare the results. Exact value of $f(1.25) = 3.0096$.

| $x_i$ | $f(x_i)$ |
|---|---|
| $x_0 = 1.05$ | $f(x_0) = 1.7433$ |
| $x_1 = 1.20$ | $f(x_1) = 2.5722$ |
| $x_2 = 1.30$ | $f(x_2) = 3.6021$ |
| $x_3 = 1.43$ | $f(x_3) = 8.2381$ |

**Solution.** First we construct the (Newton) divided difference table as follows,

| $x_i$ | Zeroth divided difference $f(x_i) = f[x_i]$ | First divided difference $f[x_i, x_{i+1}] = \frac{f[x_i] - f[x_{i+1}]}{x_i - x_{i+1}}$ | Second divided difference $f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_i, x_{i+1}] - f[x_{i+1}, x_{i+2}]}{x_i - x_{i+2}}$ | Third divided difference $f[x_i, x_{i+1}, x_{i+2}, x_{i+3}] = \frac{f[x_i, x_{i+1}, x_{i+2}] - f[x_{i+1}, x_{i+2}, x_{i+3}]}{x_i - x_{i+3}}$ |
|---|---|---|---|---|
| $x_0 = 1.05$ | $f[x_0] = 1.7433$ | | | |
| | | $f[x_0, x_1] = \frac{f[x_0] - f[x_1]}{x_0 - x_1} = 5.526$ | | |
| $x_1 = 1.20$ | $f[x_1] = 2.5722$ | | $f[x_0, x_1, x_2] = \frac{f[x_0, x_1] - f[x_1, x_2]}{x_0 - x_2} = 19.092$ | |
| | | $f[x_1, x_2] = \frac{f[x_1] - f[x_2]}{x_1 - x_2} = 10.299$ | | $f[x_0, x_1, x_2, x_3] = \frac{f[x_0, x_1, x_2] - f[x_1, x_2, x_3]}{x_0 - x_3} = 158.346\,666\,7$ |
| $x_2 = 1.30$ | $f[x_2] = 3.6021$ | | $f[x_1, x_2, x_3] = \frac{f[x_1, x_2] - f[x_2, x_3]}{x_1 - x_3} = 82.430\,666\,68$ | |
| | | $f[x_2, x_3] = \frac{f[x_2] - f[x_3]}{x_2 - x_3} = 30.906\,666\,67$ | | |
| $x_3 = 1.45$ | $f[x_3] = 8.2381$ | | | |

We know, the Newton's interpolating divided difference formula is

$$P_n(x) = \sum_{i=0}^{n} f[x_0, x_1, \ldots, x_i] \prod_{j=0}^{i-1} (x - x_j)$$

In this case, $n = 3$

$$\begin{aligned}
\therefore P_3(x) &= \sum_{i=0}^{3} f[x_0, x_1, \ldots, x_i] \prod_{j=0}^{i-1} (x - x_j) \\
&= f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) \\
&= 1.7433 + 5.526(x - 1.05) + 19.092(x - 1.05)(x - 1.20) + 158.346\,666\,7(x - 1.05)(x - 1.30)(x - 1.30) \\
&= 1.7433 + 5.526(x - 1.05) + 19.092(x^2 - 2.25x + 1.26) + 158.346\,666\,7(x^2 - 2.25x + 1.26)(x - 1.30) \\
&= 1.7433 + 5.526(x - 1.05) + 19.092(x^2 - 2.25x + 1.26) + 158.346\,666\,7(x^3 - 3.55x^2 + 4.185x - 1638) \\
&= 158.346\,666\,7x^3 - 543.038\,666\,8x^2 + 625.249\,800\,1x - 239.374\,920\,1 \\
&\approx f(x)
\end{aligned}$$

$\therefore f(1.25) = 2.960\,24$

# Chapter 4

# Interpolation With Equal Intervals

## 4.1 Newton's (Gregory) Forward Difference Formula

This is called 'forward' interpolation formula because this formula contains values of the tabulated function from $f(a)$ onward to the right, used mainly for interpolating the values of $y = f(x)$ near the beginning of set of tabulated values and for extrapolating values of $f(x)$ a short distance to the left of $f(a)$.

Let $y = f(x)$ takes values $f(a), f(a+h), f(a+2h), f(a+3h), \ldots, f(a+nh)$.
ie. $x_0 = a, x_1 = a+h, x_2 = a+2h \ldots, x_n = a+nh$ where $x_0, x_1, \ldots, x_n$ are equivalent points.

$$P_n(x) = A_0 + A_1(x-a) + A_2(x-a)(x-a-h) + \cdots + A_n(x-a)(x-a-h)\ldots(x-a-(n-1)h)$$

Where,

$$P_n(a) = A_0 = f(a)$$

$$\begin{aligned}
P_n(a+h) &= A_0 + A_1 h = f(a+h) \\
\Rightarrow A_1 &= \frac{f(a+h) - f(a)}{h} = \frac{\Delta f(a)}{h}
\end{aligned}$$

$$\begin{aligned}
P_n(a+2h) &= A_0 + A_1 \cdot 2h + A_2 \cdot 2h \cdot h = f(a+2h) \\
\Rightarrow f(a+2h) &= A_0 + 2A_1 h + 2A_2 h^2 \\
&= f(a) + 2\{f(a+h) - f(a)\} + 2A_2 h^2 \\
\Rightarrow A_2 &= \frac{f(a+2h) - f(a) - 2\{f(a+h) - f(a)\}}{2h^2} \\
\Rightarrow A_2 &= \frac{\{f(a+2h) - f(a+h)\} - \{f(a+h) - f(a)\}}{2h^2} \\
\Rightarrow A_2 &= \frac{1}{2!\, h^2} \Delta^2 f(a)
\end{aligned}$$

Similarly,
$A_3 = \frac{1}{3!\,h^3}\Delta^3 f(a)$
$A_4 = \frac{1}{4!\,h^4}\Delta^4 f(a)$
$A_n = \frac{1}{n!\,h^n}\Delta^n f(a)$
Thus if $u = \frac{x-a}{h}$ then

$$\begin{aligned} P_n(x) &= P_n(a+hu) \\ &= f(a) + u\Delta f(a) + \frac{u(u-1)}{2!}\Delta^2 f(a) + \frac{u(u-1)(u-2)}{3!}\Delta^3 f(a) + \cdots + \frac{u(u-1)\ldots(u-n+1)}{n!}\Delta^n f(a) \end{aligned}$$

Where,
$\Delta^i f(a) = i$th difference
$u = \frac{x-a}{h}\, x_0 = a$, $h =$ interval
$x =$ the point at which $f(x)$ to be interpolated
This known as N-G formula for forward interpolation.

**Problem 4.1.1.** Given the following table; estimate the number of candidates who obtained marks between 40 and 45.

| Marks | No. of students |
|---|---|
| $30-40$ | 31 |
| $40-50$ | 42 |
| $50-60$ | 51 |
| $60-70$ | 35 |
| $70-80$ | 31 |

**Solution.**
*(i)* First prepare the cumulative frequency table

| Marks less than $(x)$ | No. of students $f(x)$ |
|---|---|
| 40 | 31 |
| 50 | 73 |
| 60 | 124 |
| 70 | 159 |
| 80 | 190 |

*(ii)* Prepare the difference table

| $x$ | $f(x)$ | $\Delta f(x)$ | $\Delta^2 f(x)$ | $\Delta^3 f(x)$ | $\Delta^4 f(x)$ | $\Delta^5 f(x)$ |
|---|---|---|---|---|---|---|
| 40 | 31 | | | | | |
| | | 42 | | | | |
| 50 | 73 | | 9 | | | |
| | | 51 | | -25 | | |
| 60 | 124 | | -16 | | 37 | |
| | | 35 | | 12 | | |
| 70 | 159 | | -4 | | | |
| | | 31 | | | | |
| 80 | 190 | | | | | |

Now,

$$\begin{aligned} u &= \frac{x-a}{h} \\ \therefore u &= \frac{45-40}{10} \\ &= \frac{5}{10} \\ &= 5 \end{aligned} \qquad \left| \qquad \begin{aligned} \text{Where, } x &= 45 \\ a &= 40 \\ h &= 10 \end{aligned} \right.$$

So no. of students with mark less than 45 is

$$P_n(x) \approx f(45)$$

$$\begin{aligned} \therefore f(45) &= f(a) + u\Delta f(a) + \frac{u(u-1)}{2!}\Delta^2 f(a) + \frac{u(u-1)(u-2)}{3!}\Delta^3 f(a) + \frac{u(u-1)(u-2)(u-3)}{4!}\Delta^4 f(a) \\ &= 31 + (0.5)(42) + \frac{0.5(0.5-1)}{2!}(9) + \frac{0.5(0.5-1)(0.5-2)}{3!}(-25) + \frac{0.5(0.5-1)(0.5-2)(0.5-3)}{4!}(37) \\ &= 47.867\,188 \end{aligned}$$

i.e. no. of students with marks less than 45 = 48
no. of students with marks less than 40 = 31
So no. of students with marks between 40 and 45 = 48 − 31 = 17

**Problem 4.1.2.** The following table gives the population of a town. Estimate the increase in the population during the period from 1946 to 1948

| Year | Population (in thousands) |
|---|---|
| 1911 | 12 |
| 1921 | 15 |
| 1931 | 20 |
| 1941 | 27 |
| 1951 | 39 |
| 1961 | 52 |

using the N-G formula for forward interpolation.

**Solution.** The difference table for the given data is as follows

| $x$ | $f(x)$ | $\Delta f(x)$ | $\Delta^2 f(x)$ | $\Delta^3 f(x)$ | $\Delta^4 f(x)$ | $\Delta^5 f(x)$ |
|---|---|---|---|---|---|---|
| 1911 | 12 | | | | | |
| | | 3 | | | | |
| 1921 | 15 | | 2 | | | |
| | | 5 | | 0 | | |
| 1931 | 20 | | 2 | | 3 | |
| | | 7 | | 3 | | -10 |
| 1941 | 27 | | 5 | | -7 | |
| | | 12 | | -4 | | |
| 1951 | 39 | | 4 | | | |
| | | 13 | | | | |
| 1961 | 52 | | | | | |

$$\text{Since } u = \frac{x-a}{h} \qquad \text{Where, } x = 1946,\ a = 1911,\ h = 10$$

$$\text{For } f(1946), u = \frac{1946-1911}{10} = 3.5$$

Now from Newton's formula for forward interpolation, we get

$$P_5(1946) \approx f(1946)$$

$$\begin{aligned}
\therefore f(1946) &= f(a) + u\Delta f(a) + \frac{u(u-1)}{2!}\Delta^2 f(a) + \frac{u(u-1)(u-2)}{3!}\Delta^3 f(a) + \frac{u(u-1)(u-2)(u-3)}{4!}\Delta^4 f(a) \\
&\quad + \frac{u(u-1)(u-2)(u-3)(u-4)}{5!}\Delta^5 f(a) \\
&= 12 + (3.5)(3) + \frac{3.5(3.5-1)}{2!}(2) + \frac{3.5(3.5-1)(3.5-2)}{3!}(0) + \frac{3.5(3.5-1)(3.5-2)(3.5-3)}{4!}(3) \\
&\quad + \frac{3.5(3.5-1)(3.5-2)(3.5-3)(3.5-4)}{5!}(-10)
\end{aligned}$$

$$\Rightarrow f(1946) = 32.343\,75$$

Again, to find $f(1948)$, $u = \frac{1948-1911}{10} = 3.7$

$$P_5(1948) \approx f(1948)$$

$$\begin{aligned}
\therefore f(1948) &= f(a) + u\Delta f(a) + \frac{u(u-1)}{2!}\Delta^2 f(a) + \frac{u(u-1)(u-2)}{3!}\Delta^3 f(a) + \frac{u(u-1)(u-2)(u-3)}{4!}\Delta^4 f(a) \\
&\quad + \frac{u(u-1)(u-2)(u-3)(u-4)}{5!}\Delta^5 f(a) \\
&= 12 + (3.7)(3) + \frac{3.7(3.7-1)}{2!}(2) + \frac{3.7(3.7-1)(3.7-2)}{3!}(0) + \frac{3.7(3.7-1)(3.7-2)(3.7-3)}{4!}(3) \\
&\quad + \frac{3.7(3.7-1)(3.7-2)(3.7-3)(3.7-4)}{5!}(-10)
\end{aligned}$$

$$\Rightarrow f(1948) = 34.873\,215$$

Therefore increase in the population during the period from 1946 to 1948

$$\begin{aligned}
&= f(1948) - f(1946) = 34.873\,215 - 32.343\,75 \\
&= 2.529\,465 \text{ thousand} \\
&= 2.5295 \text{ thousand}
\end{aligned}$$

**Problem 4.1.3.** Use Newton's formula for interpolation to find the net premium at age 25 from the table given below

| Age $(x)$ | Premium $f(x)$ |
|---|---|
| 20 | 0.014 27 |
| 24 | 0.015 81 |
| 28 | 0.017 72 |
| 32 | 0.019 96 |

**Solution.** The difference table for the given data is

| Age $x$ | Premium $f(x)$ | $\Delta f(x)$ | $\Delta^2 f(x)$ | $\Delta^3 f(x)$ |
|---|---|---|---|---|
| 20 | 0.014 27 | | | |
| | | 0.001 55 | | |
| 24 | 0.015 81 | | 0.0037 | |
| | | 0.001 91 | | −0.000 04 |
| 28 | 0.017 72 | | 0.000 33 | |
| | | 0.002 24 | | |
| 32 | 0.019 96 | | | |

Now we have to find $f(25)$
Since

$$\begin{aligned} u &= \frac{x-a}{h} \\ \therefore u &= \frac{25-20}{4} \\ &= 1.25 \end{aligned}$$

$$\begin{aligned} \text{Where, } x &= 15 \\ a &= 20 \\ h &= 4 \end{aligned}$$

$$\begin{aligned} P_n(25) &\approx f(25) \\ \therefore f(25) &= f(a) + u\Delta f(a) + \frac{u(u-1)}{2!}\Delta^2 f(a) + \frac{u(u-1)(u-2)}{3!}\Delta^3 f(a) \\ &= 0.014\,27 + (1.25)(0.001\,45) + \frac{1.25(1.25-1)}{2!}(0.000\,37) + \frac{1.25(1.25-1)(1.25-2)}{3!}(-0.000\,04) \\ &= 0.016\,141\,8 \end{aligned}$$

## 4.2 Newton-Gregory Backward Interpolation Formula For Equal Interval

To derive this formula we write

$$\begin{aligned} P_n(x) = A_0 &+ A_1\{x-(a+nh)\} + A_2\{x-(a+nh)\}\{x-(a+(n-1)h)\} \\ &+ \cdots + A_n\{x-(a+nh)\}\{x-(a+(n-1)h)\}\ldots(x-h) \end{aligned} \tag{4.1}$$

Where $A_0, A_1, \ldots, A_n$ are constants which are to be determined.
Put $x = a+nh, a+(n-1)h, \ldots, a$
and $P_n(a+nh) = f(a+nh), \ldots$
etc in (4.1)
We get the co efficient $A_0, A_1, \ldots, A_n$ as:

$$\begin{aligned} P_n(a+nh) &= A_0 = f(a+nh) \\ \Rightarrow A_0 &= f(a+nh) \end{aligned}$$

$$\begin{aligned} P_n(a+(n-1)h) &= A_0 + A_1(-h) = f(a+(n-1)h) \\ \Rightarrow A_1 &= \frac{f(a+nh) - f(a+(n-1)h)}{h} \\ \Rightarrow A_1 &= \frac{1}{h}\nabla f(a+nh) \end{aligned}$$

Similarly,

$$A_2 = \frac{1}{2!\,h^2}\nabla^2 f(a+nh)$$
$$A_n = \frac{1}{n!\,h^n}\nabla^n f(a+nh)$$

By substituting these in (4.1)

$$P_n(x) = f(a+nh) + \frac{1}{h}\nabla f(a+nh)\{x-(a+nh)\} + \frac{1}{2!\,h^2}\nabla^2 f(a+nh)\{x-(a+nh)\}\{x-(a+(n-1)h)\}$$
$$+\cdots+\frac{1}{n!\,h^n}\nabla^n f(a+nh)\{x-(a+nh)\}\{x-(a+(n-1)h)\}\ldots(x-h) \tag{1.2}$$

This is known as Newton-Gregory backward interpolating formula.
*Working Formula*
Put $u = \frac{x-(a+nh)}{h} \Rightarrow x = a+nh+hu$ in (1.2)
So (1.2) becomes,

$$\begin{aligned}P_n(x) &= P_n(a+nh+hu)\\ &= f(a+nh) + u\nabla f(a+nh) + \frac{u(u+1)}{2!}\nabla^2 f(a+nh) + \frac{u(u+1)(u+2)}{3!}\nabla^3 f(a+nh)\\ &+\cdots+\frac{u(u+1)\ldots(u+n-1)}{n!}\nabla^n f(a+nh)\end{aligned}$$

# Chapter 5

# Solution of System of Linear Equations

## 5.1 Solutions of system of linear equations

Consider the following system of linear equations

$$\left.\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\ a_{31}x_1 + a_{32}x_2 + \cdots + a_{3n}x_n = b_3 \end{aligned}\right\} \tag{5.1}$$

Let the coefficient matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}, \quad B = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}, \quad X = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

then the system (5.1) reduces to $AX = B$. To find the solution of $AX = B \Rightarrow X = A^{-1}B$, there are two method solving the system (5.1) namely (i) Direct method and (ii) Iteration method.
Direct or Gauss-Elimination method is used when the coefficient matrix $A$ is a dense matrix and the iteration method is used when the coefficient matrix $A$ is large ans sparse.

## 5.2 Gauss-Elimination Method

In this method, we use $k$th equation to eliminate $x_k$ from equations $(K+1), (K+2), \ldots, n$ during the $k$th step $(K = 1, 2, \ldots, n)$.

By this process the system is reduced to an upper triangular form. This is possible only if at the beginning of the $k$th step the coefficient $a_{kk} \neq 0$. Otherwise, straight forward reduction does not work. Then rearrangement is necessary.

Thus in an $n \times m$ matrix, the value of the element and its position is hence important.

**Example.** Solve the system of equations:

$$x_1 + x_2 + x_3 = 1 \tag{5.2}$$

$$x_1 + x_2 + 2x_3 = 2 \tag{5.3}$$

$$x_1 + 2x_2 + 2x_3 = 1 \tag{5.4}$$

$$
\begin{aligned}
& & x_1 + x_2 + x_3 &= 1 && (5.5)\\
&(5.3)\text{-}(5.2) & x_3 &= 1 && (5.6)\\
&(5.4)\text{-}(5.2) & x_2 + x_3 &= 0 && (5.7)
\end{aligned}
$$

Since $a_{22}^{'} = 0$, rearrangement is necessary (5.6)$\longleftrightarrow$(5.7)

$$
\begin{aligned}
x_1 + x_2 + x_3 &= 1 && (5.8)\\
x_2 + x_3 &= 0 && (5.9)\\
x_3 &= 1 && (5.10)
\end{aligned}
$$

Back substitution starts

$$
\begin{aligned}
(5.10) \Rightarrow & x_3 = 1\\
(5.9) \Rightarrow & x_2 = -x_3 = -1\\
(5.8) \Rightarrow & x_1 = 1 - x_3 - x_2 = 1
\end{aligned}
$$

So the solutions is $x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$

**Example.** Solve the system

$$x_2, x_3 = 1,\ x_1 + x_3 = 1,\ x_1 + x_2 = 1$$

**Example.** Solve the system of equations:

$$
\begin{aligned}
x_1 + x_2 + x_3 &= 1 && (5.11)\\
x_1 + 1.0001x_2 + 2x_3 &= 2 && (5.12)\\
x_1 + 2x_2 + 2x_3 &= 1 && (5.13)
\end{aligned}
$$

$$
\begin{aligned}
& & x_1 + x_2 + x_3 &= 1 && (5.14)\\
&(5.12)\text{-}(5.11) & 0.0001x_2 + x_3 &= 1 && (5.15)\\
&(5.13)\text{-}(5.11) & x_2 + x_3 &= 0 && (5.16)
\end{aligned}
$$

$$
\begin{aligned}
& & x_1 + x_2 + x_3 &= 1 && (5.17)\\
& & 0.0001x_2 + x_3 &= 0 && (5.18)\\
&10\,000\times\ (5.15)\text{-}(5.16) & 9999x_3 &= 100\,000 && (5.19)
\end{aligned}
$$

By back substitution,

$$
\begin{aligned}
(5.19) \Rightarrow & x_3 = \frac{10\,000}{9\,999} = 1.000\,100\,1 \approx 1 \text{ (using 3 significant digit)}\\
(5.18) \Rightarrow & x_2 = \frac{1-1}{0.0001} = 0\\
(5.17) \Rightarrow & x_1 = 1 - 0 - 1 = 0
\end{aligned}
$$

So the solutions is $x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

Alternatively

$$x_1 + x_2 + x_3 = 1 \tag{5.20}$$
$$x_1 + 1.0001x_2 + 2x_3 = 2 \tag{5.21}$$
$$x_1 + 2x_2 + 2x_3 = 1 \tag{5.22}$$

$$x_1 + x_2 + x_3 = 1 \tag{5.23}$$
$$(5.21)\text{-}(5.20) \qquad 0.000\,1x_2 + x_3 = 1 \tag{5.24}$$
$$(5.22)\text{-}(5.20) \qquad x_2 + x_3 = 0 \tag{5.25}$$

Interchanging (5.24) and (5.25) we get

$$x_1 + x_2 + x_3 = 1 \tag{5.26}$$
$$x_2 + x_3 = 0 \tag{5.27}$$
$$0.000\,1x_2 + x_3 = 1 \tag{5.28}$$

$$x_1 + x_2 + x_3 = 1 \tag{5.29}$$
$$x_2 + x_3 = 0 \tag{5.30}$$
$$(5.28)\text{-}0.000\,1(5.27) \qquad 0.999\,9x_3 = 1 \tag{5.31}$$

By back substitution,

$$\begin{aligned}(5.31) &\Rightarrow x_3 = \frac{1}{0.999\,9} = 1.000\,100\,1 \approx 1 \\ (5.30) &\Rightarrow x_2 = -x_3 = -1 \\ (5.29) &\Rightarrow x_1 = 1 - (-1) - 1 = 1\end{aligned}$$

So the solutions is $x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$ (correct result)

*Remark.* In this problem, we see that there are different solution in different way. It is caused by using different pivot equation which is discusses below.

