

NUMERICAL METHODS

VI SEMESTER

CORE COURSE

B Sc MATHEMATICS

(2011 Admission)



UNIVERSITY OF CALICUT

SCHOOL OF DISTANCE EDUCATION

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SCHOOL OF DISTANCE EDUCATION

STUDY MATERIAL

Core Course

B Sc Mathematics

VI Semester

NUMERICAL METHODS

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SYLLABUS

B.Sc. DEGREE PROGRAMME

MATHEMATICS

MM6B11 : NUMERICAL METHODS

4 credits

30 weightage

Text :

S.S. Sastry : Introductory Methods of Numerical Analysis, Fourth Edition, PHI.

Module I : Solution of Algebraic and Transcendental Equation

- 2.1 Introduction
- 2.2 Bisection Method
- 2.3 Method of false position
- 2.4 Iteration method
- 2.5 Newton-Raphson Method
- 2.6 Ramanujan's method
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Finite Differences

- 3.1 Introduction
 - 3.3.1 Forward differences
 - 3.3.2 Backward differences
 - 3.3.3 Central differences
 - 3.3.4 Symbolic relations and separation of symbols
- 3.5 Differences of a polynomial

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- 3.6 Newton's formulae for intrapolation
- 3.7 Central difference interpolation formulae
 - 3.7.1 Gauss' Central Difference Formulae
- 3.9 Interpolation with unevenly spaced points
 - 3.9.1 Langrange's interpolation formula
- 3.10 Divided differences and their properties
 - 3.10.1 Newton's General interpolation formula

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Numerical Differentiation and Integration

5.1 Introduction

5.2 Numerical differentiation (using Newton's forward and backward formulae)

5.4 Numerical Integration

5.4.1 Trapezoidal Rule

5.4.2 Simpson's 1/3-Rule

5.4.3 Simpson's 3/8-Rule

Module III : Matrices and Linear Systems of equations

6.3 Solution of Linear Systems – Direct Methods

6.3.2 Gauss elimination

6.3.3 Gauss-Jordan Method

6.3.4 Modification of Gauss method to compute the inverse

6.3.6 LU Decomposition

6.3.7 LU Decomposition from Gauss elimination

6.4 Solution of Linear Systems – Iterative methods

6.5 The eigen value problem

6.5.1 Eigen values of Symmetric Tridiagonal matrix

Module IV : Numerical Solutions of Ordinary Differential Equations

7.1 Introduction

7.2 Solution by Taylor's series

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7.4 Euler's method

7.4.2 Modified Euler's Method

7.5 Runge-Kutta method

7.6 Predictor-Corrector Methods

7.6.1 Adams-Moulton Method

7.6.2 Milne's method

References

1. S. Sankara Rao : Numerical Methods of Scientists and Engineer, 3rd ed., PHI.
2. F.B. Hidebrand : Introduction to Numerical Analysis, TMH.
3. J.B. Scarborough : Numerical Mathematical Analysis, Oxford and IBH.

1

FIXED POINT ITERATION METHOD

Nature of numerical problems

Solving mathematical equations is an important requirement for various branches of science. The field of numerical analysis explores the techniques that give approximate solutions to such problems with the desired accuracy.

Computer based solutions

The major steps involved to solve a given problem using a computer are:

1. Modeling: Setting up a mathematical model, i.e., formulating the problem in mathematical terms, taking into account the type of computer one wants to use.
2. Choosing an appropriate numerical method (algorithm) together with a preliminary error analysis (estimation of error, determination of steps, size etc.)
3. Programming, usually starting with a flowchart showing a block diagram of the procedures to be performed by the computer and then writing, say, a C++ program.
4. Operation or computer execution.
5. Interpretation of results, which may include decisions to rerun if further data are needed.

Errors

Numerically computed solutions are subject to certain errors. Mainly there are three types of errors. They are inherent errors, truncation errors and errors due to rounding.

1. *Inherent errors or experimental errors* arise due to the assumptions made in the mathematical modeling of problem. It can also arise when the data is obtained from certain physical measurements of the parameters of the problem. i.e., errors arising from measurements.
2. *Truncation errors* are those errors corresponding to the fact that a finite (or infinite) sequence of computational steps necessary to produce an exact result is “truncated” prematurely after a certain number of steps.
3. *Round of errors* are errors arising from the process of rounding off during computation. These are also called *chopping*, i.e. discarding all decimals from some decimals on.

Error in Numerical Computation

Due to errors that we have just discussed, it can be seen that our numerical result is an approximate value of the (sometimes unknown) exact result, except for the rare case where the exact answer is sufficiently simple rational number.

If \tilde{a} is an approximate value of a quantity whose exact value is a , then the difference $\varepsilon = \tilde{a} - a$ is called the absolute error of \tilde{a} or, briefly, the error of \tilde{a} . Hence, $\tilde{a} = a + \varepsilon$, i.e.

Approximate value = True value + Error.

For example, if $\tilde{a} = 10.52$ is an approximation to $a = 10.5$, then the error is $\varepsilon = 0.02$. The relative error, ε_r , of \tilde{a} is defined by

$$|r| = \frac{| \varepsilon |}{|a|} = \frac{|\text{Error}|}{|\text{Truevalue}|}$$

For example, consider the value of $\sqrt{2}(=1.414213\dots)$ up to four decimal places, then

$$\sqrt{2} = 1.4142 + \text{Error}.$$

$$|\text{Error}| = |1.4142 - 1.41421| = .00001,$$

taking 1.41421 as true or exact value. Hence, the relative error is

$$r = \frac{0.00001}{1.4142}.$$

We note that

$$r \approx \frac{\varepsilon}{\tilde{a}} \quad \text{if } |\varepsilon| \text{ is much less than } |\tilde{a}|.$$

We may also introduce the quantity $\gamma = a - \tilde{a} = -\varepsilon$ and call it the correction, thus, $a = \tilde{a} + \gamma$, i.e.

True value = Approximate value + Correction.

Error bound for \tilde{a} is a number β such that $|\tilde{a} - a| \leq \beta$ i.e., $|\varepsilon| \leq \beta$.

Number representations

Integer representation

Floating point representation

Most digital computers have two ways of representing numbers, called **fixed point** and **floating point**. In a fixed point system the numbers are represented by a fixed number of decimal places e.g. 62.358, 0.013, 1.000.

In a floating point system the numbers are represented with a fixed number of significant digits, for example

$$0.6238 \times 10^3 \qquad 0.1714 \times 10^{-13} \quad -0.2000 \times 10^1$$

also written as $0.6238 \text{ E}03$ $0.1714 \text{ E} -13$ $-0.2000 \text{ E}01$

or more simply $0.6238 +03$ $0.1714 -13$ $-0.2000 +01$

Significant digits

Significant digit of a number c is any given digit of c , except possibly for zeros to the left of the first nonzero digit that serve only to fix the position of the decimal point. (Thus, any other zero is a significant digit of c). For example, each of the number 1360, 1.360, 0.01360 has 4 significant digits.

Round off rule to discard the $k + 1$ th and all subsequent decimals

- (a) **Rounding down** If the number at $(k + 1)^{\text{th}}$ decimal to be discarded is less than half a unit in the k^{th} place, leave the k^{th} decimal unchanged. For example, rounding of 8.43 to 1 decimal gives 8.4 and rounding of 6.281 to 2 decimal places gives 6.28.
- (b) **Rounding up** If the number at $(k + 1)^{\text{th}}$ decimal to be discarded is greater than half a unit in the k^{th} place, add 1 to the k^{th} decimal. For example, rounding of 8.48 to 1 decimal gives 8.5 and rounding of 6.277 to 2 decimals gives 6.28.
- (c) If it is exactly half a unit, round off to the nearest even decimal. For example, rounding off 8.45 and 8.55 to 1 decimal gives 8.4 and 8.6 respectively. Rounding off 6.265 and 6.275 to 2 decimals gives 6.26 and 6.28 respectively.

Example Find the roots of the following equations using 4 significant figures in the calculation.

(a) $x^2 - 4x + 2 = 0$ and (b) $x^2 - 40x + 2 = 0$.