## 5.3 Pivot Strategy

If $a_{kk}^{(k)} = 0$ in the $k$th step for some $k = 1, 2, \ldots, n-1$ then from the $k$th row to the $n$th row is searched for the first non-zero entry.

If $a_{pk}^{(k)} \neq 0$ for some $p$, $k+1 \leq p \leq n$, then perform $E_k \longleftrightarrow E_p$ (interchange) where $E_k$ is the $k$th equation in the system.

If $a_{pk}^{(k)} = 0$, $p = k, k+1, \ldots, n$ then the system does not have unique solution and the procedure fails.

So obtaining a zero for the pivot element, necessarily takes a row interchange. But in practice it is often desirable to perform row interchanges involving pivot elements even when they are non-zero.

**Problem 5.3.1.** Solve

$$E_1 : 0.003x_1 + 29.140x_2 = 59.17$$
$$E_2 : \quad 5.291x_1 - 6.130x_2 = 46.78$$

Use 4 digits arithmetic to find its solution. Exact solution is $x_1 = 10.00$, $x_2 = 1.00$

**Solution.** Use $a_{11} = 0.003\,0$ as pivot element,
Find the multiplier $m = \frac{a_{21}}{a_{11}} = \frac{5.291\,0}{0.003} = 1\,763.666\,6 \approx 1764$
Eliminate $x_1$ from $E_2$ by $(E_2 - mE_1) \to E_2^{'}$

$$E_1^{'} : 0.003x_1 + 59.140x_2 = 59.17$$
$$E_2^{'} : \qquad -104\,329x_2 = -104\,329.1$$

By back substitution,

$$x_2 = 1.000\,000\,959 \approx 1.001$$
$$\therefore E_1 = \frac{59.19 - 59.140 \times 1.001}{0.003\,0} = -9.7133 \approx -10.0$$

The large error in the solution of $x_1$ resulted from the small error in solving $x_2$. The errors magnified 20000 times in the solution of $x_1$. This happened due to division by pivot element $0.003\,0$.

This sort of difficulties arise in choosing the pivot element $a_{kk}^{(k)}$ (in the $k$th step) when they are relatively small, compared to the other entries, $a_{ij}^{(k)}$ for $k \leq i \leq n$, $k \leq j \leq n$.

So we choose a new pivot element $a_{pq}^{(k)}$ (in the $k$th step).

Pivot Strategies in general are accomplished by selecting a new element for the pivot $a_{pq}^{(k)}$ and interchanging the $k$the row and $p$th rows, followed by interchanging $k$th and $p$th column if necessary.

The simplest way is to choose the element in the same column, that is below the diagonal and has the largest absolute value; that is, we choose $p$ such that,

$$a_{pk}^{(k)} = \max_{k \leq i \leq n} \left| a_{ik}^{(k)} \right|$$

Then perform $E_k \longleftrightarrow E_p$. In this case no interchange of column is necessary.

**Solution.**

$$E_1 : 0.003x_1 + 59.140x_2 = 59.17$$
$$E_2 : \quad 5.291x_1 - 6.130x_2 = 46.78$$

By the pivot Strategy: Find $(k = 1)$

$$\begin{aligned} \max\left\{ \left| a_{11}^{(1)} \right|, \left| a_{21}^{(1)} \right| \right\} &= \max\left\{ |1.003|, |5.291| \right\} \\ &= 5.291 \\ &= a_{21}^{(1)} \end{aligned}$$

The operation $E_2 \longleftrightarrow E_1$ is performed to give the system

$$E_1 \qquad 5.291x_1 - 6.13x_2 = 46.78$$
$$E_2 : 0.003x_1 + 59.140x_2 = 59.17$$

The multiplier for this system is

$$m = \frac{a_{21}^{(1)}}{a_{11}^{(1)}} = \frac{0.003}{5.291} = 0.000\,567$$

and the operation $(E_2 - mE_1) \to E_2'$ reduces the system to

$$\begin{aligned} E_1' &: 5.29x_1 - 6.130x_2 = 46.78 \\ E_2' &: \qquad\qquad 59.14x_2 = 59.14 \end{aligned}$$

Then by back substitution $x_2 = 1.000$, $x_1 = 10.00$.
Which is the correct solution.

This technique is known as maximal-column pivoting or partial pivoting.

**Problem 5.3.2.** Solve the following system using 4 digits arithmetic, once with the 1st equation as pivot equation and then 2nd equation as pivot equation and then compare the results with exact solution $x_1 = 1.00$, $x_2 = 0.2500$.

$$\begin{aligned} E_1 &: 0.1410 \times 10^{-2}x_1 + 0.400\,4 \times 10^{-1}x_2 = 0.114\,2 \times 10^{-1} \\ E_2 &: \quad 0.200\,0 \times 10^{0}x_1 + 0.491\,2 \times 10^{1}x_2 = 0.142\,8 \times 10^{1} \end{aligned}$$

## 5.4 Gauss-Seidal Iterative Method

An iterative technique here starts with an initial approximation $X^{(0)}$ of the solution $X$ and generates a sequence of vectors $\left\{X^{(k)}, k = 0, 1, 2, \dots\right\}$ that converges to $X$.

In this case first we transform the system $AX = B$ into an equivalent system of the form $X = TX + C$ for some $n \times n$ matrix $T$ and a vector $C$ and we suppose

$$\left.\begin{array}{lll} E_1: & x_1 = -\dfrac{a_{12}}{a_{11}}x_2 - \dfrac{a_{13}}{a_{11}}x_3 - \cdots - \dfrac{a_{1n}}{a_{11}}x_n + \dfrac{b_1}{a_{11}} \\ E_2: & x_2 = -\dfrac{a_{21}}{a_{22}}x_1 - \dfrac{a_{23}}{a_{22}}x_3 - \cdots - \dfrac{a_{2n}}{a_{22}}x_n + \dfrac{b_2}{a_{22}} \\ E_2: & x_3 = -\dfrac{a_{31}}{a_{33}}x_1 - \dfrac{a_{32}}{a_{34}}x_4 - \cdots - \dfrac{a_{3n}}{a_{33}}x_n + \dfrac{b_3}{a_{33}} \\ \dots & \dots \quad \dots \quad \dots \quad \dots \\ E_n: & x_n = -\dfrac{a_{na}}{a_{nn}}x_1 - \dfrac{a_{n2}}{a_{nn}}x_2 - \cdots - \dfrac{a_{n\cdot n-1}}{a_{nn}}x_{n-1} + \dfrac{b_n}{a_{nn}} \end{array}\right\} \tag{5.32}$$

In this case, it is reasonable to compute $x_i^{(k)}$ using these most recently calculated values i.e.,

1. First substitute $x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}$ in the first equation $E_1$ in the right-hand side of (5.32) and we get the new value $x_1^{(1)}$.

2. Then substitute $x_1^{(1)}, x_2^{(0)}, x_3^{(0)} \dots, x_n^{(0)}$ in the second equation $E_2$ in the right-hand side of (5.32) and we get the new value $x_2^{(1)}$.

3. Then substitute $x_1^{(1)}, x_2^{(1)}, x_3^{(0)} \dots, x_n^{(0)}$ in the third equation $E_3$ in the right-hand side of (5.32) and we get the new value $x_3^{(1)}$.

4. Continuing in this way we put $x_1^{(1)}, x_2^{(1)}, \ldots, x_n^{(0)}$ in the last equation of (5.32)

Then the first iteration is complete.
Repeat the entire process till $(x_1, x_2, \ldots, x_n)$ is obtained.
This method is known as Gauss-Seidal iterative method.

**Problem 5.4.1.** Solve the system

$$\left.\begin{aligned} 10x_1 - x_2 + 2x_3 &= 6 \\ -x_1 + 11x_2 - x_3 + 3x_4 &= 25 \\ 2x_1 - x_2 + 10x_3 - x_4 &= -11 \\ 3x_2 - x_3 + 8x_4 &= 15 \end{aligned}\right\} \tag{5.33}$$

using Gauss-Seidal method.

**Solution.** The given system can be written as

$$\begin{aligned} E_1 &: \quad x_1 = \frac{1}{10}x_2 - \frac{2}{10}x_3 + \frac{6}{10} \\ E_2 &: \quad x_2 = \frac{1}{11}x_1 + \frac{1}{11}x_3 - \frac{3}{11}x_4 + \frac{25}{11} \\ E_3 &: \quad x_3 = -\frac{2}{10}x_1 + \frac{1}{10}x_2 + \frac{1}{10}x_4 - \frac{11}{10} \\ E_4 &: \quad x_4 = -\frac{3}{8}x_2 + \frac{1}{8}x_3 + \frac{15}{8} \end{aligned}$$

which is of the form $X = TX + C$
Where,

$$T = \begin{pmatrix} 0 & \frac{1}{10} & \frac{-2}{10} & 0 \\ \frac{1}{11} & 0 & \frac{1}{11} & \frac{-3}{11} \\ \frac{-2}{10} & \frac{1}{10} & 0 & \frac{1}{10} \\ 0 & \frac{-3}{8} & \frac{1}{8} & 0 \end{pmatrix}$$

and

$$C = \begin{pmatrix} \frac{6}{10} \\ \frac{25}{11} \\ -\frac{11}{10} \\ \frac{15}{8} \end{pmatrix}$$

Suppose the initial approximation is $X^{(0)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

from $X^{(1)} = TX^{(0)} + C \Rightarrow X^{(1)} = \begin{pmatrix} \frac{6}{10} \\ \\ \frac{25}{11} \\ \\ -\frac{11}{10} \\ \\ \frac{15}{8} \end{pmatrix}$.

Similarly, we calculate the other approximation which are shown in the following iteration table

| k→ | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|---|
| $x_1^{(k)}$ | 0 | 0.6000 | 1.0302 | 1.0066 | 1.0004 | 1.0001 | 1.0000 |
| $x_2^{(k)}$ | 0 | 2.3273 | 2.0370 | 2.0036 | 2.0003 | 2.0000 | 2.0000 |
| $x_3^{(k)}$ | 0 | $-0.9873$ | $-1.0145$ | $-1.0025$ | $-1.0003$ | $-1.0000$ | $-1.0000$ |
| $x_4^{(k)}$ | 0 | 0.8789 | 0.4843 | 0.9984 | 0.9998 | 1.0000 | 1.0000 |

Therefore, the required solution is

$$X = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ -1 \\ 1 \end{pmatrix}$$

**Problem 5.4.2.** Solve the following system by Gauss-Seidal method

$$\begin{aligned} 21x_1 + 6x_2 - x_3 &= 85 \\ 6x_1 + 15x_2 + 2x_3 &= 72 \\ x_1 + x_2 + 54x_3 &= 110 \end{aligned}$$

# Chapter 6

# System of Linear Equations

## 6.1 Introduction

System of linear equations occur in a variety of applications in the fields like elasticity, electrical engineering, statistical analysis. The techniques and methods for solving system of linear equations belong to two categories: direct and iterative methods.

Some of the direct methods are Gauss elimination method, matrix inverse method, LU factorization and Cholesky method. Elimination approach reduces the given system of equations to a form from which the solution can be obtained by simple substitution. Since calculators and computers have some limit to the number of digits for their use. This may lead to round off errors and produces poorer results. It will be assumed that readers are familiar with some of the direct methods suitable for small systems. Handling of large systems are also time-consuming.

Iterative methods provide an alternative to the direct methods for solving system of linear equations. This method involves assumptions of some initial values which are then refined repeatedly till they reach some accepted range of accuracy.

In this chapter we shall consider Gauss elimination method and iterative methods suitable for numerical calculations.

## 6.2 Linear System of Equations

Consider a system of $n$ linear equations in the $n$ unknowns $x_1, x_2, \ldots, x_n$

$$\begin{aligned} E_1:&\ \ a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ E_2:&\ \ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\ & \qquad\qquad \ldots \quad \ldots \quad \ldots = \ldots \\ E_n:&\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n \end{aligned} \tag{6.1}$$

Where $a_{ij}, b_i \in \mathbb{R}$

Exactly one of the following three cases must occur:

(a) The system has a unique solution.

(b) The system has no solution.

(c) The system has an infinite number of solutions.

In matrix notation, we can write the system as

$$AX = B \tag{6.2}$$

where

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} = (a_{ij})$$

$$X = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}^\top$$

$$B = \begin{bmatrix} b_1 & b_2 & \dots & b_n \end{bmatrix}^\top$$

The solution of the system exists and is unique if $|A| \neq 0$.
The solution (6.2) may then be written as

$$X = A^{-1}B$$

where $A^{-1}$ is the inverse of $A$.

## 6.3 Method of Elimination

*Equivalent Systems:* Two systems of equations are called equivalent if and only if they have the same solution set.

*Elementary Transformations:* A system of equations is transformed into an equivalent system if the following elementary operations are applied on the system:

1. two equations are interchanged
2. an equation is multiplied by a non-zero constant
3. an equation is replaced by the sum of that equation and a multiple of any other equation.

*Gaussian Elimination*

The process which eliminates an unknown from succeeding equations using elementary operations is known as Gaussian elimination.
The equation which is used to eliminate an unknown from the succeeding equations is known as the *pivotal equation*. The coefficient of the eliminated variable in a pivotal equation is known as the *pivot*. If the pivot is zero, it cannot be used to eliminate the variable from the other equations. However, we can continue the elimination process by interchanging the equation with a nonzero pivot.

*Solution of a Linear System*

A systematic procedure for solving a linear system is to reduce a system that is easier to solve. One such system is the echelon form. The *back substitution* is then used to solve the system in reverse order.

A system is in *echelon form* or *upper triangular form* if

(i) all equations containing nonzero terms are above any equation with zeros only.

(ii) The first nonzero term in every equation occurs to the right of the first nonzero term in the equation above it.

## 6.4 Pivotal Elimination Method

Computers and calculators use fixed number of digits in its calculation and we may need to round the numbers. This introduces error in the calculations. Also, when two nearly equal numbers are subtracted, the accuracy in the calculation is lost. To reduce the propagation of errors, pivoting strategy is to be used.

### 6.4.1 Partial Pivoting (Partial Column Pivoting)

In partial pivoting, at any time we use the maximum magnitude of coefficient of the eliminating variable as the pivot. The process is continued for resulting subsystems. Pivotal equation is divided throughout by the pivot to reduce to build up large coefficients when solving a system. The method is illustrated with an example.

**Example.** Solve the following linear system by the Gaussian elimination with partial pivoting, giving your answers to 3 decimal places. $5x + 12y + 9z = 5, 8x + 11y + 20z = 35, 16x + 5y + 7z = 29$

Taking first equation as the pivotal equation we can write the system as

| | Coefficient of | | | | | |
|---|---|---|---|---|---|---|
| Operation | $x$ | $y$ | $z$ | R.H.S | Eq. # | Check sum |
| | 16.0000 | 5.0000 | 7.0000 | 29.0000 | Eq1 | 57.0000 |
| | 5.0000 | 12.0000 | 9.0000 | 5.0000 | Eq2 | 31.0000 |
| | 8.0000 | 11.0000 | 20.0000 | 35.0000 | Eq3 | 74.0000 |
| Eq 1/16 | 1.0000 | 0.3125 | 0.4375 | 1.8125 | Eq4* | 3.5625 |
| Eq 2/5 | 1.0000 | 2.4000 | 1.8000 | 1.0000 | Eq5 | 6.2000 |
| Eq 3/8 | 1.0000 | 1.3750 | 2.5000 | 4.3750 | Eq6 | 9.2500 |
| Eq 5 - Eq 4 | | 2.0875 | 1.3625 | −0.8125 | Eq7 | 2.6375 |
| Eq 6 - Eq 4 | | 1.0625 | 2.0625 | 2.5625 | Eq8 | 5.6875 |
| Eq 7/2.0875 | | 1.0000 | 0.6527 | −0.3892 | Eq9* | 1.2635 |
| Eq 8/1.0625 | | 1.0000 | 1.9412 | 2.4118 | Eq10 | 5.3530 |
| Eq 10 - Eq 9 | | | 1.2885 | 2.8010 | Eq11* | 4.0895 |

Solution of the system is obtained by the back substitution as follows:

$$z = 2.8010/1.2885 = 2.1738$$
$$y = -0.3892 - 0.6527 \times 2.1738 = -1.8080$$
$$x = 1.8124 - 0.3125 \times (-1.8080) - 0.4375 \times 2.1738 = 1.4264$$

To check the calculations an extra column headed by *check sum* is included which is the sum of the numbers in the row. It is also worked out in exactly the same way as the other numbers in the line.

### 6.4.2 Total Pivoting

Partial pivoting is adequate for most of the simultaneous equations which arise in practice. But we may encounter sets of equations where wrong or incorrect solutions may occur. To improve the calculation in such cases total pivoting is used. In total pivoting, maximum magnitude of the coefficients is used for the pivot in each case.

**Example.** Solve the system of equation from previous example using total pivoting.

| | Coefficient of | | | | | |
|---|---|---|---|---|---|---|
| Operation | $x$ | $y$ | $z$ | R.H.S | Eq. # | Check sum |
| | 5.0000 | 12.0000 | 9.0000 | 5.0000 | Eq1 | 31.0000 |
| | 8.0000 | 11.0000 | 20.0000 | 35.0000 | Eq2 | 74.0000 |
| | 16.0000 | 5.0000 | 7.0000 | 29.0000 | Eq3 | 57.0000 |
| Eq 2/20 | 0.4000 | 0.5500 | 1.0000 | 1.7500 | Eq4* | 3.7000 |
| Eq 3/7 | 0.2857 | 0.7143 | 1.0000 | 4.1429 | Eq5 | 8.1429 |
| Eq 1/9 | 0.5556 | 1.3333 | 1.0000 | 0.5556 | Eq6 | 3.4445 |
| Eq 5 - Eq 4 | 1.8857 | 0.1643 | 0.0000 | 2.3929 | Eq7 | 4.4429 |
| Eq 6 - Eq 4 | 0.1556 | 0.7833 | 0.0000 | $-1.1944$ | Eq8 | $-0.2555$ |
| Eq 7/1.8857 | 1.0000 | 0.0871 | 0.0000 | 1.2690 | Eq9* | 2.3561 |
| Eq 8/0.1556 | 1.0000 | 5.0341 | 0.0000 | $-7.6761$ | Eq10 | $-1.6420$ |
| Eq 10 - Eq 9 | 0.0000 | 4.9470 | 0.0000 | $-8.9451$ | Eq11* | $-3.9981$ |

Solution of the system is

$$y = \frac{-8.9451}{4.94470} = -1.8082$$
$$x = 1.2690 - 0.0871 \times (-1.8082) = 1.4265$$
$$z = 1.7500 - 0.4000 \times 1.4265 - 0.5500 \times (-1.8042) = 2.1739$$

Solutions of the system are summarized below for comparison

| | Using Maxima | with Partial Pivoting | with Total Pivoting |
|---|---|---|---|
| $x$ | 1.4265 | 1.4264 | 1.4265 |
| $y$ | $-1.8081$ | $-1.8080$ | $-1.8082$ |
| $z$ | 2.1739 | 2.1738 | 2.1739 |

## 6.5 Solution by Triangular Factorization

In Gaussian elimination process, a linear system is reduced to an upper-triangular system and then solved by backward substitution. The linear system $AX = B$ can effectively be solved by expressing the coefficient matrix $A$ as the product of a lower-triangular matrix $L$ and an upper-triangular matrix $U$ :

$$A = LU$$

When this is possible we say that $A$ has an LU-decomposition. In this case the equation can be written as

$$LUX = B$$

and the solution can be obtained by defining $Y = UX$ and then solving the two systems

(i) $LY = B$ for $Y$, and

(ii) $UX = Y$ for $X$.

LU-decomposition of a non-singular matrix (when it exists) is not unique.
For example,

$$\begin{array}{ccccc}
A & & L & & U \\
\begin{pmatrix} 2 & 0 & -2 \\ 2 & 1 & -3 \\ 4 & -1 & 5 \end{pmatrix} & = & \begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 2 & -2 & 1 \end{pmatrix} & & \begin{pmatrix} 0 & 0 & -2 \\ 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & 8 \end{pmatrix} \\
 & = & \begin{pmatrix} 2 & 0 & 0 \\ 2 & 1 & 0 \\ 4 & -1 & 8 \end{pmatrix} & & \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix} \\
 & = & \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -1 & 1 \end{pmatrix} & & \begin{pmatrix} 2 & 0 & -2 \\ 0 & 1 & -1 \\ 0 & 0 & 8 \end{pmatrix} \\
 & & \text{and so on} & &
\end{array}$$

It can be shown that the non-singular matrix $B = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 1 \\ -1 & 0 & 2 \end{pmatrix}$ cannot be decomposed into LU form. But by interchanging 2nd and 3rd row the resulting matrix can be factored as follows:

$$\begin{pmatrix} 1 & 2 & 3 \\ -1 & 0 & 2 \\ 2 & 4 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 2 & 0 \\ 2 & 0 & -5 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & \frac{5}{2} \\ 0 & 0 & 1 \end{pmatrix}$$

To check for the LU-decomposition, we may use the idea of principal minor of the matrix.