Solution

A formula for the roots x_1, x_2 of a quadratic equation $ax^2 + bx + c = 0$ is

$$(i) \quad x_1 = \frac{1}{2a}(-b + \sqrt{b^2 - 4ac}) \quad \text{and} \quad x_2 = \frac{1}{2a}(-b - \sqrt{b^2 - 4ac}).$$

Furthermore, since $x_1x_2 = c/a$, another formula for these roots is

$$(ii) \quad x_1 = \frac{1}{2a}(-b + \sqrt{b^2 - 4ac}), \quad \text{and} \quad x_2 = \frac{c}{ax_1}$$

For the equation in (a), formula (i) gives,

$$x_1 = 2 + \sqrt{2} = 2 + 1.414 = 3.414,$$

$$x_2 = 2 - \sqrt{2} = 2 - 1.414 = 0.586$$

and formula (ii) gives,

$$x_1 = 2 + \sqrt{2} = 2 + 1.414 = 3.414,$$

$$x_2 = 2.000/3.414 = 0.5858.$$

For the equation in (b), formula (i) gives,

$$x_1 = 20 + \sqrt{398} = 20 + 19.95 = 39.95,$$

$$x_2 = 20 - \sqrt{398} = 20 - 19.95 = 0.05$$

and formula (ii) gives,

$$x_1 = 20 + \sqrt{398} = 20 + 19.95 = 39.95,$$

$$x_2 = 20.000/39.95 = 0.05006.$$

Example Convert the decimal number (which is in the base 10) 81.5 to its binary form (of base 2).

Solution Note that $(81.5)_{10} = 8 \cdot 10^1 + 1 \cdot 10^0 + 5 \cdot 10^{-1}$

$$\text{Now } 81.5 = 64 + 16 + 1 + 0.5 = 2^6 + 2^4 + 2^0 + 2^{-1} = (1010001.1)_2.$$

	Remainder	Product	Integer part	
2	81	0.5×2	1.0	1 ↓
2	40			1
2	20			0
2	10			0
2	5			0
2	2			1
2	1			0
	0			1

Example Convert the binary number 1010.101 to its decimal form.

Solution

$$\begin{aligned}(1010.101)_2 &= 1 \cdot 2^3 + 1 \cdot 2^1 + 1 \cdot 2^{-1} + 1 \cdot 2^{-3} \\ &= 8 + 2 + 0.5 + 0.125 = (10.625)_{10}\end{aligned}$$

Numerical Iteration Method

A **numerical iteration method** or simply **iteration method** is a mathematical procedure that generates a sequence of improving approximate solutions for a class of problems. A specific way of implementation of an iteration method, including the termination criteria, is called an algorithm of the iteration method. In the problems of finding the solution of an equation an iteration method uses an initial guess to generate successive approximations to the solution.

Since the iteration methods involve repetition of the same process many times, computers can act well for finding solutions of equation numerically. Some of the iteration methods for finding solution of equations involves (1) Bisection method, (2) Method of false position (Regula-falsi Method), (3) Newton-Raphson method.

A numerical method to solve equations may be a long process in some cases. If the method leads to value close to the exact solution, then we say that the method is convergent. Otherwise, the method is said to be divergent.

Solution of Algebraic and Transcendental Equations

One of the most common problem encountered in engineering analysis is that given a function $f(x)$, find the values of x for which $f(x) = 0$. The solution (values of x) are known

as the **roots** of the equation $f(x) = 0$, or the **zeroes** of the function $f(x)$. The roots of equations may be real or complex.

In general, an equation may have any number of (real) roots, or no roots at all. For example, $\sin x - x = 0$ has a single root, namely, $x = 0$, whereas $\tan x - x = 0$ has infinite number of roots ($x = 0, \pm 4.493, \pm 7.725, \dots$).

Algebraic and Transcendental Equations

$f(x) = 0$ is called an **algebraic equation** if the corresponding $f(x)$ is a polynomial. An example is $7x^2 + x - 8 = 0$. $f(x) = 0$ is called **transcendental equation** if the $f(x)$ contains trigonometric, or exponential or logarithmic functions. Examples of transcendental equations are $\sin x - x = 0$, $\tan x - x = 0$ and $7x^3 + \log(3x - 6) + 3e^x \cos x + \tan x = 0$.

There are two types of methods available to find the roots of algebraic and transcendental equations of the form $f(x) = 0$.

1. Direct Methods: Direct methods give the exact value of the roots in a finite number of steps. We assume here that there are no round off errors. Direct methods determine all the roots at the same time.

2. Indirect or Iterative Methods: Indirect or iterative methods are based on the concept of successive approximations. The general procedure is to start with one or more initial approximation to the root and obtain a sequence of iterates x_k which in the limit converges to the actual or true solution to the root. Indirect or iterative methods determine one or two roots at a time. The indirect or iterative methods are further divided into two categories: bracketing and open methods. The bracketing methods require the limits between which the root lies, whereas the open methods require the initial estimation of the solution. Bisection and False position methods are two known examples of the bracketing methods. Among the open methods, the Newton-Raphson is most commonly used. The most popular method for solving a non-linear equation is the

Newton-Raphson method and this method has a high rate of convergence to a solution.

In this chapter and in the coming chapters, we present the following indirect or iterative methods with illustrative examples:

1. Fixed Point Iteration Method
2. Bisection Method
3. Method of False Position (Regula Falsi Method)
4. Newton-Raphson Method (Newton's method)

Fixed Point Iteration Method

Consider

$$f(x) = 0 \quad \dots (1)$$

Transform (1) to the form,

$$x = w(x). \quad \dots (2)$$

Take an arbitrary x_0 and then compute a sequence x_1, x_2, x_3, \dots recursively from a relation of the form

$$x_{n+1} = \phi(x_n) \quad (n = 0, 1, \dots) \quad \dots (3)$$

A **solution** of (2) is called **fixed point** of w . To a given equation (1) there may correspond several equations (2) and the behaviour, especially, as regards speed of convergence of iterative sequences $x_0, x_1, x_2, x_3, \dots$ may differ accordingly.

Example Solve $f(x) = x^2 - 3x + 1 = 0$, by fixed point iteration method.

Solution

Write the given equation as

$$x^2 = 3x - 1 \quad \text{or} \quad x = 3 - 1/x.$$

Choose $w(x) = 3 - \frac{1}{x}$. Then $w'(x) = \frac{1}{x^2}$ and $|w'(x)| < 1$ on the interval $(1, 2)$.

Hence the iteration method can be applied to the Eq. (3).

The iterative formula is given by

$$x_{n+1} = 3 - \frac{1}{x_n} \quad (n = 0, 1, 2, \dots)$$

Starting with, $x_0 = 1$, we obtain the sequence

$$x_0 = 1.000, x_1 = 2.000, x_2 = 2.500, x_3 = 2.600, x_4 = 2.615, \dots$$

Question : Under what assumptions on w and x_0 , does Algorithm 1 converge ? When does the sequence (x_n) obtained from the iterative process (3) converge ?

We answer this in the following theorem, that is a sufficient condition for convergence of iteration process

Theorem Let α be a root of $f(x)=0$ and let I be an interval containing the point α . Let $w(x)$ be continuous in I , where $w(x)$ is defined by the equation $x=w(x)$ which is equivalent to $f(x)=0$. Then if $|w'(x)| < 1$ for all x in I , the sequence of approximations $x_0, x_1, x_2, \dots, x_n$ defined by

$$x_{n+1} = w(x_n) \quad (n = 0, 1, \dots)$$

converges to the root α , provided that the initial approximation x_0 is chosen in I .

Example Find a real root of the equation $x^3 + x^2 - 1 = 0$ on the interval $[0, 1]$ with an accuracy of 10^{-4} .

To find this root, we rewrite the given equation in the form

$$x = \frac{1}{\sqrt{x+1}}$$

Take

$$w(x) = \frac{1}{\sqrt{x+1}}. \text{ Then } w'(x) = -\frac{1}{2} \frac{1}{(x+1)^{3/2}}$$

$$\max_{[0,1]} |w'(x)| = \left| \frac{1}{2\sqrt{8}} \right| = k = 0.17678 < 0.2.$$

Choose $w(x) = 3 - \frac{1}{x}$. Then $w'(x) = \frac{1}{x^2}$ and $|w'(x)| < 1$ on the interval $(1, 2)$.