*Principal Minor:* The $r$th principal minor of a square matrix $A$ is the determinant of the sub-matrix $A_r$ formed by the first $r$ rows and $r$ columns of $A$.

Consider the $n \times n$ matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3n} \\ \dots & \dots & \dots & \ddots & \dots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{pmatrix}$$

The first principal minor of $A$ is $\quad \left|A_1\right| = \left|a_{11}\right|$

The second principal minor of $A$ is $\quad \left|A_2\right| = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}$

The third principal minor of $A$ is $\quad \left|A_3\right| = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$

and so on.

*Theorem* 6.5.1. Let $A$ be an invertible $n \times n$ matrix (non-singular). Then $A$ has an LU-factorization if and only if all the principal minors $\left|A_r\right|$, $r = 1, 2, 3, \ldots, n$ are non-zero.

In matrix $A = \begin{pmatrix} 2 & 0 & -2 \\ 2 & 1 & -3 \\ 4 & -1 & 5 \end{pmatrix}$, the principal minors are

$$\left|A_1\right| = \left|2\right| = 2, \qquad \left|A_2\right| = \begin{vmatrix} 2 & 0 \\ 2 & 1 \end{vmatrix} = 2, \qquad \left|A_3\right| = \begin{vmatrix} 2 & 0 & -2 \\ 2 & 1 & -3 \\ 4 & -1 & 5 \end{vmatrix} = 16$$

and hence $A$ has LU-decomposed. In matrix $B = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 1 \\ -1 & 0 & 2 \end{pmatrix}$ the principal minors are,

$$\left|B_1\right| = \left|1\right| = 1, \qquad \left|B_2\right| = \begin{vmatrix} 1 & 2 \\ 2 & 4 \end{vmatrix} = 0$$

are not non-zero and hence $B$ has no LU-decomposition.

### 6.5.1 Solution by LU-factorization

For unique factorization we may impose conditions on the elements of $L$ and $U$. In particular, if all the diagonal elements of $L$ are 1, it is called a *Doolittle factorization* and if all the diagonal elements of $U$ are 1, then it is called a *Crout factorization*. This may be used for a unique factorization.

***Crout's factorization*** method is explained by the following example:

**Problem 6.5.1.** Given that

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 4 & 11 \\ 5 & 14 & 12 \end{pmatrix}, \quad B = \begin{pmatrix} 5 \\ 21 \\ 15 \end{pmatrix}, \quad X = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

(i) Determine a lower triangular matrix $L$ and an upper triangular matrix $U$ such that $LU = A$.

(ii) Use the above factorization to solve the equation $AX = B$.

**Solution.** (i) Let,

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 4 & 11 \\ 5 & 14 & 12 \end{pmatrix} = LU = \begin{pmatrix} a & 0 & 0 \\ b & c & 0 \\ d & e & f \end{pmatrix} \begin{pmatrix} 1 & l & m \\ 0 & 1 & n \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} a & al & am \\ b & bl + c & bm + cn \\ d & dl + e & dm + en + f \end{pmatrix}$$

Equating the corresponding elements of the two matrices we have,

$$
\begin{aligned}
&a = 1 \\
&b = 3 \\
&d = 5 \\
&al = 2 && \text{or,} \quad l = \frac{2}{1} = 2 \\
&am = 3 && \text{or,} \quad m = \frac{3}{1} = 2 \\
&bl + c = 4 && \text{or,} \quad c = 4 - 3(2) = -2 \\
&dl + e = 14 && \text{or,} \quad e = 14 - 5(2) = 4 \\
&bm + cn = 11 && \text{or,} \quad n = \frac{11 - 3(3)}{-2} = -1 \\
&dm + en + f = 12 && \text{or,} \quad f = 12 - 5(3) - 4(-1) = 1
\end{aligned}
$$

Thus,

$$
L = \begin{pmatrix} 1 & 0 & 0 \\ 3 & -2 & 0 \\ 5 & 4 & 1 \end{pmatrix} \qquad U = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix}
$$

(ii) The equation can be written as

$$
AX = LUX = LY = B
$$

Where,

$$
UX = Y \qquad \text{and } Y = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}
$$

Consider the solution of

$$
\begin{aligned}
&LY = B \\
\Rightarrow &\begin{pmatrix} 1 & 0 & 0 \\ 3 & -2 & 0 \\ 5 & 4 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 5 \\ 21 \\ 15 \end{pmatrix}
\end{aligned}
$$

Using forward elimination, we have,

$$
y_1 = 5, \quad y_2 = -3, \quad y_3 = 2
$$

Now consider the solution of,

$$
\begin{aligned}
&UX = Y \\
\Rightarrow &\begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 5 \\ -3 \\ 2 \end{pmatrix}
\end{aligned}
$$

Using backward elimination, we have

$$
x = 1, \quad y = -1, \quad z = 2
$$

and hence

$$
X = \begin{pmatrix} 1 \\ -1 \\ 2 \end{pmatrix}
$$

### 6.5.2 Positive Definite

*Quadratic Forms:* A quadratic form $Q$ in $n$-unknowns is

$$Q = a_{11}x_1^2 + a_{12}x_1x_2 + a_{13}x_1x_3 + \cdots + a_{n,n-1}x_nx_{n-1} + a_{n,n}x_n^n = \sum_{1\le i,j\le n} a_ia_jx_ix_j$$

may be written in matrix representation as

$$Q = x^\top Ax$$

where $x = (x_1, x_2, x_3, \ldots, x_n)^\top$ and $A = (a_{ij})$, the $n \times n$ matrix.
For example, the quadratic form $x^2 - 6xy$ can be written as

$$x^2 - 6xy = \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 1 & -2 \\ -4 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

This can also be written as

$$x^2 - 6xy = \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 1 & -3 \\ -3 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

Note that in the second representation the matrix is symmetric.

*Positive definite:* A matrix $A$ is positive definite if its quadratic form is greater than zero for all non-zero vector $x$, i.e. $x^\top Ax > 0$.

It is hard to check the positive definiteness using this definition. Direct verification using definition is considered for the simple cases of $2 \times 2$ matrices.

**Example.** Show that the matrix $A = \begin{pmatrix} 1 & 1 \\ 2 & 3 \end{pmatrix}$ is positive definite but $B = \begin{pmatrix} 1 & 5 \\ -1 & 1 \end{pmatrix}$ is not.

Consider

$$\begin{aligned} x^\top Ax &= \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = x^2 + 3xy + 3y^2 \\ &= \left(x + \frac{3}{2}y\right)^2 + \frac{3}{4}y^2 > 0 \qquad \text{for all non-zero } x. \end{aligned}$$

Thus, $A$ is positive definite. Principal minors of $A$ are

$$\left|A_1\right| = \left|1\right| = 1 \quad \text{and} \left|A_2\right| = \begin{vmatrix} 1 & 1 \\ 2 & 3 \end{vmatrix} = 1$$

both are positive and non-zero. Now consider

$$\begin{aligned} x^\top Bx &= \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 1 & 5 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = x^2 + 4xy + 3y^2 \\ &= (x+y)^2 + 2xy = -5 \qquad \text{for } x = 2 \text{ and } y = -1. \end{aligned}$$

Thus, $B$ is not positive definite. Principal minors of $B$ are

$$\left|B_1\right| = \left|1\right| = 1 \quad \text{and} \left|B_2\right| = \begin{vmatrix} 1 & 5 \\ -1 & 1 \end{vmatrix} = 6$$

both are positive and non-zero. Note that positive values of principal minors does not imply positive definiteness.

**Example.** Show that the symmetric matrix $A = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$ is positive definite but $B = \begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix}$ is not.

Consider

$$\begin{aligned} x^\top Ax &= \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 2x^2 + 2xy + 3y^2 \\ &= 2\left(x + \frac{1}{2}y\right)^2 + \frac{5}{2}y^2 > 0 \qquad \text{for all non-zero } x. \end{aligned}$$

Thus, $A$ is positive definite.
Principal minors of A are

$$\left|A_1\right| = \left|2\right| = 2 \quad \text{and} \left|A_2\right| = \begin{vmatrix} 2 & 1 \\ 1 & 3 \end{vmatrix} = 5$$

both are positive and non-zero.
Now consider

$$\begin{aligned} x^\top Bx &= \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = x^2 + 4xy + 3y^2 \\ &= -1 \qquad \text{for } x = 2 \text{ and } y = -1. \end{aligned}$$

Thus, $B$ is not positive definite. Principal minors of B are

$$\left|B_1\right| = \left|1\right| = 1 \quad \text{and} \left|B_2\right| = \begin{vmatrix} 1 & 2 \\ 2 & 3 \end{vmatrix} = -1$$

Not that all the principal minors are not positive and hence it is not positive definite.

*Remark.* Any quadratic form can be represented by a symmetric matrix.

*Theorem* 6.5.2. A symmetric matrix A is positive definite if and only if all its principal minors are strictly positive.

**Definition 1.** A symmetric matrix $A$ and the quadratic form $x^\top Ax$ are called

| | |
|---|---|
| positive semi-definite | if $x^\top Ax \geq 0$ for all $x$ |
| negative definite | if $x^\top Ax < 0$ for $x \neq 0$ |
| negative semi-definite | if $x^\top Ax \leq 0$ for all $x$ |
| indefinite | if $x^\top Ax$ has both positive and negative values. |

### 6.5.3 Solution by Cholesky Factorization

A symmetric positive definite matrix $A$ may be decomposed into

$$A = LL^\top$$

This is the Cholesky decomposition.
The solution of a linear system $AX = B$ with $A$ symmetric and positive definite can be obtained by first computing the Cholesy decomposition $A = LL^\top$, then solving $LY = B$ for $Y$ and finally solving

$L^\top X = Y$ for $X$.
In this case the inverse $A^{-1}$ can be obtained as follows:

$$A^{-1} = \left(LL^\top\right)^{-1} = \left(L^\top\right)^{-1} L^{-1} = \left(L^{-1}\right)^\top L^{-1}$$

Recall that inverse of a lower triangular matrix is also a lower triangular matrix. This property may be used to find $L^{-1}$.
For a third order lower triangular matrix L, we may write the relation $LL^{-1} = I$ as

$$\begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{11} & l_{22} & l_{33} \end{pmatrix} \begin{pmatrix} b_{11} & 0 & 0 \\ b_{21} & b_{22} & 0 \\ b_{11} & b_{22} & b_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Comparing two sides we may then find the unknowns $b_{ij}$. Then use the relation

$$A^{-1} = \left(L^{-1}\right)^\top L^{-1}$$

to find $A^{-1}$.

**Problem 6.5.2.** Solve the following system of equations

$$x + 3y + 5z = 10, \quad 3x + 13y + 23z = 46, \quad 5x + 23y + 45z = 94$$

by the Cholesky decomposition.
Find the inverse of the coefficient matrix using Cholesky factor.

**Solution.** In matrix notation, the equation can be written as

$$\begin{aligned} & AX = B \\ \text{or,} \quad & \begin{pmatrix} 1 & 3 & 5 \\ 3 & 13 & 23 \\ 5 & 23 & 45 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 10 \\ 46 \\ 94 \end{pmatrix} \end{aligned}$$

Here the matrix $A$ is symmetric and positive definite. Thus, $A$ can be factorized into $\mathbf{A} = \mathbf{L}\mathbf{L}^\top$.

$$\begin{aligned} \begin{pmatrix} 1 & 3 & 5 \\ 3 & 13 & 23 \\ 5 & 23 & 45 \end{pmatrix} &= \begin{pmatrix} a & 0 & 0 \\ b & d & 0 \\ c & e & f \end{pmatrix} \begin{pmatrix} a & b & c \\ 0 & d & e \\ 0 & 0 & f \end{pmatrix} \\ &= \begin{pmatrix} a^2 & ab & ac \\ ab & b^2 + d^2 & bc + de \\ ac & bc + de & c^2 + e^2 + f^2 \end{pmatrix} \end{aligned}$$

Equating like elements, we have

$$\begin{aligned} & a^2 = 1 && \text{or,} \quad a = 1 \\ & ab = 3 && \text{or,} \quad b = 3 \\ & ac = 5 && \text{or,} \quad c = 5 \\ & b^2 + d^2 = 13 && \text{or,} \quad d = 2 \\ & bc + de = 23 && \text{or,} \quad e = 4 \\ & c^2 + e^2 + f^2 = 45 && \text{or,} \quad f = 2 \end{aligned}$$

Thus,

$$\mathbf{L} = \begin{pmatrix} 1 & 0 & 0 \\ 3 & 2 & 0 \\ 5 & 4 & 2 \end{pmatrix}$$

The equation can be written as

$$\mathbf{L}\mathbf{L}^\top\mathbf{X} = \mathbf{B} \quad \text{or } \mathbf{L}\mathbf{Y} = \mathbf{B} \quad \text{where } \mathbf{L}^\top\mathbf{X} = \mathbf{Y}$$

$$\mathbf{L}\mathbf{Y} = \begin{pmatrix} 1 & 0 & 0 \\ 3 & 2 & 0 \\ 5 & 4 & 2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \mathbf{B} = \begin{pmatrix} 10 \\ 46 \\ 94 \end{pmatrix}$$

Using forward elimination, we have

$$y_1 = 10, \qquad y_2 = 8, \qquad y_3 = 6$$

Now consider the solution of $\mathbf{L}^\top\mathbf{X} = \mathbf{Y}$.

$$\begin{pmatrix} 1 & 3 & 5 \\ 0 & 2 & 4 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 10 \\ 8 \\ 6 \end{pmatrix}$$

Using backward elimination, we have

$$z = 3, \qquad y = -2, \qquad x = 1$$

Inverse of the matrix $\mathbf{A}$ can be obtained from the relation $\mathbf{A}^{-1} = \left(\mathbf{L}^{-1}\right)^\top \mathbf{L}^{-1}$.
Note that the inverse of a triangular matrix is also a triangular matrix.
Thus, we may use the relation

$$\mathbf{L}\mathbf{L}^{-1} = \mathbf{I}$$

$$\text{or,} \quad \begin{pmatrix} 1 & 0 & 0 \\ 3 & 2 & 0 \\ 5 & 4 & 2 \end{pmatrix} \begin{pmatrix} l & 0 & 0 \\ m & p & 0 \\ n & q & r \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\text{or,} \quad \begin{pmatrix} l & 0 & 0 \\ 3l + 2m & 2p & 0 \\ 5l + 4m + 2n & 4p + 2q & 2r \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Equating like elements, we have

$$\begin{aligned}
&l = 1 \\
&p = \tfrac{1}{2} \\
&r = \tfrac{1}{2} \\
&3l + 2m = 0 && \text{or} \quad m = -\tfrac{3}{2} \\
&5l + 4m + 2n = 0 && \text{or} \quad n = \tfrac{1}{2} \\
&4p + 2q = 0 && \text{or} \quad q = -1
\end{aligned}$$

Thus,

$$\mathbf{L}^{-1} = \frac{1}{2}\begin{pmatrix} 2 & 0 & 0 \\ -3 & 1 & 0 \\ 1 & -2 & 1 \end{pmatrix}$$

Using the relation $\mathbf{A}^{-1} = (\mathbf{L}^{-1})^{\top}\mathbf{L}^{-1}$, we have

$$\mathbf{A}^{-1} = \frac{1}{2}\begin{pmatrix} 2 & -3 & 1 \\ 0 & 1 & -2 \\ 0 & 0 & 1 \end{pmatrix} \times \frac{1}{2}\begin{pmatrix} 2 & 0 & 0 \\ -3 & 1 & 0 \\ 1 & -2 & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 14 & -5 & 1 \\ -5 & 5 & -2 \\ 1 & -2 & 1 \end{pmatrix}$$

## 6.6 Solution of Linear System by Iterative Method

Iterative method for linear system is similar as the method of fixed-point iteration for an equation in one variable, To solve a linear system by iteration, we solve each equation for one of the variables, in turn, in terms of the other variables. Starting from an approximation to the solution, if convergent, derive a new sequence of approximations. Repeat the calculations till the required accuracy is obtained. An iterative method converges, for any choice of the first approximation, if every equation satisfies the condition that the magnitude of the coefficient of solving variable is greater than the sum of the absolute values of the coefficients of the other variables. A system satisfying this condition is called diagonally dominant. A linear system can always be reduced to diagonally dominant form by elementary operations.

For example in the following system, we have

$$\begin{aligned} 12x - 2y + 5z &= 20 \qquad (E1) \qquad & |12| &> |-2| + |5| \\ 4x + 5y + 11z &= 8 \qquad (E2) \qquad & |5| &< |4| + |11| \\ 7x + 12y + 10z &= 27 \qquad (E3) \qquad & |10| &< |7| + |12| \end{aligned}$$

and is not diagonally dominant. Rearranging as $(E1), (E3) - (E2), (E2)$, we have

$$\begin{aligned} &12x - 2y + 5z = 20 \qquad & |12| &> |-2| + |5| \\ &3x + 7y - z = 19 \qquad & |7| &> |3| + |-1| \\ &4x + 5y + 11z = 8 \qquad & |11| &> |4| + |5| \end{aligned}$$

The system reduces to diagonally dominant form.
Two commonly used iterative process are discussed below:

### 6.6.1 Jacobi Iterative Method:

In this method, a fixed set of values is used to calculate all the variables and then repeated for the next iteration with the values obtained previously. The iterative formulas of the above system are

$$\begin{aligned} x_{n+1} &= \frac{1}{12}\left(20 + 2y_n - 5z_n\right) \\ y_{n+1} &= \frac{1}{7}\left(19 - 3x_n + z_n\right) \\ z_{n+1} &= \frac{1}{11}\left(8 - 4x_n - 5y_n\right) \end{aligned}$$

Starting with initial values

$$x_0 = 0, \quad y_0 = 0, \quad z_0 = 0$$

we get

$$x_1 = \frac{1}{12}[20 + 0 + 0] = 1.67$$
$$y_1 = \frac{1}{7}[19 + 0 + 0] = 2.71$$
$$z_1 = \frac{1}{11}[8 + 0 + 0] = 0.73$$

Second approximation is

$$x_2 = \frac{1}{12}[20 + 2(2.71) - 5(0.73)] = 1.81$$
$$y_2 = \frac{1}{7}[19 - 3(1.67) + 0.73] = 2.10$$
$$z_2 = \frac{1}{11}[8 - 4(1.67) - 5(2.71)] = -1.11$$

and so on. Results are summarized below.

| $n$ | 0 | 1 | 2 | 3 | 4 | ... | 9 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|
| $x_n$ | 0 | 1.67 | 1.81 | 2.48 | 2.33 | ... | 2.29 | 2.29 | 2.29 |
| $y_n$ | 0 | 2.71 | 2.10 | 1.78 | 1.52 | ... | 1.62 | 1.61 | 1.61 |
| $z_n$ | 0 | 0.73 | −1.11 | −0.89 | −0.98 | ... | −0.84 | −0.84 | 0.84 |

Table 6.1: Successive iterates of solution (Jacobi Method)

### 6.6.2 Gauss-Seidel Iterative Method:

In this method, the values of each variable is calculated using the most recent approximations to the values of the other variables. The iterative formulas of the above system are

$$x_{n+1} = \frac{1}{12}\left(20 + 2y_n - 5z_n\right)$$
$$y_{n+1} = \frac{1}{7}\left(19 - 3x_{n+1} + z_n\right)$$
$$z_{n+1} = \frac{1}{11}\left(8 - 4x_{n+1} - 5y_{n+1}\right)$$

Starting with initial values

$$x_0 = 0, \quad y_0 = 0, \quad z_0 = 0$$

we get the solutions as follows:
First approximation:

$$x_1 = \frac{1}{12}[20 + 0 + 0] = 1.67$$
$$y_1 = \frac{1}{7}[19 - 3(1.67) + 0] = 2.00$$
$$z_1 = \frac{1}{11}[8 - 4(1.67) - 5(2)] = -0.79$$

Second approximation:

$$
\begin{aligned}
x_2 &= \frac{1}{12}[20 + 2(2.00) - 5(-0.79)] = 2.33 \\
y_2 &= \frac{1}{7}[19 - 3(2.33) - 0.79] = 1.60 \\
z_2 &= \frac{1}{11}[8 - 4(2.33) - 5(1.60)] = -0.89
\end{aligned}
$$

Third approximation:

$$
\begin{aligned}
x_3 &= \frac{1}{12}[20 + 2(1.60) - 5(-0.85)] = 2.29 \\
y_3 &= \frac{1}{7}[19 - 3(2.29) - 0.85] = 1.61 \\
z_3 &= \frac{1}{11}[8 - 4(2.29) - 5(1.61)] = -0.84
\end{aligned}
$$

Fourth approximation:

$$
\begin{aligned}
x_4 &= \frac{1}{12}[20 + 2(1.61) - 5(-0.84)] = 2.29 \\
y_4 &= \frac{1}{7}[19 - 3(2.29) - 0.84] = 1.61 \\
z_4 &= \frac{1}{11}[8 - 4(2.29) - 5(1.61)] = -0.84
\end{aligned}
$$

which gives the results correct to 2 decimal point.
It can be observed that the Gauss-Seidel method converges twice as fast as the Jacobi method.

## 6.7 Exercise

1. The linear system

$$
\begin{aligned}
0.003x + 71.08y &= 71.11 \\
4.231x - 8.16y &= 34.15
\end{aligned}
$$

   has the exact solution $x = 10$ and $y = 1$.
   Solve the above system using four-digit rounding arithmetic by Gaussian elimination

   (a) without changing the order of equations,

   (b) with partial pivoting,

   (c) by multiplying the first equation by 104,

   (d) with scaled-column pivoting.

   Comment on the results obtained in different cases.

2. Solve the following system of equations by the Gauss elimination method with partial pivoting, giving your answers to 2 decimal places.