Hence the iteration method gives:

n	x_n	$\sqrt{x_n + 1}$	$x_{n+1} = 1/\sqrt{x_n + 1}$
0	0.75	1.3228756	0.7559289
1	0.7559289	1.3251146	0.7546517
2	0.7546617	1.3246326	0.7549263

At this stage,

$$|x_{n+1} - x_n| = 0.7549263 - 0.7546517 = 0.0002746,$$

which is less than 0.0004. The iteration is therefore terminated and the root to the required accuracy is 0.7549.

Example Use the method of iteration to find a positive root, between 0 and 1, of the equation $xe^x = 1$.

Writing the equation in the form

$$x = e^{-x}$$

We find that $w(x) = e^{-x}$ and so $w'(x) = -e^{-x}$.

Hence $|w'(x)| < 1$ for $x < 1$, which assures that the iterative process defined by the equation $x_{n+1} = w(x_n)$ will be convergent, when $x < 1$.

The iterative formula is

$$x_{n+1} = \frac{1}{e^{x_n}} \quad (n = 0, 1, \dots)$$

Starting with $x_0 = 1$, we find that the successive iterates are given by

$$x_1 = 1/e = 0.3678794, \quad x_2 = \frac{1}{e^{x_1}} = 0.6922006,$$

$$x_3 = 0.5004735, \quad x_4 = 0.6062435,$$

$$x_5 = 0.5453957, \quad x_6 = 0.5796123,$$

We accept 6.5453957 as an approximate root.

Example Find the root of the equation $2x = \cos x + 3$ correct to three decimal places.

We rewrite the equation in the form

$$x = \frac{1}{2}(\cos x + 3)$$

so that

$$w = \frac{1}{2}(\cos x + 3),$$

and

$$|w'(x)| = \left| \frac{\sin x}{2} \right| < 1.$$

Hence the iteration method can be applied to the eq. (3) and we start with $x_0 = f/2$. The successive iterates are

$$x_1 = 1.5, \quad x_2 = 1.535, \quad x_3 = 1.518,$$

$$x_4 = 1.526, \quad x_5 = 1.522, \quad x_6 = 1.524,$$

$$x_7 = 1.523, \quad x_8 = 1.524.$$

We accept the solution as 1.524 correct to three decimal places.

Example Find a solution of $f(x) = x^3 + x - 1 = 0$, by fixed point iteration.

$x^3 + x - 1 = 0$ can be written as $x(x^2 + 1) = 1$, or $x = \frac{1}{x^2 + 1}$.

Note that

$$|w'(x)| = \frac{2|x|}{(1+x^2)^2} < 1 \text{ for any real } x,$$

so by the Theorem we can expect a solution for any real number x_0 as the starting point.

Choosing $x_0 = 1$, and undergoing calculations in the iterative formula

$$x_{n+1} = w(x_n) = \frac{1}{1+x_n^2} \quad (n = 0, 1, \dots), \quad \dots(4)$$

we get the sequence

$$\begin{aligned} x_0 &= 1.000, & x_1 &= 0.500, & x_2 &= 0.800, & x_3 &= 0.610, \\ x_4 &= 0.729, & x_5 &= 0.653, & x_6 &= 0.701, \dots \end{aligned}$$

and we choose 0.701 as an (approximate) solution to the given equation.

Example Solve the equation $x^3 = \sin x$. Considering various $w(x)$, discuss the convergence of the solution.

How do the functions we considered for $w(x)$ compare? Table shows the results of several

iterations using initial value $x_0 = 1$ and four different functions for $w(x)$. Here x_n is the value of x

on the n th iteration.

Answer:

When $w(x) = \sqrt[3]{\sin x}$, we have:

$$\begin{aligned} x_1 &= 0.94408924124306; & x_2 &= 0.93215560685805 \\ x_3 &= 0.92944074461587; & x_4 &= 0.92881472066057 \end{aligned}$$

When $w(x) = \frac{\sin x}{x^2}$, we have:

$$\begin{aligned} x_1 &= 0.84147098480790; & x_2 &= 1.05303224555943 \\ x_3 &= 0.78361086350974; & x_4 &= 1.14949345383611 \end{aligned}$$

Referring to Theorem, we can say that for $w(x) = \frac{\sin x}{x^2}$, the iteration doesn't converge.