(a) $15x - 8y - 4z = 26, \qquad 25x - 6y + 12z = 27, \qquad 12x + 11y + 9z = 32$

(b) $10x + 19y + 13z = 42, \qquad 8x + 15y + 29z = 73, \qquad 28x + 12y + 9z = 9$

3. Solve the following system of equations.

   (a) $x - 2y + z = 6.7, \qquad x - 4y + 3z = 12.1, \qquad -2x + 5y - 6z = -21.2$

   (b) $x - 2y + 2z = 8.8, \qquad x - y + 5z = 13.9, \qquad 2x - 3y + 4z = 16.1$

   (c) $x - 2y + 3z = 11.4, \qquad 3x - 8y + 11z = 42.4, \qquad 2x - 4y + 3z = 16.8$

      i. by Gaussian elimination,

      ii. by **LU** factorization method.

4. Consider a symmetric matrix $A = \begin{pmatrix} 1 & 2 & -1 \\ 2 & 13 & 1 \\ -1 & 1 & 6 \end{pmatrix}$, determine a lower triangular matrix $\mathbf{L}$ such that $\mathbf{L}\mathbf{L}^\top = \mathbf{A}$.
   Hence, obtain the solution $X$ of the equation $AX = \begin{pmatrix} 1 & 13 & 14 \end{pmatrix}^\top$.

5. Given $A = \begin{pmatrix} 1 & 2 & -1 \\ 2 & 5 & 1 \\ -1 & 1 & 14 \end{pmatrix}, B = \begin{pmatrix} 6 \\ 17 \\ 13 \end{pmatrix}, X = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$

   (a) Find the Cholesky factorization of $A$.

   (b) Solve the equation $AX = B$ by the Cholesky method.

   (c) Find the inverse of the matrix A by the Cholesky method.

6. Use three-digit rounding arithmetic to solve the following system by

   (a) Jacobi's iteration method,

   (b) Gauss-Seidel iteration method.

$$5x - 4y + 14z = 16, \qquad 15x - 4y + 6z = 24, \qquad 4x + 16y + 6z = 33$$

   (i) Without changing the order of the equations.

   (ii) By rearranging the system to diagonally dominant form.

7. Reduce the following system to an equivalent system which is diagonally dominant:

$$5x + 18y - 6z = 24, \qquad 11x + 10y + 15z = -8, \qquad 16x + 7y - 5z = 25.$$

   With the starting values $x_0 = -1$, $y_0 = 2$, $z_0 = 1$, use Gauss-Seidel iteration to find roots correct to 3 significant figures.

8. Reduce the following system to an equivalent system which is diagonally dominant. Find the solution of the system, correct to 2 decimal places, using

   (i) Jacobi iteration,

   (ii) Gauss-Seidel iteration

   (a) $2x + y + 10z = 10, \qquad 10x - y + z = -24, \qquad 5x + 11y + 8z = 31$

   (b) $7x + 11y - 8z = 21, \qquad 3x - 7y + 5z = 6, \qquad 2x - 4y - 10z = 24$

   (c) $8x - 7y + 2z = 7, \qquad 4x + 5y - 6z = 19, \qquad 6x - 3y - 8z = 17$

# Chapter 7

# Numerical Differentiation

## 7.1 Introduction

In previous chapters we have considered the problem of interpolation, i.e. given the set of values of $(x_0, y_0)$, $(x_1, y_1), \ldots,$ $(x_n, y_n)$ of $x$ and $y$, to find a polynomial $p(x)$ of the lowest degree such that $y(x)$ and $p(x)$ agree at the set of tabulated points. In this chapter we shall consider the derivative at a point using those set of tabulated values. Numerical differentiation formulas can be derived by using the Taylor series expansion or by differentiating the interpolating polynomials. Here we shall consider both way of deriving the derivative formulas.

## 7.2 Derivative Formula from Taylor Series

From the Taylor series expansion of $f(x)$ about $x = x_0$, we have

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f'''(x_0)$$
$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2!}f''(x_0) - \frac{h^3}{3!}f'''(x_0)$$

From the expansion of $f(x_0 + h)$, we have

$$\frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0) + \frac{h}{2!}f''(x_0) + \frac{h^2}{3!}f'''(x_0)$$
$$\Rightarrow \frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0) + O(h)$$

and from $f(x_0 - h)$, we have

$$f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h} + O(h)$$

Similarly $f(x_0 + h) - f(x_0 - h)$ gives

$$\frac{f(x_0 + h) - f(x_0 - h)}{2h} = f'(x_0) + O(h^2)$$

Also $f(x_0 + h) + f(x_0 - h)$ gives

$$\frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} = f''(x_0) + O(h^2)$$

Using different combinations we get different formulas for derivatives.

## 7.3 Derivative Formula from Interpolating Polynomials

Numerical differentiation formulas can also be derived by differentiating the interpolating polynomial. The method is illustrated with the Newton-Gregory forward difference formula.
Consider the Newton-Gregory forward difference formula:

$$f(x) = f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 f_0 + \dots$$

where

$$s = \frac{1}{h}(x - x_0) \qquad \text{and} \qquad f(x_0) = f_0$$

Then

$$\begin{aligned} f'(x) &= \frac{\mathrm{d}}{\mathrm{d}\,s}f(x)\frac{\mathrm{d}\,s}{\mathrm{d}\,x} \\ &= \frac{1}{h}\left[\Delta f_0 + \frac{2s-1}{2}\Delta^2 f_0 + \frac{3s^2-6s+2}{6}\Delta^3 f_0 + \dots\right] \end{aligned}$$

The formula can be used for computing the values of $f'(x)$ for non-tabular values of $x$. For tabular values of $x$, the formula takes a simpler form. For example, by setting $x = x_0$, we obtain $s = 0$ and hence

$$f'(x_0) = \frac{1}{h}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \dots\right]$$

With one term we have

$$f'(x_0) \approx \frac{f_1 - f_0}{h}$$

Using two terms we get the 3-point formula

$$\begin{aligned} f'(x_0) &\approx \frac{1}{h}\left[f_1 - f_0 - \frac{1}{2}\Delta(f_1 - f_0)\right] \\ &\approx \frac{1}{h}\left[f_1 - f_0 - \frac{1}{2}(f_2 - f_1 - (f_1 - f_0))\right] \\ &\approx \frac{1}{h}[-3f_0 + 4f_1 - f_2] \end{aligned}$$

Differentiating $f'(x)$ once again we obtain

$$f''(x) = \frac{1}{h^2}\left[\Delta^2 f_0 + \frac{6s-6}{6}\Delta^3 f_0 + \frac{12s^2-36s+22}{24}\Delta^4 f_0 + \dots\right]$$

from which we obtain

$$f''(x_0) = \frac{1}{h^2}\left[\Delta^2 f_0 - \Delta^3 f_0 + \frac{11}{12}\Delta^4 f_0 - \dots\right]$$

Formulas for higher derivatives may be obtained by successive differentiation. In a similar way, different formulas can be derived by starting with other interpolating formulas.

Newton-Gregory backward difference formula gives

$$f'(x_n) = \frac{1}{h}\left[\nabla f_n + \frac{1}{2}\nabla^2 f_n + \frac{1}{3}\nabla^3 f_n + \dots\right]$$

and

$$f''(x_n) = \frac{1}{h^2}\left[\nabla^2 f_n + \nabla^3 f_n + \frac{11}{12}\nabla^4 f_n - \dots\right]$$

## 7.4 Richardson Extrapolation

Suppose $M(h)$ is an estimate of order $h^n$ for $M = \lim_{h\to 0} M(h)$ with step size $h$. Then error can be expressed as

$$M - M(h) = a_n h^n + a_p h^p + a_q h^q + \dots, \quad a_n \neq 0,\, n < p < q$$

The exact value $M$ can be written as

$$M = M(h) + a_n h^n + O(h^p) \tag{7.1}$$

where the notation $O(h^p)$ is used to stand for "a sum of terms of order $h^p$ and higher".

Neglecting the higher order error term $O(h^p)$ from Eq. (8.6), we have

$$M = M(h) + a_n h^n \tag{7.2}$$

Using another step size $rh$ instead of $h$, we get

$$M = M(rh) + a_n (rh)^n \tag{7.3}$$

The coefficient $a_n$ in Eqs. (8.7) and (7.3) are not usually same for different step sizes. Apart from a small change, we shall assume they are equal.
Subtracting (8.7) and (7.3) we can estimate the error term $a_n h^n$ as follows

$$(r^n - 1) a_n h^n = M(h) - M(rh)$$

or

$$a_n h^n = \frac{M(h) - M(rh)}{r^n - 1}$$

Substituting the value of $a_n h^n$ in (8.6) we get $M$ as

$$M = M(h) + \frac{M(h) - M(rh)}{r^n - 1} + O(h^p)$$

An approximate value $M_1(h)$ of $M$ defined by

$$M_1(h) = M(h) + \frac{M(h) - M(rh)}{r^n - 1}$$

is called the Richardson extrapolation of $M(h)$ and it is an estimate of order $h^p$ with $p > n$.
Thus, we can write

$$M = M_1(h) + O(h^p)$$

The process can be repeated to remove more error terms to get better approximations.
Eliminating the next leading error term of order $h^p$, next approximation to $M$ is

$$M_2(h) = M_1(h) + \frac{M_1(h) - M_1(rh)}{r^p - 1}$$

If $M_i(h)$ is an estimate of order $h^m$ for $M$, then

$$M = M_i(h) + O(h^m)$$

A general recurrence relation can be defined for $(i+1)$th approximation by

$$M_(i+1)(h) = M_i + \frac{M_i(h) - M_i(rh)}{r^m - 1} = \frac{r^m M_i(h) - M_i(rh)}{r^m - 1}$$

## 7.5 Formulas for Computing Derivatives

**First Derivatives**

$$
\begin{aligned}
f'(x_0) &\approx \frac{f_1 - f_0}{h}, && O(h) && 2-\text{points forward difference}\\
f'(x_0) &\approx \frac{f_0 - f_(-1)}{h}, && O(h) && 2-\text{points backward difference}\\
f'(x_0) &\approx \frac{f_1 - f_(-1)}{2h}, && O(h^2) && 3-\text{points central difference}\\
f'(x_0) &\approx \frac{1}{2h}[-3f_0 + 4f_1 - f_2], && O(h^2) && 3-\text{points forward difference}\\
f'(x_0) &\approx \frac{1}{2h}[3f_0 - 4f_{-1} + f_{-2}], && O(h^2) && 3-\text{points backward difference}
\end{aligned}
$$

**Second Derivatives**

$$
\begin{aligned}
f''(x_0) &\approx \frac{1}{h^2}[f_{-1} - 2f_0 + f_1], && O(h^2) && 3-\text{point central difference}\\
f''(x_0) &\approx \frac{1}{h^2}[f_0 - 2f_1 + f_2], && O(h) && 3-\text{point forward difference}\\
f''(x_0) &\approx \frac{1}{h^2}[f_0 - 2f_{-1} + f_{-2}], && O(h) && 3-\text{point backward difference}
\end{aligned}
$$

Lower order formula and Richardson extrapolation can be used to deduce the higher order formula.

**Example.** Derive 5-point central difference formula for $f'(x_0)$ using 3-point central difference formula and Richardson extrapolation.

For convenience, we shall use the notation $f'(x_0, h)$ instead of $f'(x_0)$ to indicate clearly the step size $h$.
From 3-point central difference formula, we have

$$
\begin{aligned}
f'(x_0, h) &= \frac{f(x_0 + h) - f(x_0 - h)}{2h} = \frac{f_1 - f_(-1)}{2h}\\
f'(x_0, 2h) &= \frac{f(x_0 + 2h) - f(x_0 - 2h)}{2 \times 2h} = \frac{f_2 - f_(-2)}{4h}
\end{aligned}
$$

Using Richardson extrapolation

$$
\begin{aligned}
f'_R(x_0) &= \frac{2^2 f'(x_0, h) - f'(x_0, 2h)}{2^2 - 1} = \frac{1}{3}\left[\frac{4(f_1 - f_(-1))}{2h} - \frac{f_2 - f_(-2)}{4h}\right]\\
&= \frac{1}{12h}(-f_2 + 8f_1 - 8f_{-1} + f_{-2})
\end{aligned}
$$

which is the five point central derivative formula for first derivative.

**Example.** Estimate $f'(1)$ and $f''(1)$ using three point formula and extrapolation for the following set of values of $x$ and $f(x)$.

| $x$ | $f(x)$ |
|---|---|
| 0.8 | 1.5505 |
| 0.9 | 1.5289 |
| 1.0 | 1.4687 |
| 1.1 | 1.3627 |
| 1.2 | 1.2031 |

Using 3 point central for $f'(1)$, we have

$$\begin{aligned} f'(1.0, 0.1) &= \frac{f(1.1) - f(0.9)}{2(0.1)} \\ &= \frac{1.3627 - 1.5289}{0.2} \\ &= -0.8310 \\ f'(1.0, 0.2) &= \frac{f(1.2) - f(0.8)}{2(0.2)} \\ &= \frac{1.2031 - 1.5505}{0.4} \\ &= -0.8685 \end{aligned}$$

Thus,

$$\begin{aligned} f'(1.0) \approx f'_R(1.0) &= \frac{2^2 f'(1.0, 0.1) - f'(1.0, 0.2)}{2^2 - 1} \\ &= \frac{4(-0.8310) - (-0.8685)}{3} \\ &= -0.8185 \end{aligned}$$

[The data were constructed from $f(x) = e^x \cos x$ and exact value of $f'(1.0) = -0.818\,66$]

Also, for $f''(1)$, we have

$$\begin{aligned} f''(1, 0.1) &= \frac{f(1.1) - 2f(1.0) + f(0.9)}{(0.1)^2} \\ &= \frac{1.3627 - 2 \times 1.4687 + 1.5289}{0.01} \\ &= -4.580 \\ f''(1, 0.2) &= \frac{f(1.2) - 2f(1.0) + f(0.8)}{(0.2)^2} \\ &= \frac{1.2031 - 2 \times 1.4687 + 1.5505}{0.04} \\ &= -4.595 \end{aligned}$$

Richardson's extrapolated estimates is

$$\begin{aligned} f''(1,0) \approx f''_R(1,0) &= \frac{2^2 f''(1.0,0.1) - f''(1.0,0.2)}{2^2-1} \\ &= \frac{4(-4.580) + 4.595}{3} \\ &= -4.575 \end{aligned}$$

[The exact value of $f''(1) = -4.574\,71$]

**Problem 7.5.1.** The distance $D = D(t)$ traveled by an object is given in the table below:

| $t$ | $D(t)$ |
|---|---|
| 8.0 | 17.453 |
| 9.0 | 21.460 |
| 10.0 | 25.752 |
| 11.0 | 30.301 |
| 12.0 | 35.084 |

Using repeated Richardson extrapolation find

(a) the velocity $V(10)$,

(b) the velocity $V(8)$,

(c) In each case compare your results with exact results obtained from

$$D(t) = -70 + 7t + 70e^{\frac{-t}{10}}$$

**Solution.** (a) Using three point central formula at $t = 10$
with $h = 1$:

$$D'(10,1) = \frac{D(11) - D(9)}{2(1)} = \frac{30.301 - 21.460}{2} = 4.4205$$

with $h = 2$:

$$D'(10,2) = \frac{D(12) - D(8)}{2(2)} = \frac{35.084 - 17.453}{4} = 4.4078$$

Using extrapolation,

$$\begin{aligned} V(10) \approx D'_R(10) &= D'(10,1) + \frac{D'(10,1) - D'(10,2)}{2^2-1} \\ &= 4.4205 + \frac{4.4205 - 4.4078}{3} \\ &= 4.4247 \end{aligned}$$

(b) Using two point forward difference formula at $t = 8$
with $h = 1$:

$$D'(8,1) = \frac{D(9) - D(8)}{(1)} = 21.460 - 17.453 = 4.0070$$

with $h = 2$:

$$D'(8,2) = \frac{D(10) - D(8)}{(2)} = \frac{25.752 - 17.453}{2} = 4.1495$$

with $h = 4$:

$$D'(8,4) = \frac{D(12) - D(8)}{(4)} = \frac{35.084 - 17.453}{4} = 4.4077$$

Applying the Richardson extrapolation

$$g_{i+1}(h) = g_i(h) + \frac{g_i(h) - g_i(2h)}{2^m - 1}$$

where $i$ denotes $i$th iterate and $m$ is the order of the error. Thus,

**Extrapolation Table**

| $h$ | $O(h)$ | $O(h^2)$ | $O(h^3)$ |
|---|---|---|---|
| 4 | 4.4077 | | |
| 2 | 4.1495 | 3.8913 | |
| 1 | 4.400 70 | 3.8645 | 3.8556 |

(c) Comparison with exact results
Velocity is given by

$$V(t) = \frac{\mathrm{d}\,D}{\mathrm{d}\,t} = 7 - 7e^{\frac{-t}{10}}$$

Thus,

$$V_t(10) = 4.4248$$

**% of Errors for 3-point central difference formula**

| $h$ | $O(h^2)$ | $O(h^2)$ |
|---|---|---|
| 2 | 0.38% | |
| 1 | $9.7 \times 10^{-2}$ | $2.3 \times 10^{-3}$ |

From the exact derivative

$$V(8) = 3.8547$$

**% of Errors for 2-point forward difference formula**

| $h$ | $O(h)$ | $O(h^2)$ | $O(h^3)$ |
|---|---|---|---|
| 4 | 14.35% | | |
| 2 | 7.65% | 0.95% | |
| 1 | 3.95% | 0.25% | 0.25% |

**Problem 7.5.2.** The distance $D = D(t)$ traveled by an object is given in the table below:

| $t$ | $D(t)$ |
|---|---|
| 8.0 | 17.453 |
| 9.0 | 21.460 |
| 10.0 | 25.752 |
| 11.0 | 30.301 |
| 12.0 | 35.084 |

(a) Estimate the velocity and acceleration at $t = 10.4$ using three suitable points.

(b) Estimate the velocity and acceleration at $t = 10.4$ using four suitable points.

In each case compare your results with exact results obtained from

$$D(t) = -70 + 7t + 70e^{\frac{-t}{10}}$$

**Solution.** To construct polynomial through the given points, the divided difference table is as follows:

| $t$ | $D(t)$ | $D^1(t)$ | $D^2(t)$ | $D^3(t)$ |
|---|---|---|---|---|
| 9 | 21.46 | | | |
| 10 | 25.752 | 4.292 | | |
| 11 | 30.301 | 4.549 | 0.1285 | |
| 12 | 35.084 | 4.783 | 0.117 | −0.003 83 |

(a) We need to consider 3 points that are closest to $t = 10.4$ and we choose the points as $t = 9$, $t = 10$ and $t = 11$. Then

$$\begin{aligned} D(t) &= 21.46 + 4.292(t-9) + 0.1285(t-9)(t-10), \qquad 9 \le t \le 11 \\ v(t) &= \frac{\mathrm{d}\,D}{\mathrm{d}\,t} = 4.292 + 0.1285(2t - 9 - 10) \\ a(t) &= \frac{\mathrm{d}^2 D}{\mathrm{d}\,t^2} = 0.1285(2) = 0.257 \end{aligned}$$

Thus

$$v(10.4) = 4.5233 \qquad \text{and} \qquad a(10.4) = 0.257$$

(b) We need to consider 4 points that are closest to $t = 10.4$ and we choose the points as $t = 9$, $t = 10$, $t = 11$ and $t = 12$. Then

$$\begin{aligned} D(t) &= 21.46 + 4.292(t-9) + 0.1285(t-9)(t-10) - 0.00383(t-9)(t-10)(t-12), \qquad 9 \le t \le 12 \\ v(t) &= \frac{\mathrm{d}\,D}{\mathrm{d}\,t} = 4.292 + 0.1285(2t - 9 - 10) - 0.00383[3t^2 - 2t(9 + 10 + 12) + (90 + 108 + 120)] \\ a(t) &= \frac{\mathrm{d}^2 D}{\mathrm{d}\,t^2} = 0.1285(2) - 0.00383[6t - 2(31)] \end{aligned}$$

Thus

$$v(10.4) = 4.5322 \qquad \text{and} \qquad a(10.4) = 0.2554$$

**Error estimation:**
From the exact expression for distance we have

$$\frac{\mathrm{d}\,D}{\mathrm{d}\,t} = 7 - 7e^{\frac{-t}{10}} \qquad \text{and} \qquad \frac{\mathrm{d}^{\,2}D}{\mathrm{d}\,t^2} = \frac{7}{10}e^{\frac{-t}{10}}$$

which gives,

$$v(10.4) = 4.5258 \qquad \text{and} \qquad a(10.4) = 0.2474$$

Error with 3-point polynomial:

$$\text{Absolute error in velocity} = \left|\frac{4.5233 - 4.5258}{4.5258}\right| \times 100 = 0.055\%$$
$$\text{Absolute error in acceleration} = \left|\frac{0.257 - 0.2474}{0.2474}\right| \times 100 = 3.88\%$$

Error with 4-point polynomial:

$$\text{Absolute error in velocity} = \left|\frac{4.5322 - 4.5258}{4.5258}\right| \times 100 = 0.14\%$$
$$\text{Absolute error in acceleration} = \left|\frac{0.2554 - 0.2474}{0.2474}\right| \times 100 = 3.23\%$$

## 7.6 Exercise

1. The values of $f(x)$ are given in the following table:

| $x$ | $f(x)$ |
|---|---|
| 1.2 | 4.448 |
| 1.3 | 3.567 |
| 1.4 | 2.624 |
| 1.5 | 1.625 |
| 1.6 | 0.576 |

   (a) Using two-point formulae estimate the values of $f'(1.2)$, $f'(1.4)$, $f'(1.6)$.

   (b) Using three-point formulae estimate the values of $f'(1.4)$ and $f''(1.4)$.