When $w(x) = x + \sin x - x^3$, we have:

$$x_1 = 0.84147098480790; \quad x_2 = 0.99127188988250$$

$$x_3 = 0.85395152069647; \quad x_4 = 0.98510419085185$$

When $w(x) = x - \frac{\sin x - x^3}{\cos x - 3x^2}$, we have:

$$x_1 = 0.93554939065467; \quad x_2 = 0.92989141894368$$

$$x_3 = 0.92886679103170; \quad x_4 = 0.92867234089417$$

Example Give all possible transpositions to $x = w(x)$, and solve $f(x) = x^3 + 4x^2 - 10 = 0$.

Possible Transpositions to $x = w(x)$, are

$$x = w_1(x) = x - x^3 - 4x^2 + 10,$$

$$x = w_2(x) = \sqrt{\frac{10}{x} - 4x},$$

$$x = w_3(x) = \frac{1}{2}\sqrt{10 - x^3}$$

$$x = w_4(x) = \sqrt{\frac{10}{4 + x}}$$

$$x = w_5(x) = x - \frac{x^3 + 4x^2 - 10}{3x^2 + 8x}$$

For $x = w_1(x) = x - x^3 - 4x^2 + 10$, numerical results are:

$$x_0 = 1.5; \quad x_2 = -0.875$$

$$x_3 = 6.732; \quad x_4 = -469.7;$$

Hence doesn't converge.

For $x = w_2(x) = \sqrt{\frac{10}{x} - 4x}$, numerical results are:

$$x_0 = 1.5; \quad x_2 = 0.8165$$

$$x_3 = 2.9969; \quad x_4 = (-8.65)^{1/2};$$

For $x = w_3(x) = \frac{1}{2}\sqrt{10 - x^3}$, numerical results are:

$$\begin{array}{ll} x_0 = 1.5; & x_2 = 1.2869 \\ x_3 = 1.4025; & x_4 = 1.3454 \end{array};$$

Exercises

Solve the following equations by iteration method:

- $\sin x = \frac{x+1}{x-1}$
- $x^4 = x + 0.15$
- $3x - \cos x - 2 = 0$
- $x^3 - 5x + 3 = 0,$
- $x^3 + x + 1 = 0$
- $x = \frac{1}{6}(x^3 + 3)$
- $3x = 6 + \log_{10} x$
- $x = \frac{1}{5}(x^3 + 3)$
- $2x - \log_{10} x = 7$
- $x^3 = 2x^2 + 10x = 20$
- $2 \sin x = x$
- $\cos x = 3x - 1$
- $x^3 + x^2 = 100$
- $3x + \sin x = e^x$

2

BISECTION AND REGULA FALSI METHODS

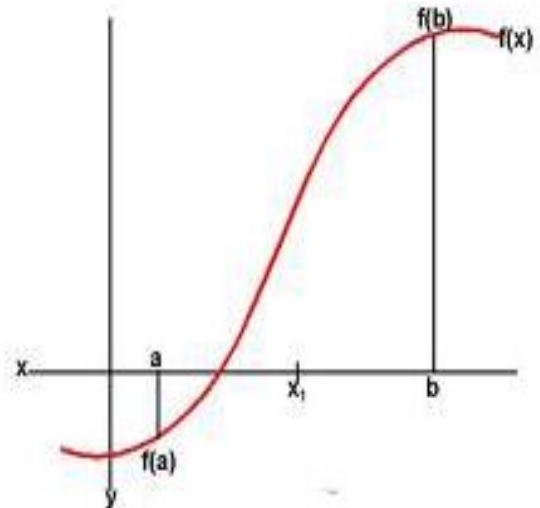
Bisection Method

The bisection method is one of the bracketing methods for finding roots of an equation. For a given a function $f(x)$, guess an interval which might contain a root and perform a number of iterations, where, in each iteration the interval containing the root is get halved.

The **bisection method** is based on the intermediate value theorem for continuous functions.

Intermediate value theorem for continuous functions: If f is a continuous function and $f(a)$ and $f(b)$ have opposite signs, then at least one root lies in between a and b . If the interval (a, b) is small enough, it is likely to contain a single root.

i.e., an interval $[a, b]$ must contain a zero of a continuous function f if the product $f(a)f(b) < 0$. Geometrically, this means that if $f(a)f(b) < 0$, then the curve f has to cross the x -axis at some point in between a and b .