2. The table below shows the values of $f(x)$ at different values of $x$:

| $x$ | $f(x)$ |
|---|---|
| 1.4 | 1.3796 |
| 1.5 | 1.4962 |
| 1.6 | 1.5993 |
| 1.7 | 1.6858 |
| 1.8 | 1.7629 |

(a)

| $x$ | $f(x)$ |
|---|---|
| 0.7 | 1.297 |
| 0.8 | 1.597 |
| 1.0 | 2.287 |
| 1.2 | 3.094 |
| 1.3 | 3.536 |

(b)

| $x$ | $f(x)$ |
|---|---|
| 0.7 | 1.297 |
| 0.9 | 1.927 |
| 1.0 | 2.287 |
| 1.1 | 2.677 |
| 1.3 | 3.536 |

(a) Derive three-point forward and backward difference formulae for the first and second derivatives using two-point first derivative formula.
Use three-point formulae to estimate the values of $f'(1.4)$, $f'(1.8)$, $f''(1.4)$ and $f''(1.8)$.

(b) Derive five-point central difference formula for $f'(x_0)$ and $f''(x_0)$ using three-point central difference formula with Richardson extrapolation.
Use five-points formulae to estimate the values of $f'(1.6)$ and $f''(1.6)$.
[The table is constructed for $f(x) = x \sin x$]

3. Estimate $f'(1.2)$ and $f''(1.2)$ using Richardson extrapolation for the following data:

| $x$ | $f(x)$ |
|---|---|
| 0.8 | 0.9548 |
| 1.0 | 1.6487 |
| 1.2 | 2.6239 |
| 1.4 | 3.9470 |
| 1.6 | 5.6974 |

Compare your result with the exact value $f'(1.2) = 5.6850$ and $f''(1.2) = 8.6733$ correct to 4 decimal places.
[The table is constructed for $f(x) = x^2 e^{\frac{x}{2}}$]

4. Use the following table of values of $f(x)$ to estimate $f'(1.0)$ and $f''(1.0)$ by using three point central difference formulae with Richardson extrapolation. [The table is constructed for $f(x) = e^x \sin x$]

5. The voltage $E = E(t)$ in an electric circuit obeys the differential equations

$$E(t) = L\frac{\mathrm{d}I}{\mathrm{d}t} + RI,$$

where $R$ is the resistance and $L$ is the inductance. Use $L = 0.05$ and $R = 2$ and the $I(t)$ in the table

| $t$ | $I(t)$ |
|---|---|
| 1.0 | 8.2277 |
| 1.1 | 7.2428 |
| 1.2 | 5.9908 |
| 1.3 | 4.5260 |
| 1.4 | 2.9122 |

(a) Find $I'(1.2)$ by numerical differentiation as accurately as possible and use it to compute $E(1.2)$.

(b) Compare your result with the exact solution $I(t) = 10e^{\frac{-t}{10}} \sin 2t$.

6. Derive three-point forward and backward formulae for first derivative.
The table below gives the values of the distance traveled by a car at various time intervals during its journey

| Time, $t$ (min) | Distance traveled $s(t)$ (km) |
|---|---|
| 4 | 7.5 |
| 5 | 11.0 |
| 6 | 15.0 |
| 7 | 19.5 |
| 8 | 24.0 |

(a) Estimate the velocity, $v = \frac{ds}{dt}$, at time $t = 4$, $t = 6$ and $t = 8$ using three-point formulae with Richardson extrapolation.

(b) Estimate the velocity and acceleration at time $t = 4.5$ and $6.5$ using 3 and 4 suitable points.

# Chapter 8

# Numerical Differentiation

## 8.1 Introduction

Recall the definition of the derivative of a function

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

For finite $\Delta x$,

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

To find the derivative at $x = x_i$, we choose another point $x_{i+1} = x_i + h$ ahead of $x_i$. This gives two point forward difference formulae

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i)}{h} \tag{8.1}$$

If $\Delta x$ is chosen as a negative number, say $\Delta x = -h (h > 0)$, we have

$$f'(x_i) \approx \frac{f(x_i - h) - f(x_i)}{-h} \approx \frac{f(x_i) - f(x_i - h)}{h} \tag{8.2}$$

This is backward difference formula for first derivative. Adding Eq.(8.1) and Eq.(8.2), we have

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i - h)}{2h} \tag{8.3}$$

which is a-point central difference formula for first derivative.

## 8.2 Derivative Formula from Taylor Series

For clear idea about the different formulas and their order of errors we may use the Taylor series expansion of $f(x)$.
From Taylor series expansion for $h > 0$, we have

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!} f''(x_0) + \frac{h^3}{3!} + \dots \tag{8.4}$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2!} f''(x_0) - \frac{h^3}{3!} + \dots \tag{8.5}$$

From the expansion of $f(x_0+h)$, we have

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2!}f''(x_0) - \frac{h^2}{3!} - \dots$$

which leads to the two-point forward difference formula for $f'(x_0)$ as

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} + E$$

where the error series is

$$E = -\left[\frac{h}{2!}f''(x_0) + \frac{h^2}{3!} + \dots\right]$$

From the expansion of $f(x_0-h)$, we have 2-point backward difference formula

$$f'(x_0) = \frac{f(x_0)-f(x_0-h)}{h} + E$$

with error term

$$E = \frac{h}{2!}f''(x_0) - \frac{h^2}{3!} + \dots$$

In the two point formula the error series is of the form

$$E = a_1h + a_2h^2 + a_3h^3 + \dots$$

where $a$'s does not depend on $h$.

By subtraction, we obtain

$$f(x_0+h) - f(x_0-h) = 2hf(x_0) + \frac{2}{3!}h^3f'''(x_0) + \frac{2}{5!}h^5f^{(v)}(x_0) + \dots$$

This leads to the 3-point central formula for approximating $f'(x_0)$

$$f'(x_0) = \frac{f(x_0+h)-f(x_0-h)}{2h} + E$$

with

$$E = -\left[\frac{1}{3!}h^2f'''(x_0) + \frac{1}{5!}h^4f^{(v)}(x_0) + \dots\right]$$

Adding the Taylor series for $f(x_0+h)$ and $f(x_0-h)$, we get

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

When this is rearranged, we get 3-point central difference formula for $f''(x_0)$

$$f''(x_0) = \frac{f(x_0+h)-2f(x_0)+f(x_0-h)}{h^2} + E$$

where the error series is

$$E = -2\left[\frac{1}{4!}h^2f^{(4)}(x_0) + \frac{1}{6!}h^4f^{(6)}(x_0)\dots\right]$$

In the three point central difference formula the error series is of the form

$$E = a_2h^2 + a_4h^4 + a_6h^6 + \dots$$

## 8.3 Formulas for Computing Derivatives

**First Derivatives**

$$f'(x_0) \approx \frac{f_1 - f_0}{h}, \qquad O(h) \qquad 2-\text{points forward difference}$$
$$f'(x_0) \approx \frac{f_0 - f_(-1)}{h}, \qquad O(h) \qquad 2-\text{points backward difference}$$
$$f'(x_0) \approx \frac{f_1 - f_(-1)}{2h}, \qquad O(h^2) \qquad 3-\text{points central difference}$$
$$f'(x_0) \approx \frac{1}{2h}[-3f_0 + 4f_1 - f_2], \qquad O(h^2) \qquad 3-\text{points forward difference}$$
$$f'(x_0) \approx \frac{1}{2h}[3f_0 - 4f_{-1} + f_{-2}], \qquad O(h^2) \qquad 3-\text{points backward difference}$$

**Second Derivatives**

$$f''(x_0) \approx \frac{1}{h^2}[f_{-1} - 2f_0 + f_1], \qquad O(h^2) \qquad 3-\text{point central difference}$$
$$f''(x_0) \approx \frac{1}{h^2}[f_0 - 2f_1 + f_2], \qquad O(h) \qquad 3-\text{point forward difference}$$
$$f''(x_0) \approx \frac{1}{h^2}[f_0 - 2f_{-1} + f_{-2}], \qquad O(h) \qquad 3-\text{point backward difference}$$

## 8.4 Richardson Extrapolation

If the two approximations of order $O(h^n)$ for $M$ are $M(h)$ and $M(rh)$, then the Richardson's extrapolated estimate $M_R$ of $M$ can be written as

$$M_R = M(h) + Ah^n \tag{8.6}$$
$$M_R = M(rh) + A(rh)^n \tag{8.7}$$

where we have assumed the constant multiplicative factor is same.
Subtracting (8.6) from (8.7),

$$0 = M(rh) - M(h) + Ah^n(r^n - 1)$$
$$\Rightarrow \; Ah^n = \frac{M(h) - M(rh)}{r^n - 1}$$

Substituting in (8.6), we have

$$M_R = M(h) + \frac{M(h) - M(rh)}{r^n - 1}$$

which is the *Richardson extrapolation* formula.

Lower order formula and Richardson extrapolation can be used to deduce the higher order formula. For convenience, we have used the notation $f'(x_0, h)$ to indicate clearly the approximation of $f'(x_0)$ with step size $h$ and $f(x_0 + rh) = f_r$. Thus, the 3-point central difference formula for first derivative will be written as

$$f'(x_0, h) = \frac{f_1 - f_{-1}}{2h}$$

**Problem 8.4.1.** Derive three-point forward difference formulas for the first and second derivative using two point derivative formula
The values of distance at various times are given below

| Time ($t$) | Distance($s$) |
|---|---|
| 6 | 7.38 |
| 7 | 12.07 |
| 8 | 18.37 |
| 9 | 26.42 |
| 10 | 36.40 |

Estimate the velocity $v = \frac{\mathrm{d}\, s}{\mathrm{d}\, t}$ and acceleration $a = \frac{\mathrm{d}^2 s}{\mathrm{d}\, t^2}$ at time $t = 6$ using three point formula and extrapolation.

**Solution.** Three point forward derivate formula:
From 2-point forward difference formula, we have

$$\begin{aligned} f'(x_0, h) &= \frac{f(x_0+h) - f(x_0)}{h} = \frac{f_1 - f_0}{h} \\ f'(x_0, 2h) &= \frac{f(x_0+2h) - f(x_0)}{2h} = \frac{f_2 - f_0}{2h} \end{aligned}$$

Using Richardson extrapolation

$$\begin{aligned} f_R'(x_0) &= f'(x_0, h) + \frac{f'(x_0, h) - f'(x_0, 2h)}{2^1 - 1} \\ &= \frac{f_1 - f_0}{h} + \left[\frac{f_1 - f_0}{h} - \frac{f_2 - f_0}{2h}\right] \\ &= \frac{1}{2h}(4f_1 - 4f_0 - f_2 + f_0) \\ &= \frac{1}{2h}(-3f_0 + 4f_1 - f_2) \end{aligned}$$

which is the three point forward difference formula for first derivative and its order of error is two $O(h^2)$.

Froward derivative formula for second derivatve:
Differentiating two-point first derivative formula we have

$$\begin{aligned} f''(x_0, h) &= \frac{f'(x_0+h) - f'(x_0)}{h} \\ &= \frac{1}{h}\left[\frac{f(x_0+2h) - f(x_0+h)}{h} - \frac{f(x_0+h) - f(x_0)}{h}\right] \\ &= \frac{1}{h^2}[f(x_0+2h) - 2f(x_0+h) + f(x_0)] \\ &= \frac{1}{h^2}(f_0 - 2f_1 + f_2) \end{aligned}$$

Here error term is not eliminated by extrapolation and hence the order of the error is $O(h)$.

Velocity at $t = 6$

$$\begin{aligned}
v(6,1) &= \frac{1}{2(1)}[-3s(6) + 4s(7) - s(8)] \\
&= \frac{1}{2}[-3(7.38) + 4(12.07) - 18.37] \\
&= 3.885 \\
v(6,2) &= \frac{1}{2(2)}[-3s(6) + 4s(8) - s(10)] \\
&= \frac{1}{2}[-3(7.38) + 4(18.37) - 36.40] \\
&= 3.735
\end{aligned}$$

Extrapolated value is

$$v_R(6) = v(6,1) + \frac{v(6,1) - v(6,2)}{2^2 - 1} = 3.885 + \frac{3.885 - 3.735}{3} = 3.935$$

Acceleration at $t = 6$

$$\begin{aligned}
a(6,1) &= \frac{1}{(1)^2}[s(6) - 2s(7) + s(8)] \\
&= [7.38 - 2(12.07) + 18.37] \\
&= 1.61 \\
a(6,2) &= \frac{1}{(2)^2}[s(6) - 2s(8) + s(10)] \\
&= \frac{1}{4}[7.38 - 2(18.37) + 36.40] \\
&= 1.76
\end{aligned}$$

Extrapolated value is

$$a_R(6) = a(6,1) + \frac{a(6,1) - a(6,2)}{2^1 - 1} = 1.61 + \frac{1.61 - 1.76}{1} = 1.46$$

## 8.5 Derivatives from Interpolating Polynomials

We can fit a polynomial through the data points and then by differentiating we may find the derivatives at a point. This is useful when the data values are not evenly distributed or derivatives are required at points other than tabulated points.
The method is discussed with an example.

**Problem 8.5.1.** The distance $D = D(t)$ traveled by an object is given in the table below:

(a) Estimate the velocity and acceleration at $t = 10.4$ using three suitable points.

(b) Estimate the velocity and acceleration at $t = 10.4$ using four suitable points.

In each case compare your results with exact results obtained from

$$D(t) = -70 + 7t + 70e^{\frac{-t}{10}}$$

| $t$ | $D(t)$ |
|---|---|
| 8.0 | 17.453 |
| 9.0 | 21.460 |
| 10.0 | 25.752 |
| 11.0 | 30.301 |
| 12.0 | 35.084 |

| $t$ | $D(t)$ | $D^1(t)$ | $D^2(t)$ | $D^3(t)$ |
|---|---|---|---|---|
| 9 | 21.460 | | | |
| 10 | 25.752 | 4.292 | | |
| 11 | 30.301 | 4.549 | 0.1285 | |
| 12 | 35.084 | 4.783 | 0.117 | −0.003 83 |

**Solution.** To construct polynomial through the given points, the divided difference table is as follows:

(a) We need to consider 3 points that are closest to $t = 10.4$ and we choose the points as $t = 9$, $t = 10$ and $t = 11$. Then

$$\begin{aligned} D(t) &= 21.46 + 4.292(t-9) + 0.1285(t-9)(t-10), \qquad 9 \le t \le 11 \\ v(t) &= \frac{\mathrm{d}\,D}{\mathrm{d}\,t} \\ &= 4.292 + 0.1285(2t-9-10) \\ a(t) &= \frac{\mathrm{d}^2 D}{\mathrm{d}\,t^2} \\ &= 0.1285(2) \\ &= 0.257 \end{aligned}$$

Thus,

$$v(10.4) = 4.5233 \qquad \text{and} \qquad a(10.4) = 0.257$$

(b) We need to consider 4 points that are closest to $t = 10.4$ and we choose the points as $t = 9$, $t = 10$, $t = 11$ and $t = 12$. Then

$$\begin{aligned} D(t) &= 21.46 + 4.292(t-9) + 0.1285(t-9)(t-10) - 0.003\,83(t-9)(t-10)(t-12), \qquad 9 \le t \le 12 \\ v(t) &= \frac{\mathrm{d}\,D}{\mathrm{d}\,t} \\ &= 4.292 + 0.1285(2t-9-10) - 0.003\,83\left[3t^2 - 2t(9+10+12) + (90+108+120)\right] \\ a(t) &= \frac{\mathrm{d}^2 D}{\mathrm{d}\,t^2} \\ &= 0.1285(2) - 0.003\,83[6t - 2(31)] \end{aligned}$$

Thus

$$v(10.4) = 4.5322 \qquad \text{and} \qquad a(10.4) = 0.2554$$

**Error estimation:**
From the exact expression for distance we have

$$\frac{\mathrm{d}\,D}{\mathrm{d}\,t} = 7 - 7e^{\frac{-t}{10}} \qquad \text{and} \qquad \frac{\mathrm{d}^{\,2}D}{\mathrm{d}\,t^2} = \frac{7}{10}e^{\frac{-t}{10}}$$

which give

$$v(10.4) = 4.5258 \qquad \text{and} \qquad a(10.4) = 0.2474$$

Error with 3-point polynomial:

$$\text{Absolute error in velocity} = \left|\frac{4.5233 - 4.5258}{4.5258}\right| \times 100 = 0.055\%$$

$$\text{Absolute error in acceleration} = \left|\frac{0.257 - 0.2474}{0.2474}\right| \times 100 = 3.88\%$$

Error with 4-point polynomial:

$$\text{Absolute error in velocity} = \left|\frac{4.5322 - 4.5258}{4.5258}\right| \times 100 = 0.14\%$$

$$\text{Absolute error in acceleration} = \left|\frac{0.2554 - 0.2474}{0.2474}\right| \times 100 = 3.23\%$$

## 8.6 Exercise

1. The values of $f(x)$ are given in the following table:

| $x$ | $f(x)$ |
|---|---|
| 1.2 | 4.448 |
| 1.3 | 3.567 |
| 1.4 | 2.624 |
| 1.5 | 1.625 |
| 1.6 | 0.576 |

   (a) Using two-point formulae estimate the values of $f'(1.2)$, $f'(1.4)$, $f'(1.6)$.

   (b) Using three-point formulae estimate the values of $f'(1.4)$ and $f''(1.4)$.

2. The table below shows the values of $f(x)$ at different values of $x$:

| $x$ | $f(x)$ |
|---|---|
| 1.4 | 1.3796 |
| 1.5 | 1.4962 |
| 1.6 | 1.5993 |
| 1.7 | 1.6858 |
| 1.8 | 1.7629 |

   (a) Derive three-point forward and backward difference formulae for the first and second derivatives using two-point first derivative formula.
   Use three-point formulae to estimate the values of $f'(1.4)$, $f'(1.8)$, $f''(1.4)$ and $f''(1.8)$.

| $x$ | $f(x)$ |
|---|---|
| 0.8 | 0.9548 |
| 1.0 | 1.6487 |
| 1.2 | 2.6239 |
| 1.4 | 3.9470 |
| 1.6 | 5.6974 |

(a)

| $x$ | $f(x)$ |
|---|---|
| 0.7 | 1.297 |
| 0.8 | 1.597 |
| 1.0 | 2.287 |
| 1.2 | 3.094 |
| 1.3 | 3.536 |

(b)

| $x$ | $f(x)$ |
|---|---|
| 0.7 | 1.297 |
| 0.9 | 1.927 |
| 1.0 | 2.287 |
| 1.1 | 2.677 |
| 1.3 | 3.536 |

(b) Derive five-point central difference formula for $f'(x_0)$ and $f''(x_0)$ using three-point central difference formula with Richardson extrapolation.
Use five-points formulae to estimate the values of $f'(1.6)$ and $f''(1.6)$.

[The table is constructed for $f(x) = x \sin x$]

3. Estimate $f'(1.2)$ and $f''(1.2)$ using Richardson extrapolation for the following data: Compare your result with the exact value $f'(1.2) = 5.6850$ and $f''(1.0)$ correct to 4 decimal places.
   [The table is constructed for $f(x) = x^2 e^{\frac{x}{2}}$]

4. Use the following table of values of $f(x)$ to estimate $f'(1.0)$ and $f''(1.0)$ by using three point central difference formulae with Richardson extrapolation. [The table is constructed for $f(x) = e^x \sin x$]

5. The voltage $E = E(t)$ in an electric circuit obeys the differential equations

$$E(t) = L\frac{\mathrm{d}\,I}{\mathrm{d}\,t} + RI,$$

where $R$ is the resistance and $L$ is the inductance. Use $L = 0.05$ and $R = 2$ and the $I(t)$ in the table

| $t$ | $I(t)$ |
|---|---|
| 1.0 | 8.2277 |
| 1.1 | 7.2428 |
| 1.2 | 5.9908 |
| 1.3 | 4.5260 |
| 1.4 | 2.9122 |

(a) Find $I'(1.2)$ by numerical differentiation as accurately as possible and use it to compute $E(1.2)$.

(b) Compare your result with the exact solution $I(t) = 10e^{\frac{-t}{10}} \sin 2t$.

6. Using Taylor series expansion derive three-point forward derivative formulas for the first and second derivatives.
In each case estimate the order of the errors.

7. The table below gives the values of the distance traveled by a car at various time intervals during its journey

| Time, $t$ (min) | Distance traveled $s(t)$ (km) |
|---|---|
| 4 | 7.5 |
| 5 | 11.0 |
| 6 | 15.0 |
| 7 | 19.5 |
| 8 | 24.0 |

Estimate the velocity, $v = \frac{\mathrm{d}\,s}{\mathrm{d}\,t}$ and acceleration $v = \frac{\mathrm{d}^2 s}{\mathrm{d}\,t^2}$, at time $t = 4$, $t = 6$ and $t = 8$ using three-point formulae with Richardson extrapolation.

8. The following data shows the distance of a particle from a fixed point at different time.

| Time, $t$ (sec) | Distance $s(t)$ $(m)$ |
|---|---|
| 4 | 16 |
| 5 | 20 |
| 8 | 128 |
| 10 | 340 |

   (a) Find the initial velocity and acceleration of the particle.
   (b) Find the velocity and acceleration of the particle at time $t = 6$ and $t = 8$.
   (c) Find the times when the particle is at rest.

9. Find the velocity and acceleration at time $t = 4.5$ and $6.5$ using 3 and 4 suitable points for the data of 7

10. Estimate the first and second derivatives at $x = 3$ and at $x = 6$ for the function represented by the following tabular data.

| $x$ | $f(x)$ |
|---|---|
| 2 | 2.704 |
| 3 | 4.841 |
| 5 | 9.625 |
| 8 | 17.407 |

# Chapter 9

# Numerical Integration

The process of computing the value of a definite integral from a set of numerical values of the integrand is called *Numerical Integration*. When applied to the integration of a function of a single variable, the process is known as quadrature.

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

## 9.1 A General Quadrature Formula for Equidistant Ordinates

Let $I = \int_a^b y \, \mathrm{d}\, x$ where $y = f(x)$. Let $f(x)$ be given for certain equidistant value of $x$ say $x_0, x_0 + h, x_0 + 2h, \ldots$. Let the range $(a, b)$ be divided into $n$ equal parts, each of width $h$ so that $b - a = nh$.
Let $x_0 = a$, $x_1 = x_0 + h = a + h$, $x_2 = a + 2h$, $\ldots$, $x_n = a + nh = b$. We have assumed that the $n+1$ ordinates $y_0$, $y_1, \ldots, y_n$ are at equal intervals.

$$\therefore\ I = \int_a^b y \, \mathrm{d}\, x = \int_{x_0}^{x_0+nh} y_x \, \mathrm{d}\, x$$

Let, $u = \frac{x - x_0}{h}$ $\quad \therefore\ \mathrm{d}\, x = h \, \mathrm{d}\, u$
when $x = x_0$, $\quad u = 0$

$x = x_0 + nh, \quad u = n$

Now we have (from Newton's forward formula)

$$y_{x_0+uh} = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \ldots$$

$$\therefore\ I = h\int_0^n \left[ y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \ldots \right] \mathrm{d}\, u$$

$$\Rightarrow\ I = h\left[ ny_0 + \frac{n^2}{2}\Delta y_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 y_0}{2!} + \ldots \text{ upto } (n+1) \text{ terms} \right] \tag{9.1}$$

This is the general quadrature formula.
We can deduce a number of formulae from thus by putting $n = 1, 2, \ldots$.

## 9.2 Kinds of Rule for Determining Numerical Integration

### 9.2.1 The Trapezoidal Rule

Putting $n = 1$ in the formula (9.1) and neglecting second and higher order differences, we get

$$\int_{x_0}^{x_0+h} y \, \mathrm{d}\, x = h \left[ y_0 + \frac{1}{2} (y_1 - y_0) \right] = \frac{h[y_0 + y_1]}{2}$$

Similarly,

$$\int_{x_0+h}^{x_0+2h} y \, \mathrm{d}\, x = h \, \frac{y_1 + y_2}{2}$$
$$\int_{x_0+(n-1)h}^{x_0+nh} y \, \mathrm{d}\, x = h \, \frac{y_{n-1} + y_n}{2}$$

Adding these $n$ integrals we get

$$\begin{aligned}
\int_{x_0}^{x_0+nh} y \, \mathrm{d}\, x &= h \left[ \frac{1}{2} \left\{ (y_0 + y_n) + (y_1 + y_2) + \cdots + (y_{n-1} + y_n) \right\} \right] \\
&= h \left[ \frac{1}{2} (y_0 + y_n) + (y_1 + y_2 + \cdots + y_{n-1}) \right] \\
&= \text{ distance between two consecutive ordinates} \times \{\text{mean of the 1st and last ordinates} \\
&+ \text{ sum of all the intermediate ordinates}\}
\end{aligned}$$

This rule is known as the Trapezoidal Rule.

### 9.2.2 Simpson's $^1/_3$ Rule (Simpson's rule)

Putting $n = 2$ in the formula (9.1) and neglecting third and higher order differences, we get

$$\begin{aligned}
\int_{x_0}^{x_0+2h} y \, \mathrm{d}\, x &= h \left[ 2y_0 + \frac{4}{2} \Delta y_0 + \left( \frac{8}{3} - \frac{4}{2} \right) \frac{\Delta^2 y_0}{2} + \ldots \right] \\
&= h \left[ 2y_0 + 2(y_1 - y_0) + \frac{1}{3} \left\{ 4(y_1 - y_0) \right\} \right] \\
&= h \left[ 2y_0 + 2y_1 - 2y_0 + \frac{1}{3} (y_2 - y_1 - (y_1 - y_0)) \right] \\
&= \frac{h}{3} [6y_1 + y_2 - y_1 - y_1 + y_0] \\
&= \frac{h}{3} [y_0 + 4y_1 + y_2]
\end{aligned}$$

Similarly,

$$\int_{x_0+2h}^{x_0+4h} y \, \mathrm{d}\, x = \frac{h}{3} [y_2 + 4y_3 + y_4]$$
$$\int_{x_0+(n-2)h}^{x_0+nh} y \, \mathrm{d}\, x = \frac{h}{3} [y_{n-2} + 4y_{n-1} + y_n] \qquad [n \text{ is even}]$$

Adding all the integrals we get,

$$\begin{aligned}\int_{x_0}^{x_0+nh} y\,\mathrm{d}\,x &= \frac{h}{3}\left[(y_0+4y_1+y_2)+(y_2+4y_3+y_4)+\cdots+(y_{n-2}+4y_{n-1}+y_n)\right]\\ &= \frac{h}{3}\left[(y_0+y_n)+4(y_1+y_3+y_5+\cdots+y_{n-1})+2(y_2+y_4+\cdots+y_{n-2})\right]\end{aligned}$$

This formula is known as Simpson's ${}^1/_3$ -rule also known as Simpson's rule.

### 9.2.3 Simpson's ${}^3/_8$ Rule

Putting $n=3$ in the formula (9.1) and neglecting fourth and higher order differences, we get

$$\begin{aligned}\int_{x_0}^{x_0+3h} y\,\mathrm{d}\,x &= h\left[3y_0+\frac{9}{2}\Delta y_0+\left(\frac{27}{3}-\frac{9}{2}\right)\frac{\Delta^2 y_0}{2!}+\left(\frac{81}{4}-27+9\right)\frac{\Delta^3 y_0}{3!}\right]\\ &= h\left[3y_0+\frac{9}{2}(y_1-y_0)+\frac{9}{2}\cdot\frac{1}{2}(y_2-2Y_1+y_0)+\frac{81-104+36}{4}\cdot\frac{1}{6}\Delta(y_2-2y_1+y_0)\right]\\ &= h\left[3y_0+\frac{9}{2}(y_1-y_0)+\frac{9}{4}(y_2-2y_1+y_0)+\frac{9}{4}\cdot\frac{1}{6}(y_3-y_2-2y_2+2y_1+y_1-y_0)\right]\\ &= \frac{3h}{8}\left[y_0+3y_1+3y_2+y_3\right]\end{aligned}$$

Similarly,

$$\begin{aligned}\int_{x_0+3h}^{x_0+6h} y\,\mathrm{d}\,x &= \frac{3h}{8}\left[y_3+3y_4+3y_5+y_6\right]\\ \int_{x_0+(n-3)h}^{x_0+nh} y\,\mathrm{d}\,x &= \frac{3h}{8}\left[y_{n-3}+3y_{n-2}+3y_{n-1}+y_n\right]\end{aligned}$$

Adding all the integrals we get,

$$\int_{x_0}^{x_0+nh} y\,\mathrm{d}\,x = \frac{3h}{8}\left[(y_0+y_n)+3(y_1+y_2+y_4+\cdots+y_{n-2}+y_{n-1})+2(y_3+y_6+\cdots+y_{n-3})\right]$$

This formula is known as Simpson's ${}^3/_8$ rule.

**Problem 9.2.1.** Calculate the value of the integral

$$\int_4^{5.2} \log_e x\,\mathrm{d}\,x$$

by

(i) Trapezoidal rule

(ii) Simpson's ${}^1/_3$ rule

(iii) Simpson's ${}^3/_8$ rule

(iv) Weddle's rule

After finding the true value of the integral, compare the errors in tn the four cases.

**Solution.** Divide the range of integration $(4, 5.2)$ in 6 equal parts each of width $\frac{5.2-4}{6} = 0.2$, so that $h = 0.2$. The value of the function $f(x) = \ln x$ for each point of sub-division are given below:

| $x$ | $y = f(x) = \ln x$ |
|---|---|
| $x_0 = 4.0$ | $y_0 = 1.386\,294\,4$ |
| $x_0 + h = 4.2$ | $y_1 = 1.435\,084\,5$ |
| $x_0 + 2h = 4.4$ | $y_2 = 1.481\,604\,5$ |
| $x_0 + 3h = 4.6$ | $y_3 = 1.526\,056\,3$ |
| $x_0 + 4h = 4.8$ | $y_4 = 1.568\,615\,9$ |
| $x_0 + 5h = 5.0$ | $y_5 = 1.609\,437\,9$ |
| $x_0 + 6h = 5.2$ | $y_6 = 1.648\,658\,6$ |

(i) We have from Trapezoidal rule

$$\int_{x_0}^{x_0+nh} y \,\mathrm{d}\,x = h\left[\frac{1}{2}(y_0 + y_n) + (y_1 + y_2 + \cdots + y_{n-1})\right]$$

In this case:

$$\begin{aligned}\int_4^{5.2} \ln x \,\mathrm{d}\,x &= 0.2\,[1.517\,476\,5 + 7.620\,799\,2]\\ &= 1.827\,655\,1\end{aligned}$$

(ii) By Simpson's $^1/_3$ rule:

$$\int_{x_0}^{x_0+nh} y \,\mathrm{d}\,x = \frac{h}{3}\,[(y_0 + y_n) + 4(y_1 + y_3 + y_5 + \cdots + y_{n-1}) + 2(y_2 + y_4 + \cdots + y_{n-2})]$$

In this case:

$$\begin{aligned}\int_4^{5.2} \ln x \,\mathrm{d}\,x &= \frac{0.2}{3}\,[3.034\,953\,0 + 18.282\,314\,9 + 6.100\,844\,09]\\ &= 1.827\,847\,2\end{aligned}$$

(iii) By Simpson's $^3/_8$ rule:

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

In this case:

$$\begin{aligned}\int_4^{5.2} \ln x \,\mathrm{d}\,x &= \frac{3 \times 0.2}{8}\,[3.034\,953\,0 + 18.284\,228\,7 + 3.052\,112\,6]\\ &= 1.827\,847\end{aligned}$$

Actual value of

$$\begin{aligned}\int_4^{5.2} \ln x \,\mathrm{d}\,x &= (x \ln x - x)\Big|_4^{5.2}\\ &= 1.827\,847\,5\end{aligned}$$

Hence the errors are:

(i) 0.000 192 4

(ii) 0.000 000 3

(iii) 0.000 000 5

So Simpson's $^1/_3$ rule is more accurate.

Note To Self: May be missing a page

Similarly,

$$\int_{x_0+6h}^{x_0+12h} y \,\mathrm{d}\, x = \frac{3h}{10}[y_6 + 5y_7 + y_8 + 6y_9 + y_{10} + 5y_{11} + y_{12}]$$
$$\int_{x_0+(n-6)h}^{x_0+nh} y \,\mathrm{d}\, x = \frac{3h}{10}[y_{n-6} + 5y_{n-5} + y_{n-4} + 6y_{n-3} + y_{n-2} + 5y_{n-1} + y_n]$$

Adding these integrals, we get

$$\int_{x_0}^{x_0+nh} y \,\mathrm{d}\, x = \frac{3h}{10}[y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + 2y_6 + 5y_7 + y_8 + \dots]$$

This formula is known as Weddle's rule.

# Chapter 10

# Curve Fitting and Spline Interpolation

## 10.1 Curve Fitting by Least Squares Method

The method of least squares may be one of the most systematic procedure to fit a curve through given data points.
Consider the problem of fitting a set of data points

$$(x_r, y_r), \qquad r = 1, 2, 3, \ldots, m$$

to a curve $y = f(x)$ whose values depend on $n$ parameters $c_1, c_2, c_3, \ldots, c_n$. The values of the function at a point depends on the values of the parameter involved. In least square method we determine a set of values of the parameter $c_1, c_2, c_3, \ldots, c_n$ such that the sum of the squares of the error

$$E(c_1, c_2, \ldots, c_n) = \sum_{i}^{m} \left[f\left(x_i, c_1, c_2, \ldots, c_n\right) - y_i\right]^2$$

is minimum.
The necessary conditions for $E$ to have a minimum is that

$$\frac{\partial E}{\partial c_i} = 0, \qquad i = 1, 2, 3, \ldots, n$$

This condition gives a system of $n$ equations, called *normal equations*, in $n$ unknowns $c_1, c_2, c_3, \ldots, c_n$. If the parameters appear in the function in non-linear form, the normal equations become non-linear and is difficult to solve. This difficulty may be avoided if $f(x)$ is transformed to a form which is linear in parameter.

### 10.1.1 Parameters in Nonlinear Form

(a) **Power function:** Let the curve

$$y = ax^b$$

be fitted to the given data.
Taking logarithm of both sides, we get

$$\ln y = \ln a + b \ln x$$

which can be written in the form

$$Y = A + bX$$

where,

$$Y = \ln y, \quad A = \ln a, \quad X = \ln x.$$

(b) Let the curve

$$y = \frac{400}{1 + ce^{bx}}$$

be fitted to the given data.
The equation of the curve can be rewritten as

$$\frac{400}{y} - 1 = ce^{bx}$$

Taking logarithm of both sides, we get

$$\ln\left(\frac{400}{y} - 1\right) = \ln c + bx$$

which can be written in the form

$$Y = A + bx \qquad \text{where} \qquad Y = \ln\left(\frac{400}{y} - 1\right), \quad A = \ln c.$$

**Problem 10.1.1.** The average price, $P$, of a certain type of second-hand car is believed to be related to its age, $x$ years, by an equation of the form

$$P = 50 + ae^{bx}$$

where $a$ and $b$ are constants. Data from a recent newspaper give the following average price (in Taka) for used car of this type,

| $x$ | $P$ (in thousands) |
|---|---|
| 1 | 774.4 |
| 2 | 603.4 |
| 3 | 439.2 |
| 4 | 360.0 |
| 5 | 328.3 |

(a) Estimate the values of $a$ and $b$ rounded to 3 significant figures.

(b) Estimate the price of a car of this type that is 6 years old and the original new price of that car.

**Solution.** (a) The curve $P = 50 + ae^bx$ is to be fitted to the given data.
The equation of the curve can be rewritten as $P - 50 = ae^bx$
Taking logarithm of both sides, we get $\ln(P - 50) = \ln a + bx$
which can be written in the form

$$Y = A + bx \qquad \text{where} \quad Y = \ln(P - 50), \quad A = \ln a.$$

$$E(A, b) = \sum_{i=1}^{5}(A + bx_i - Y_i)^2$$

| $n$ | $x$ | $P$ | $Y$ | $xY$ | $x^2$ |
|---|---|---|---|---|---|
| 1 | 1 | 774.4 | 6.585 | 6.585 | 1 |
| 2 | 2 | 603.4 | 6.316 | 12.632 | 4 |
| 3 | 3 | 439.2 | 5.964 | 17.892 | 9 |
| 4 | 4 | 360.0 | 5.737 | 22.948 | 16 |
| 5 | 5 | 328.3 | 5.629 | 28.145 | 25 |
| Sum | 15 | | 30.231 | 88.202 | 55 |

At minimum,

$$\frac{\partial E}{\partial A} = 0 \qquad \text{and} \qquad \frac{\partial E}{\partial b} = 0$$

which give

$$2\sum[(A + bx_i - Y_i)]1 = 0$$
$$2\sum(A + bx_i - Y_i)x_i = 0$$

which can be rearranged as

$$A\sum 1 + b\sum x_i = \sum Y_i$$
$$A\sum x_i + b\sum {x_i}^2 = \sum x_x Y_i$$

The sum can be calculated in a tabular form as below: The normal equations are

$$5A + 15b = 30.231$$
$$15A + 55b = 88.202$$

Dividing 1st eq. by 5 and 2nd by 15, we have

$$A + 3b = 6.046$$
$$A + 3.667b = 5.880$$

Subtracting

$$0.667b = -0.166 \qquad \text{or} \quad b = -0.249$$

and

$$A = 5.88 - 3.667(-0.249) = 6.793$$

and hence

$$a = e^6.793 \approx 892$$

The required best fitting curve is

$$P = 50 + 892e^{-0.249x}$$

(b) When $x = 6$, we have

$$P = 50 + 892e^{-0.249\times 6} \approx 250.2$$

The price of the 6 years old car is Tk. 250.2 thousand. New price corresponds to $x = 0$ and is $50 + 892 = 942$ thousand taka.

| $x$ | $y$ |
|---|---|
| $-1$ | 1.5 |
| 0 | 3.7 |
| 2 | 6.2 |
| 4 | 8.5 |
| 5 | 12.8 |

### 10.1.2 Exercise

1. Find the least square line $y = ax + b$ to the following data

2. Students collected the following set of data to find the gravitational constant $g$. Use the relation $d = (gt^2)/2$, where $d$ is the distance in metres and $t$ is time in seconds, to find the value of $g$.

| Time ($t$) | Distance ($d$) |
|---|---|
| 0.2 | 0.2142 |
| 0.4 | 0.7789 |
| 0.6 | 1.7676 |
| 0.8 | 3.1365 |
| 5.0 | 4.9075 |

3. Fit a curve of the form $y = ax^2 + be^{-x}$ to the following data.

| $x$ | $y$ |
|---|---|
| 1 | 5.18 |
| 2 | 6.70 |
| 4 | 21.31 |
| 5 | 33.07 |
| 8 | 84.48 |

4. The temperature in a metal strip was measured at various time intervals. Given that the relation between the temperature $T(°C)$ and time $t$ (min) is of the form $T = a + be^{t/2}$. Six pairs of observations of the two variables $T$ and $t$ gave the following results.

$$\sum T = 165.5, \quad \sum e^{t/2} = 48.71, \quad \sum e^t = 656.6, \quad \sum Te^{t/2} = 1425$$

   Find the temperature after 7 minutes.

5. Given the following set of values of $x$ and $y$ :

| $x$ | $y$ |
|---|---|
| 2 | 1.14 |
| 3 | 1.45 |
| 6 | 1.97 |
| 7 | 2.41 |
| 10 | 2.99 |

(a) Fit the power equation $y = ax^b$ to the given data.

(b) Find the best fitting curve of the form $y = ae^{bx}$.

(c) Fit the saturation growth rate model $y = \frac{ax}{b+x}$ to the above data.

By finding errors determine which one of the above is the best fitting curve.

6. The following table gives the population of a certain country from 1960 to 2000 at ten yearly interval

| Year | Population $P$ (in Lac) |
|---|---|
| 1970 | 20.5 |
| 1980 | 26.4 |
| 1990 | 33.1 |
| 2000 | 40.4 |
| 2010 | 48.2 |

It is known that if environmental factors remain constant, the population size, $P$, is given by

$$P(t) = \frac{200}{1 + ce^{at}}$$

where $c$ and $a$ are constants.
Estimate, to 3 significant figures, the values of $c$ and $a$.
Hence, predict the population in the year 2015.

7. A bowl of hot water is kept in a room of constant temperature $25°C$. At 5 minutes interval temperature of the water is recorded and listed as given below.

| $t$ (in min) | $T$ (in $°C$) |
|---|---|
| 5 | 75.3 |
| 10 | 70.0 |
| 15 | 63.4 |
| 20 | 58.5 |
| 25 | 54.0 |

The law of cooling can be assumed to be of the form $T = 25 + ae^{-kt}$.
Find, to 2 significant figures, the best values of $a$ and $k$.

Estimate the initial temperature.
Hence, find the time, to the nearest minute, when the temperature of the water in the bowl will be $51°C$.

8. The pressure $p$ and volume $V$ of a fixed mass of gas are believed to be related by an equation of the form

$$pV^{\gamma} = c$$

where $\gamma$ and $c$ are constants.
In six set of experiments on the fixed mass of gas, in each of which $p$ was controlled and $V$ measured. The results are as follows:

| $p\,(Nm^{-2})$ | $V\,(m^3)$ |
|---|---|
| 0.4 | 1.894 |
| 0.6 | 1.426 |
| 0.8 | 1.166 |
| 1.0 | 0.998 |
| 1.2 | 0.878 |
| 1.4 | 0.789 |

Estimate to 2 decimal places

(i) the value of $\gamma$,

(ii) the value of $V$ when $p = 0.75Nm^{-2}$.

9. The method of least squares is used to estimate the constants $a$, $b$, $c$ in the formula

$$y = a + b\sin x + ce^{-x/5}$$

Eight pairs of data points leads to the following normal equations, where the missing numerical values are to be determined.

$$\begin{aligned} \text{\_\_\_\_\_}a - 3.616b + 5.784c &= 100.06 \\ \text{\_\_\_\_\_}a + 3.261b - 2.737c &= -46.796 \\ \text{\_\_\_\_\_}a + \text{\_\_\_\_\_}b + 4.403c &= 73.060 \end{aligned}$$

The method of Gaussian elimination leads to the following equations:

$$\begin{aligned} a - 0.452b + \text{\_\_\_\_\_}c &= \text{\_\_\_\_\_} \\ 0.450b - 0.034c &= -0.433 \\ 1.734c &= 4.895 \end{aligned}$$

Supply the missing values and complete the solution of the set of equations, giving $a$, $b$ and $c$ to two decimal places.
Using the estimated values of $a$, $b$ and $c$, find the value of $y$ given by the formula to one decimal place when $x = 4$.

10. Use a suitable substitution to derive a linearized form for the following functions:

(i)

$$y = \frac{x}{ax+b}$$

(ii)

$$y = (ax+b)^{-1}$$

(iii)

$$x = a^x b^y + 2e^y$$

(iv)

$$y = \frac{5+ax}{b+x^3}$$

(v)

$$y = \frac{x^2}{(a+bx)^2}$$

(vi)

$$y = \frac{1}{a(2^y)+b(2^{-x})}$$

(vii)

$$y = \frac{x^2}{(ax+1)(bx+2)}$$

(viii)

$$y = \frac{x}{1+ae^{bx}}$$

(ix)

$$y = \frac{1}{\sqrt{(x+a)(x+b)}}$$

## 10.2 Spline Interpolation

Spline interpolation is a form of interpolation where the interpolant is a special type of piecewise polynomial called a **spline**. Spline interpolation is preferred over polynomial interpolation because the interpolation error can be made small even when using low degree polynomials for the spline.
Divide the interval containing the tabular points as subintervals $x_0 < x_1 < x_2 < \cdots < x_n$ and replace the function $f(x)$ by some lower degree interpolating polynomial in each of the subinterval. The tabular points $x_0, x_1, x_3, \ldots, x_n$ at which the function changes its character is termed as **knots** in the theory of spline.

A function $S(x)$ of the form

$$S(x) = \begin{cases} f_0(x) & x \in [x_0, x_1] \\ f_1(x) & x \in [x_1, x_2] \\ \vdots & \\ f_{n-1}(x) & x \in [x_{n-1}, x_n] \end{cases}$$

is called a spline of degree $m$ if

(i) the domain of $S(x)$ is the interval $[x_0, x_n]$

(ii) $S(x)$, $S'(x)$, $S''(x), \ldots, S^{(m-1)}(x)$ are all continuous functions on $[x_0, x_n]$

(iii) $S(x)$ is a polynomial of degree less than equal to $m$ on each subintervals $[x_k, x_{k+1}]$, $k = 0, 1, 2, 3, \ldots, n-1$.

### 10.2.1 Linear Spline Interpolation

The simplest polynomial to use, a polynomial of degree one, produces a polygon path that consists of line segments that pass through the points. The point-slope formuala for the line segment may be used to represent this piecewise linear curve:

$$S(x) = f_k(x) = a_k(x - x_k) + b_k, \qquad \text{for } x_k \leq x \leq x_{k+1}(k = 0, 1, 2, \ldots, n-1)$$

Since the line passes through $(x_k, y_k)$ and $(x_{k+1}, y_{k+1})$ we have

$$f_k(x_k) = y_k = b_k$$

and

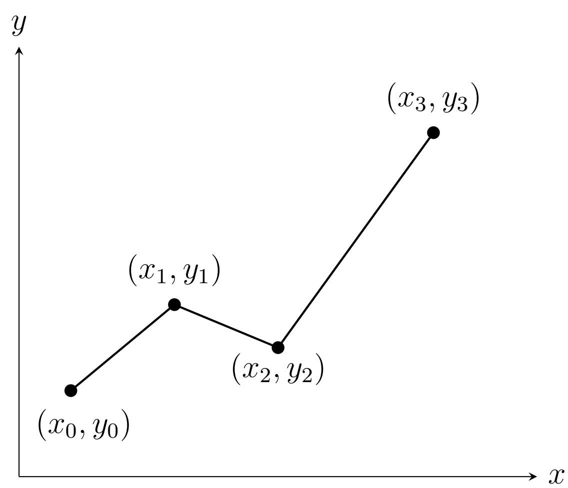
$$f_k(x_{k+1}) = y_{k+1} = a_k(x_{k+1} - x_k) + b_k$$

or

$$a_k = \frac{y_{k+1} - y_k}{x_k + 1 - x_k} = \frac{\Delta y_k}{h_k}$$

where

$$\Delta y_k = y_{k+1} - y_k \qquad \text{and} \quad h_k = x_{k+1} - x_k$$




The resulting linear spline curve $f_k(x)$ in $[x_k, x_{k+1}]$ can be written as

$$f_k(x) = \frac{\Delta y_k}{h_k}(x - x_k) + y_k, \qquad (k = 0, 1, 2, \ldots, n-1)$$

The resulting curve looks like a “broken line” as shown in the diagram.

### 10.2.2 Quadratic Spline Interpolation

For a quadratic spline through $(x_k, y_k)$ we may take $f_k(x)$ is of the form

$$f_k(x) = a_k(x - x_k)^2 + b_k(x - x_k) + c_k \tag{10.1}$$

The quadratic spline function $S(x)$ is

$$S(x) = f_k(x)$$

on the interval $[x_k, x_{k+1}]$ for $k = 0, 1, 2, \ldots, n-1$.
Each quadratic polynomial, $f_k(x)$, has three unknown constants, hence there are $3n$ unknown coefficients $a_k, b_k, c_k$ $(k = 0, 1, 2, \ldots, n-1)$.
To find $3n$ unknowns, one needs to set up $3n$ equations and then simultaneously solve them. These $3n$ equations are found as follows:

1. As the splines pass through $(x_k, y_k)$, we have

$$f_k(x_k) = c_k = y_k \qquad \text{for} \quad k = 0, 1, 2, \ldots, n-1$$

   and

$$f_{n-1}(x_n) = y_n$$

2. Continuity of $S(x)$ at the interior points gives

$$f_k(x_{k+1}) = f_{k+1}(x_{k+1}) \tag{10.2}$$

   Since there are $(n-1)$ interior points, we have $(n-1)$ such equations.

3. Continuity of $S'(x)$ at the interior points gives

$$f_k'(x_{k+1}) = f_{k+1}'(x_{k+1}) \tag{10.3}$$

Differentiating eq. (10.1) we have

$$f_k'(x) = 2a_k(x - x_k) + b_k$$

From (10.3) we have

$$2a_k h_k + b_k = b_{k+1}$$

Using the notation,

$$f_k'(x_k) = b_k = Z_k$$

we have

$$a_k = \frac{Z_{k+1} - Z_k}{2h_k}, \qquad k = 0, 1, 2, \ldots, n-1$$

From Eq. (10.2),

$$\begin{aligned}
a_k(h_k^2) + b_k(h_k) + c_k &= c_{k+1} \\
a_k h_k + b_k &= \frac{c_{k+1} - c_k}{h_k} = \frac{y_{k+1} - y_k}{h_k} \\
\frac{Z_{k+1} - Z_k}{2} + Z_k &= \frac{y_{k+1} - y_k}{h_k} \\
Z_{k+1} + Z_k &= 2\frac{\Delta y_k}{h_k}
\end{aligned}$$

Here also $(n-1)$ interior points, we have $(n-1)$ such equations.
So far, the total number of equations are

$$(2n) + (n-1) = (3n-1)$$

We still need one more equation. We can assume that the first spline is linear, that is

$$a_0 = 0$$

This gives us $3n$ equations for $3n$ unknowns. These can be solved by a number of techniques used to solve simultaneous linear equations.
It should be mentioned that the curvature of the quadratic spline changes abruptly at each knot, and the curve may not be pleasing to the eye.

### 10.2.3 Cubic Spline Interpolation

For the cubic spline through the points $(x_k, y_k)$, $k = 0, 1, 2, \dots, n$ we may take $f_k(x)$ is of the form

$$f_k(x) = a_k(x-x_k)^3 + b_k(x-x_k)^2 + c_k(x-x_k) + d_k \quad \text{in}[x_k, x_{k+1}] \tag{10.4}$$

Thus the cubic spline function $S(x)$ is of the form

$$S(x) = f_k(x) \qquad \text{on the interval} \quad [x_k, x_{k+1}] \quad \text{for } k = 0, 1, 2, 3, \dots, n-1$$

with the following properties:

(a)
$$f_k(x_k) = y_k, \qquad k = 0, 1, 2, \dots, n-1 \quad \text{and} \quad f_{n-1}(x_n) = y_n$$

(b)
$$f_k(x_{k+1}) = f_{k+1}(x_{k+1}), \qquad k = 0, 1, 2, \dots, n-1$$

(c)
$$f_k^{'}(x_{k+1}) = f_{k+1}^{'}(x_{k+1}), \qquad k = 0, 1, 2, \dots, n-1$$

(d)
$$f_k^{''}(x_{k+1}) = f_{k+1}^{''}(x_{k+1}), \qquad k = 0, 1, 2, \dots, n-1$$

Each cubic polynomial, $f_k(x)$, has four unknown constants, hence there are $4n$ coefficients to be determined. The data points supply $(n+1)$ conditions, and properties (b), (c) and (d) each supply $(n-1)$ conditions. Hence, $n+1+3(n-1) = 4n-2$ conditions are specified. Two more conditions are needed which will be discussed later.

The conditions (a) then gives

$$d_k = y_k, \qquad k = 0, 1, 2, \dots, n-1$$

From (b) we have

$$\begin{aligned} y_{k+1} &= a_k(x_{k+1}-x_k)^3 + b_k(x_{k+1}-x_k)^2 + c_k(x_{k+1}-x_k) + y_k \\ &= a_k{h_k}^3 + b_k{h_k}^2 + c_k h_k + y_k, \qquad k = 0, 1, 2, \dots, n-1 \end{aligned} \tag{10.5}$$

where $h_k = (x_{k+1} - x_k)$.
Differentiating (10.4) we have

$$f_k^{'}(x) = 3a_k(x - x_k)^2 + 2b_k(x - x_k) + c_k \tag{10.6}$$
$$f_k^{''}(x) = 6a_k(x - x_k) + 2b_k \tag{10.7}$$

Development is simplified if we write the equations in terms of the second derivatives-that is, if we use

$$M_k = f_k^{''}(x_k) \qquad \text{for } k = 0, 1, 2, \ldots, n-1 \qquad \text{and } M_n = f_k^{''}(x_k)$$

From Eq.(10.7), we have

$$M_k = 6a_k(x_k - x_k) + 2b_k = 2b_k$$
$$M_{k+1} = 6a_k(x_{k+1} - x_k) + 2b_k = 6a_k h_k + 2b_k$$

Hence we can write

$$b_k = \frac{M_k}{2}$$
$$a_k = \frac{M_{k+1} - M_k}{6h_k}$$

and from Eq.(10.5), we have

$$y_{k+1} = \left(\frac{M_{k+1} - M_k}{6h_k}\right) {h_k}^3 + \frac{M_k}{2} {h_k}^2 + c_k h_k + y_k$$
$$c_k = \frac{y_{k+1} - y_k}{h_k} - \frac{h_k}{6}(M_{k+1} + 2M_k)$$

In order to get the cubic splines, it is required to determine the second derivatives

$$M_0, M_1, M_2, \ldots, M_n$$

at the knots and can be evaluated by the continuity of the second derivatives.
From Eq. (10.4),

$$f_k^{'}(x) = 3a_k(x - x_k)^2 + 2b_k(x - x_k) + c_k$$

At the common knot $(x_{k+1}, y_{k+1})$ the first derivatives $f_k^{'}(x)$ and $f_(k+1)^{'}(x)$ should be equal i.e.

$$f_{k+1}^{'}(x_{k+1}) = f_k^{'}(x_{k+1})$$

But

$$f_{k+1}^{'}(x_{k+1}) = c_{k+1} = \frac{y_{k+2} - y_{k+1}}{h_{k+1}} - \frac{h_{k+1}}{6}(M_{k+2} + 2M_{k+1}) \tag{10.8}$$

and

$$\begin{aligned} f_k^{'}(x_{k+1}) &= 3a_k h_k^2 + 2b_k h_k + c_k \\ &= 3\left(\frac{M_{k+1} - M_k}{6h_k}\right) {h_{k-1}}^2 + 2\left(\frac{M_k}{2}\right) h_k + \frac{y_{k+1} - y_k}{h_k} - \frac{h_k}{6}(M_{k+1} + 2M_k) \\ &= \frac{y_{k+1} - y_k}{h_k} + \frac{h_k}{6}(M_{k+1} + 2M_k) \end{aligned} \tag{10.9}$$

Eq. (10.8) with Eq.(10.9),

$$h_k M_k + 2(h_k + h_{k+1})M_{k+1} + h_{k+1}M_{k+2} = 6\left[\frac{\Delta y_{k+1}}{h_{k+1}} - \frac{\Delta y_k}{h_k}\right], \qquad k = 0, 1, 2, \ldots, n-2 \tag{10.10}$$

### 10.2.4 End Points Constraints

We need to impose suitable end-conditions to get a unique cubic spline. The standard end points constraints are mentioned below.

| Description of the strategy | Equations involving $M_0$ and $M_n$ |
|---|---|
| Natural cubic spline "a relaxed curve": $S'(x_0)$ and $S''(x_n)$. | $M_0 = 0$, $M_n = 0$ |
| Clamped cubic spline: specify $S'(x_0) = A$ and $S'(x_n) = B$. | $2M_0 + M_1 = \frac{6}{h_0}\left[\frac{\Delta y_0}{h_0} - A\right]$ <br> $M_n + 2M_{n-1} = \frac{6}{h_{n-1}}6\left[B - \frac{\Delta y_{n-1}}{h_{n-1}}\right]$ |
| Extrapolated cubic spline: $M_0$ as linear extrapolation from $M_1$ and $M_2$ : $\frac{M_1-M_0}{h_0} = \frac{M_2-M_1}{h_1}$ <br> $M_n$ as linear extrapolation from $M_{n-1}$ and $M_{n-2}$: $\frac{M_n - M_{n-1}}{h_{n-1}} = \frac{M_{n-1} - M_{n-2}}{h_{n-2}}$ | $M_0 = M_1 - \frac{h_0(M_2 - M_1)}{h_1}$ <br> $M_n = M_{n-1} - \frac{h_{n-1}(M_{n-1} - M_{n-2})}{h_{n-2}}$ |
| Parabolically terminated spline ($S''(x)$ is constant near the end points) | $M_0 = M_1, \quad M_n = M_{n-1}$ |

**Problem 10.2.1.** Find the linear spline for the following data:

| $x$ | $y$ |
|---|---|
| 0 | 0.0 |
| 1 | 0.5 |
| 2 | 2.0 |
| 3 | 1.5 |

**Solution.** Here, $h_0 = h_1 = h_2 = 1$.
Linear spline functions are

$$f_0(x) = \frac{\Delta y_0}{h_0}(x - x_0) + y_0 = 0.5x \qquad 0 \le x \le 1$$

$$f_1(x) = \frac{\Delta y_1}{h_1}(x - x_1) + y_1 = 1.5(x - 1) + 0.5 \qquad 1 \le x \le 2$$

$$f_2(x) = \frac{\Delta y_2}{h_2}(x - x_2) + y_2 = -0.5(x - 2) + 2 \qquad 2 \le x \le 3$$

Linear spline function is

$$S(x) = \begin{cases} 0.5x, & 0 \leq x \leq 1 \\ 1.5(x-1) + 0.5, & 1 \leq x \leq 2 \\ -0.5(x-2) + 2, & 2 \leq x \leq 3 \end{cases}$$

**Problem 10.2.2.** Find the quadratic spline for the following data:

| $x$ | $y$ |
|---|---|
| 0 | 0.0 |
| 1 | 0.5 |
| 2 | 2.0 |
| 3 | 1.5 |

**Solution.** Here, $h_0 = h_1 = h_2 = 1$.

$$Z_{k+1} + Z_k = 2\frac{\Delta y_k}{h_k} \qquad k = 0, 1, 2$$

Using the recurrence relation, we obtain the equations

$$\begin{aligned} Z_1 + Z_0 &= 2(0.5) = 1 \\ Z_2 + Z_1 &= 2(2 - 0.5) = 3 \\ Z_3 + Z_2 &= 2(1.5 - 2) = -1 \end{aligned}$$

Using the end condition $a_0 = 0$, we have

$$\frac{Z_1 - Z_0}{2(1)} = 0 \qquad \text{or} \quad Z_1 = Z_0$$

Solving above equations, we have

$$\begin{aligned} Z_0 = Z_1 &= \frac{1}{2} = 0.5 \\ Z_2 &= 3 - 0.5 = 2.5 \\ Z_3 &= -1 - 2.5 = -3.5 \end{aligned}$$

With these values of Z's the spline coefficients the spline coefficients can be obtained as follows:
With k = 0,

$$a_0 = 0, \qquad b_0 = Z_0 = 0.5, \qquad c_0 = y_0 = 0$$

and

$$f_0(x) = 0.5x, \qquad 0 \leq x \leq 1$$

With k = 1,

$$a_1 = \frac{Z_2 - X_1}{2h_1} = \frac{2.5 - 0.5}{2(1)} = 1, \qquad b_1 = Z_1 = 0.5, \qquad c_1 = y_1 = 0.5$$

and

$$f_1(x) = (x-1)^2 + 0.5(x-1) + 0.5, \qquad 1 \leq x \leq 2$$

With k = 2,

$$a_2 = \frac{Z_3 - Z_2}{2h_2} = \frac{-3.5 - 2.5}{2(1)} = 3, \qquad b_2 = Z_2 = 2.5, \qquad c_2 = y_2 = 2$$

and

$$f_2(x) = -3(x-2)^2 + 2.5(x-2) + 2, \qquad 2 \leq x \leq 3$$

The quadratic spline function is

$$S(x) = \begin{cases} 0.5x, & 0 \leq x \leq 1 \\ (x-1)^2 + 0.5(x-1) + 0.5, & 1 \leq x \leq 2 \\ -3(x-2)^2 + 2.5(x-2) + 2, & 2 \leq x \leq 3 \end{cases}$$

**Problem 10.2.3.** Consider the points

| $x$ | $y$ |
|---|---|
| 0 | 0.0 |
| 1 | 0.5 |
| 2 | 2.0 |
| 3 | 1.5 |

(a) Find the natural cubic spline which fits the given data.

(b) Find the clamped cubic spline with conditions $S'(0) = 1$ and $S'(3) = -1$.

(c) Find the extrapolated cubic spline.

**Solution.** The governing recurrence is

$$h_k M_k + 2(h_k + h_{k+1})M_{k+1} + h_{k+1}M_{k+2} = 6\left[\frac{\Delta y_{k+1}}{h_{k+1}} - \frac{\Delta y_k}{h_k}\right], \qquad k = 0, 1, 2$$

First, compute the quantities

$$h_0 = h_1 = h_2 = 1$$

and

$$\frac{\Delta y_0}{h_0} = \frac{0.5 - 0}{1} = 0.5, \quad \frac{\Delta y_1}{h_1} = \frac{2 - 0.5}{1} = 1.5, \quad \frac{\Delta y_2}{h_2} = \frac{1.5 - 2.0}{1} = -1.5$$

(a) Using natural cubic spline
Here the end conditions are

$$M_0 = M_3 = 0$$

The equations corresponding to $k = 0, 1$ are

$$M_0 + 4M_1 + M_2 = 6(1.5 - 0.5) = 6$$

or

$$4M_1 + M_2 = 6 \tag{10.11}$$

and

$$M_1 + 4M_2 + M_3 = 6(-0.5 - 1.5) = -12$$

or

$$M_1 + 4M_2 = -12 \tag{10.12}$$

Solving (10.11) and (10.12),

$$M_1 = 2.4, \qquad M_2 = -3.6$$

With $k = 0$,

$$\begin{aligned}
a_0 &= \frac{M_1 - M_0}{6} = \frac{2.4}{6} = 0.4 \\
b_0 &= \frac{M_0}{2} = 0 \\
c_0 &= \frac{\Delta y_0}{h_0} - \frac{h_0}{6}(M_1 + 2M_0) = 0.5 - \frac{2.4}{6} = 0.1 \\
d_0 &= y_0 = 0
\end{aligned}$$

and

$$f_0(x) = 0.4x^3 + 0.1x, \qquad 0 \le x \le 1$$

With $k = 1$,

$$\begin{aligned}
a_1 &= \frac{M_2 - M_1}{6} = \frac{-6}{6} = -1 \\
b_1 &= \frac{M_1}{2} = \frac{2.4}{2} = 1.2 \\
c_1 &= \frac{\Delta y_1}{h_1} - \frac{h_1}{6}(M_2 + 2M_1) = 1.5 - \frac{1.2}{6} = 1.3 \\
d_1 &= y_1 = 0.5
\end{aligned}$$

and

$$f_1(x) = -(x-1)^3 + 1.2(x-1)^2 + 1.3(x-1) + 0.5 \qquad 0 \le x \le 1$$

With $k = 2$,

$$\begin{aligned}
a_2 &= \frac{M_3 - M_2}{6} = \frac{3.6}{6} = 0.6 \\
b_2 &= \frac{M_2}{2} = \frac{-3.6}{2} = -1.8 \\
c_2 &= \frac{\Delta y_2}{h_2} - \frac{h_2}{6}(M_3 + 2M_2) = -0.5 - \frac{-7.2}{6} = 0.7 \\
d_2 &= y_2 = 2
\end{aligned}$$

and

$$f_2(x) = 0.6(x-2)^3 - 1.8(x-2)^2 + 0.7(x-2) + 2, \qquad 0 \le x \le 1$$

The natural cubic spline function is

$$S(x) = \begin{cases} 0.4x^3 + 0.1x, & 0 \le x \le 1 \\ -(x-1)^3 + 1.2(x-1)^2 + 1.3(x-1) + 0.5, & 1 \le x \le 2 \\ 0.6(x-2)^3 - 1.8(x-2)^2 + 0.7(x-2) + 2, & 2 \le x \le 3 \end{cases}$$

(b) With clamped spline condition
The first derivative boundary conditions are:

$$S^{'}(0) = 0.2 \qquad \text{and} \qquad S^{'}(3) = -1$$

The equations involving M's are

$$\begin{aligned}
&\text{At left end:} & 2M_0 + M_1 &= 6(0.5 - 0.2) = 1.8 \\
&\text{For } k = 0: & M_0 + 4M_1 + M_2 &= 6(1.5 - 0.5) = 6 \\
&\text{For } k = 1: & M_1 + 4M_2 + M_3 &= 6(-0.5 - 1.5) = -12 \\
&\text{At right end:} & M_2 + 2M_3 &= 6(-1 + 0.5) = -3
\end{aligned}$$

Solution of the above equations are

$$M_0 = -0.36, \qquad M_1 = 2.52, \qquad M_2 = -3.72, \qquad M_3 = 0.36$$

Corresponding spline coefficients are

$$\begin{aligned}
&k = 0: & a_0 = 0.48, \quad b_0 = -0.18, \quad c_0 = 0.2, \quad d_0 = 0 \\
&k = 1: & a_1 = -1.04, \quad b_1 = 1.26, \quad c_1 = 1.28, \quad d_1 = 0.5 \\
&k = 2: & a_2 = 0.68, \quad b_2 = -1.86, \quad c_2 = 0.68, \quad d_2 = 2
\end{aligned}$$

Thus the clamped cubic spline function is

$$S(x) = \begin{cases} 0.48x^3 - 0.18x^2 + 0.2x, & 0 \le x \le 1 \\ -1.04(x-1)^3 + 1.26(x-1)^2 + 1.28(x-1) + 0.5, & 1 \le x \le 2 \\ 0.68(x-2)^3 - 1.8(x-2)^2 + 0.68(x-2) + 2, & 2 \le x \le 3 \end{cases}$$

(c) With extrapolated boundary condition
The equations involving M's are

$$\begin{aligned}
&\text{At left end:} & M_1 - M_0 &= M_2 - M_1 \\
&\text{or} & M_0 - 2M_1 + M_2 &= 0 \\
&\text{For } k = 0: & M_0 + 4M_1 + M_2 &= 6(1.5 - 0.5) = 6 \\
&\text{For } k = 1: & M_1 + 4M_2 + M_3 &= 6(-0.5 - 1.5) = -1.2 \\
&\text{At right end:} & M_3 - M_2 &= M_2 - M_1 \\
&\text{or} & M_1 - 2M_2 + M_3 &= 0
\end{aligned}$$

Solution of the above equations are

$$M_0 = 4, \qquad M_1 = 1, \qquad M_2 = -2, \qquad M_3 = -5$$

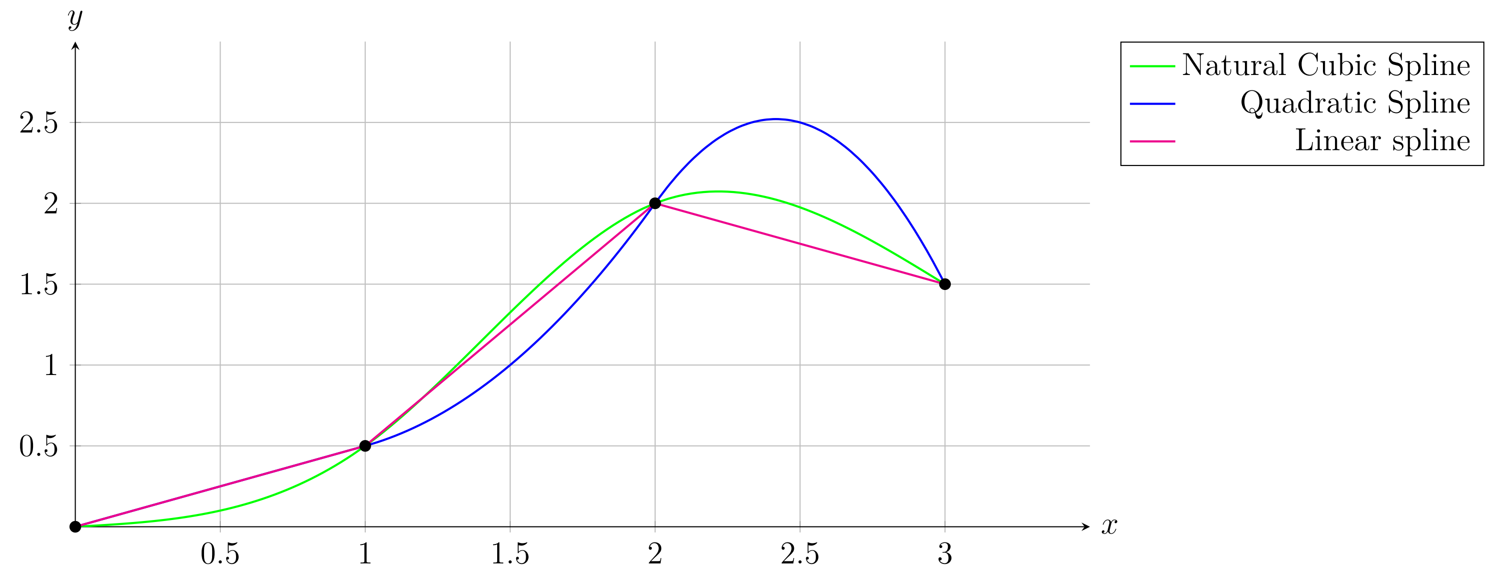
Corresponding spline coefficients are

$$\begin{aligned}
&k = 0: & a_0 = -0.5, \quad b_0 = 2, \quad c_0 = -1, \quad d_0 = 0 \\
&k = 1: & a_1 = -0.5, \quad b_1 = 0.5, \quad c_1 = 1.5, \quad d_1 = 0.5 \\
&k = 2: & a_2 = -0.5, \quad b_2 = -1, \quad c_2 = 1, \quad d_2 = 2
\end{aligned}$$

Thus the cubic spline function with extrapolated boundary condition is

$$S(x) = \begin{cases} -0.5x^3 + 2x^2 - x, & 0 \le x \le 1 \\ -0.5(x-1)^3 + 0.5(x-1)^2 + 1.5(x-1) + 0.5, & 1 \le x \le 2 \\ -0.5(x-2)^3 - (x-2)^2 + (x-2) + 2, & 2 \le x \le 3 \end{cases}$$

Comparison of the three types of spline curves are shown below:




## 10.3 EXERCISES

1. Determine whether this function is a first degree spline:

$$f(x) = \begin{cases} x, & -1 \le x \le 1 \\ 1 - 2(x-1), & 1 \le x \le 2 \\ -1 + 3(x-2), & 2 \le x \le 3 \end{cases}$$

2. Is $f(x) = |x|$ a first degree spline? Why or why not?

3. Are these functions quadratic splines? Explain why or why not.

   (a)

$$f(x) = \begin{cases} 0.1x^2, & 0 \le x \le 1 \\ 9.3x^2 - 18.4x + 9.2, & 1 \le x \le 1.3 \end{cases}$$

   (b)

$$f(x) = \begin{cases} -x^2, & x \le 0 \\ x, & x > 0 \end{cases}$$

4. Find first-degree and quadratic splines for the following data:

| $x$ | $y$ |
|---|---|
| $-1.0$ | 2 |
| 0.0 | 1 |
| 0.5 | 0 |
| 1.0 | 1 |
| 2.0 | 2 |

5. Prove that the derivative of a quadratic spline is a first degree spline.

6. Show that the indefinite integral of a first-degree spline is a second-degree spline.

7. Determine whether $f(x)$ is a cubic spline with knots -1, 0, 1 and 2:

$$f(x) = \begin{cases} 1 + 2(x+1) + (x+1)^3, & -1 \le x \le 0 \\ 4 + 5x + 3x^3, & 0 \le x \le 1 \\ 11 + 1(x-1) + 3(x-1)^2 + (x-1)^3, & 1 \le x \le 2 \end{cases}$$

8. A natural cubic spline $S$ on $[0, 2]$ is defined by

$$S(x) = \begin{cases} 1 + 2x - x^3, 0 \le x \le 1 \\ 2 + b(x-1) + c(x-1)^2 + d(x-1)^3, & 1 \le x \le 2 \end{cases}$$

Find $b$, $c$, and $d$.

9. A natural cubic spline for a function $f(x)$ on $[-1, 2]$ is defined by

$$f(x) = \begin{cases} A(x+1)^3 + B(x+1)^2 - 5(x+1) + 5, & -1 \le x \le 0 \\ x^3 + 3x^2 - 2x + 1, & 0 \le x \le 1 \\ a(x+1)^3 + b(x+1)^2 + c(x+1) + d, & 1 \le x \le 2 \end{cases}$$

Find the values of $A$, $B$, $a$, $b$, $c$ and $d$. Hence, estimate the values of $f(-0.5)$ and $f(1.5)$.

10. A clamped cubic spline for a function $f(x)$ is defined on $[1, 3]$ by

$$f(x) = \begin{cases} 3(x-1) + 2(x-1)^2 - (x-1)^3, & 0 \le x \le 1 \\ a + b(x-2) + c(x-2)^2 + d(x-2)^3, & 1 \le x \le 2 \end{cases}$$

Given $f'(1) = f'(3)$, find $a$, $b$, $c$, and $d$.

11. Find the natural cubic splines satisfying the following data points:

(a) $(0, 1)$, $(1, 1)$ and $(2, 5)$

(b) $(-1, 1)$, $(0, 2)$ and $(1, -1)$

| $x$ | $y$ |
|---|---|
| $-1$ | 9 |
| 0 | 26 |
| 3 | 56 |
| 4 | 29 |

12. Find the natural cubic spline which fits the following data:

| $x$ | $y$ |
|---|---|
| 1 | 1 |
| 2 | 5 |
| 3 | 11 |
| 4 | 8 |

and hence find the values of $y(1.5)$.

13. Find the natural cubic spline which fits the following data:

| $x$ | $f(x)$ |
|---|---|
| 1 | 6 |
| 2 | $-3$ |
| 3 | 6 |
| 4 | 2 |
| 5 | $-6$ |

Find $f(x)$ at $x = 1.3$.

14. Consider the points

    (a) Find the natural cubic spline which fits this data and hence estimate the value of $y(1)$.

    (b) Find the clamped cubic spline with conditions $S'(-1) = 1$ and $S'(4) = -1$.

    (c) Find the extrapolated cubic spline.

15. Consider the points $(0, 1)$, $(1, 4)$, $(2, 0)$ and $(3, -2)$. Find

    (a) the natural cubic spline.

    (b) the clamped cubic spline with conditions $S'(0) = 2$ and $S'(3) = 2$.

    (c) the extrapolated cubic spline.

    (d) the parabolically terminated cubic spline.

    (e) the curvature adjusted cubic spline with the second derivative boundary conditions $S''(0) = -1.5$ and $S''(3) = 3$.

# Part III

# Questions

# Questions from Previous Years

## 2012-2013 (2015)

1. Marks : $4 + 4 + 6 = 14$

   (a) Derive Newton-Raphson formula using Taylor's series expansion to solve a nonlinear equation.

   (b) Show that Newton-Raphson method converges quadratically.

   (c) Find a root, correct to three decimal places, of the equation $\cos x - xe^x = 0$ using Regula-Falsi method, and then find its percentage error.

2. Marks : $(6 + 1) + 7 = 14$

   (a) Obtain Newton's formula for backward interpolation. Discuss its drawback if any compare to Lagrange interpolation formula.

   (b) Find the Lagrange interpolation polynomial to fit the following data:

| $x$ | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| $f(x)$ | 0 | 1.7183 | 6.3891 | 19.0855 |

3. Marks : $7 + 7 = 14$

   (a) Describe the Gauss-Seidal iterative method to solve a system of linear equations numerically. Write down the conditon that for any choice of the first approximation of the Gauss-Seidal method converges.

   (b) Solve the tri-diagonal system:

$$\begin{array}{rcrcrcrl}
0.5x_1 & + & 0.25x_2 & & & & & = 0.35 \\
0.35x_1 & + & 0.8x_2 & + & 0.4x_3 & & & = 0.77 \\
 & & 0.25x_2 & + & x_3 & + & 0.5x_4 & = -0.5 \\
 & & & & x_3 & - & 2.0x_4 & = -2.25
\end{array}$$

4. Marks : $2 + 4 + 8 = 14$

   (a) What are spline functions and spline interpolation? Discuss briefly.

   (b) Derive Newton's general interpolation formula with divided difference.

(c) Fit cubic splines to the following data, and utilize the results to estimate the value at $x = 5$.

| $x$ | 2.0 | 4.5 | 7.0 | 9.0 |
|---|---|---|---|---|
| $f(x)$ | 2.5 | 1.0 | 2.5 | 0.5 |

5. Marks : $8 + 6 = 14$

(a) Derive general quadrature formula for equidistant ordinates to integrate a function numerically and hence deduce Weddle's rule.

(b) Compute the value of the integral $\int_0^3 \left(e^{x^2} - 1\right) \mathrm{d}\,x$, $n = 6$ by Trapezoidal rule and Simpson's $^1/_3$ rule.

6. Marks : $7 + 7 = 14$

(a) Derive a formula for numerical evaluation of $\frac{\mathrm{d}\,y}{\mathrm{d}\,x}$ and $\frac{\mathrm{d}^y\,2}{\mathrm{d}\,x^y}$ from a given data set of $(x, y)$.

(b) The deflection $y$, measured at various distance $x$ from one end of a cantilever, is given by

| $x:$ | 0.0 | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
|---|---|---|---|---|---|---|
| $y:$ | 0.0000 | 0.0347 | 0.1173 | 0.2160 | 0.2987 | 0.3333 |

Find $f'(0.8)$, where $y = f(x)$.

7. Marks : $7 + 7 = 14$

(a) Explain the Euler's method to solve the ordinary differential equation $\frac{\mathrm{d}\,y}{\mathrm{d}\,x} = f(x, y)$, $y(x_0) = y_0$.

(b) Use the 4th order Runge-Kutta method to solve $10\frac{\mathrm{d}\,y}{\mathrm{d}\,x} = x^2 + y^2$, $y(0) = 1$, for the interval $0 \leq x \leq 0.4$ with $h = 0.2$.

8. Marks : $7 + 7 = 14$

(a) Obtain finite difference formula for $\frac{\partial u}{\partial x}$ and $\frac{\partial^2 u}{\partial x^2}$. Derive explicit finite difference scheme to solve the BVP:

$$u''(x) + p(x)u'(x) + q(x)u(x) + r(x) = 0$$

with boundary conditions $u(x_0) = a$ and $u(x_n) = b$, $x_0 \leq x \leq x_n$.

(b) Solve the boundary value problem $y'' - y = 0$ with boundary conditions $y(0)0 = 0$ and $y(2) = 3.627$ by the finite difference method with $h = 0.5$.

## 2015-2016 (2018)

1. Marks: $(2+2)+6+4=14$

   (a) Define algebraic and transcendental equations. Discuss how the intermediate value theorem exhibits the bracketing interval.

   (b) Describe the method of iteration for finding a root of the equation $f(x)=0$. Also establish the condition of convergence of this method.

   (c) Find a real root, correct to three decimal places, of the equation $\sin^2 x = x^2 - 1$ lying in the interval $[1.3, 1.5]$ by using iteration method.

2. Marks: $7+7=14$

   (a) Write down the iteration formula of Newton-Raphson method to find a root of the equation $f(x)=0$. Then show that Newton-Raphson method converges quadratically.

   (b) Solve the equation $e^x - x - 2 = 0$ by Newton-Raphson method.

3. Marks: $5+4+5=14$

   (a) Define interpolation and extrapolation. Derive the Newton's formula for the backward interpolation.

   (b) Derive the first fourth backward difference formula and construct its backward difference table.

   (c) The population of a town in the decennial census was as given below.

   | Year: $x$ | 1981 | 1991 | 2001 | 2011 |
   |---|---|---|---|---|
   | Population: $y$ (in thousands) | 46 | 66 | 81 | 93 |

   Estimate the population for the year 1985.

4. Marks: $7+7=14$

   (a) Derive the Lagrange's interpolation formula for unequal intervals.

   (b) Given the following data:

   | $x$ | 10.1 | 22.2 | 32.0 | 41.6 | 50.5 |
   |---|---|---|---|---|---|
   | $f(x)$ | 0.17537 | 0.37784 | 0.52992 | 0.66393 | 0.63608 |

   Estimate the value of $f(27.5)$ by using divided difference formula.

5. Marks: $7+7=14$

   (a) Derive general quadrature formula for equidistance ordinates to integrate $f(x)$ numerically and hence deduce Simpson's rule.

   (b) Evaluate the value of the integral $\int_{0.2}^{1.4} (\cos x - \log_e x + e^x)\, \mathrm{d}\, x$ by

      i. Simpson's ${}^1/_3$ rule and

ii. Weddle's rule.

6. Marks: $8 + 6 = 14$

   (a) Derive cubic spline interpolating method.

   (b) Fit a natural cubic spline to the following data:

| $x$ | 1 | 2 | 3 |
|---|---|---|---|
| $y$ | $-8$ | $-1$ | 18 |

   and compute $y(1.5)$ and $y'(1)$.

7. Marks: $7 + 7 = 14$

   (a) Use the decomposition method to solve the system of equations

$$\begin{aligned} x_1 + x_2 + x_3 &= 1 \\ 4x_1 + 3x_2 - x_3 &= 6 \\ 3x_1 + 5x_2 + 3x_3 &= 4. \end{aligned}$$

   (b) Use Gauss-Seidel iteration method to solve the following system of equations:

$$\begin{aligned} 4x + y + 2z &= 4 \\ 3x + 5y + z &= 7 \\ x + y + 3z &= 3 \end{aligned}$$

   up to four decimal places.

8. Marks: $7 + 7 = 14$

   (a) Derive Euler's method to solve the IVP:

$$\frac{\mathrm{d}\,y}{\mathrm{d}\,x} = f(x, y), \quad y(x_0) = y_0$$

   Also explain its modification.

   (b) Solve the initial value problem:

$$\frac{\mathrm{d}\,u}{\mathrm{d}\,t} = -2tu^2, \quad u(0) = 1$$

   with $h = 0.2$ on the interval $[0, 0.4]$ by using the fourth-order classical Runge-Kutta method.

# 2016-2017 (2019)

1. Marks: $5+4+5$

    (a) What is meant by error in numerical analysis? Explain the following error:
    Truncation error, round-off error and inherent error.

    (b) Define bracketing interval. Derive the formula for the chord method to find a real root of a transcendental equation.

    (c) Find a root of the equation $x\log_{10} x = 4.77$ by Newton-Raphson method, correct to three decimal places.

2. Marks: $7+7$

    (a) Derive the close form formulae to solve the tridiagonal system of linear equations:

    $$a_r x_{r-1} + b_r x_r + c_r x_{r+1} = dr, \quad a_1 = c_n = 0 \quad \text{for } r = 1, 2, 3, \ldots, n$$

    (b) Apply above formulae to solve the following system of linear equations:

    $$\begin{aligned} 0.5x_1 + 0.25x_2 &= 0.35 \\ 0.35x_1 + 0.8x_2 + 0.4x_3 &= 0.77 \\ 0.25x_2 + x_3 + 0.5x_4 &= -0.50 \\ x_3 - 2.0x_4 &= -2.25 \end{aligned}$$

3. Marks: $4+5+5$

    (a) Discuss Gauss-Seidel and Gauss-Jacobi iteration methods to find solutions of the system of linear equations $Ax = b$ and write their advantages and disadvantages.

    (b) Use Gauss-Seidel iteration method to find the solutions, correct up to 3 decimal places of the following system of linear equations:

    $$\begin{aligned} 4x_1 + x_2 + 2x_3 &= 4 \\ x_1 + x_2 + 3x_3 &= 3 \\ 3x_1 + 5x_2 + x_3 &= 7 \end{aligned}$$

    (c) Solve the following system of Linear equations:

    $$\begin{aligned} 5x - 2y + z &= 4 \\ 7x + y - 5z &= 8 \\ 3x + 7y + 4z &= 10 \end{aligned}$$

    by Crout's reduction method.

4. Marks: $6+8$

    (a) Define interpolation and extrapolation. Derive the expression for the error in polynomial interpolation.

(b) The following table gives the population of a town during the last six censuses. Estimate using any suitable interpolation formula, the increase in the population during the period from 1976 to 1978.

| Year | 1941 | 1951 | 1961 | 1971 | 1981 | 1991 |
|---|---|---|---|---|---|---|
| Population (in thousand) | 12 | 15 | 20 | 27 | 39 | 52 |

5. Marks: $7 + 7$

(a) Discuss briefly the properties of cubic spline and defines its knots. Fits a cubic spline curve that passes through $(0, 0.0)$, $(1, 0.5)$. $(2, 2.0)$ and $(3, 1.5)$ with the natural-end boundary conditions.

$$S''(0) = 0, \quad S''(3) = 0$$

(b) Find interpolating polynomial for the following data using Lagrange's formula

| $x$ | 1 | 2 | $-4$ |
|---|---|---|---|
| $y = f(x)$ | 3 | $-5$ | 4 |

Hence, find $f(2.25)$.

6. Marks: $7 + 7$

(a) Derive general quaderature formula to evaluate the integral $I = \displaystyle\int_a^b y(x)\,\mathrm{d}\,x$, hence deduce the trapezoidal, Simpsons ${}^1/_3$ and Simpson's ${}^3/_8$ formula to find $I$.

(b) Compute the value of the definite integral $\displaystyle\int_0^{\frac{\pi}{2}} e^{\sin x}\,\mathrm{d}\,x$ by Simpson's ${}^3/_8$ rule and Weddle's rule. After finding the true value of the integral, compare the errors in both cases and comment which method is better.

7. Marks: $7 + 7$

(a) Define initial value problem. Derive Euler's method to solve the IVP.

$$\frac{\mathrm{d}\,y}{\mathrm{d}\,x} = (fx, y), \quad y(x_0) = y_0$$

Also explain its modification.

(b) Using modified Euler's method, obtain the solution of the differential equation $\frac{\mathrm{d}\,y}{\mathrm{d}\,x} = t + \sqrt{y}$ with the initial conditon $y(0) = 1$, for the range $0 \leq t \leq 0.6$ in steps of 0.2.

8. Marks: $6 + 8$

(a) Use fourth order Runge-Kutta method to solve numerically the initial value problem

$$\frac{\mathrm{d}\,y}{\mathrm{d}\,t} = y^2 - 100e^{-100(t-1)^2}, \quad y(0.8) = 4.9491$$

and find $y(0.85)$ taking $h = 0.01$.

(b) Find $y(0.8)$ using Milne's predictor-corrector Method, if $y(x)$ is the solution of the differential equation $\frac{\mathrm{d}\,y}{\mathrm{d}\,x} = -xy^2$, $y(0) = 2$ assuming $y(0.2) = 1.92308$, $Y(0.4) = 1.72414$ and $y(0.6) = 1.47059$.