**Algorithm : Bisection Method**

Suppose we want to find the solution to the equation $f(x) = 0$, where f is continuous.

Given a function $f(x)$ continuous on an interval $[a_0, b_0]$ and satisfying $f(a_0)f(b_0) < 0$.

For $n = 0, 1, 2, \dots$ until termination do:

Compute
$$x_n = \frac{1}{2}(a_n + b_n).$$

If $f(x_n) = 0$, accept x_n as a solution and stop.

Else continue.

If $f(a_n)f(x_n) < 0$, a root lies in the interval (a_n, x_n) .

Set $a_{n+1} = a_n, b_{n+1} = x_n$.

If $f(a_n)f(x_n) > 0$, a root lies in the interval (x_n, b_n) .

Set $a_{n+1} = x_n, b_{n+1} = b_n$.

Then $f(x) = 0$ for some x in $[a_{n+1}, b_{n+1}]$.

Test for termination.

Criterion for termination

A convenient criterion is to compute the percentage error v_r defined by

$$v_r = \left| \frac{x'_r - x_r}{x'_r} \right| \times 100\%.$$

where x'_r is the new value of x_r . The computations can be terminated when v_r becomes less than a prescribed tolerance, say v_p . In addition, the maximum number of iterations may also be specified in advance.

Some other termination criteria are as follows:

- Termination after N steps (N given, fixed)
- Termination if $|x_{n+1} - x_n| \leq \varepsilon$ ($\varepsilon > 0$ given)
- Termination if $|f(x_n)| \leq \alpha$ ($\alpha > 0$ given).

In this chapter our criterion for termination is terminate the iteration process after some finite steps. However, we note that this is generally not advisable, as the steps may not be sufficient to get an approximate solution.

Example Solve $x^3 - 9x + 1 = 0$ for the root between $x = 2$ and $x = 4$, by bisection method.

Given $f(x) = x^3 - 9x + 1$. Now $f(2) = -9$, $f(4) = 29$ so that $f(2)f(4) < 0$ and hence a root lies between 2 and 4.

Set $a_0 = 2$ and $b_0 = 4$. Then

$$x_0 = \frac{(a_0 + b_0)}{2} = \frac{2+4}{2} = 3 \quad \text{and} \quad f(x_0) = f(3) = 1.$$

Since $f(2)f(3) < 0$, a root lies between 2 and 3, hence we set $a_1 = a_0 = 2$ and $b_1 = x_0 = 3$. Then

$$x_1 = \frac{(a_1 + b_1)}{2} = \frac{2+3}{2} = 2.5 \quad \text{and} \quad f(x_1) = f(2.5) = -5.875$$

Since $f(2)f(2.5) > 0$, a root lies between 2.5 and 3, hence we set $a_2 = x_1 = 2.5$ and $b_2 = b_1 = 3$.

Then $x_2 = \frac{(a_2 + b_2)}{2} = \frac{2.5+3}{2} = 2.75$ and $f(x_2) = f(2.75) = -2.9531$.

The steps are illustrated in the following table.

n	x_n	$f(x_n)$
0	3	1.0000
1	2.5	-5.875
2	2.75	-2.9531
3	2.875	-1.1113
4	2.9375	-0.0901

Example Find a real root of the equation $f(x) = x^3 - x - 1 = 0$.

Since $f(1)$ is negative and $f(2)$ positive, a root lies between 1 and 2 and therefore we take $x_0 = 3/2 = 1.5$. Then

$f(x_0) = \frac{27}{8} - \frac{3}{2} = \frac{15}{8}$ is positive and hence $f(1)f(1.5) < 0$ and Hence the root lies between 1 and 1.5 and we obtain

$$x_1 = \frac{1+1.5}{2} = 1.25$$

$f(x_1) = -19/64$, which is negative and hence $f(1)f(1.25) > 0$ and hence a root lies between 1.25 and 1.5. Also,

$$x_2 = \frac{1.25 + 1.5}{2} = 1.375$$

The procedure is repeated and the successive approximations are

$$x_3 = 1.3125, \quad x_4 = 1.34375, \quad x_5 = 1.328125, \text{ etc.}$$

Example Find a positive root of the equation $xe^x = 1$, which lies between 0 and 1.

Let $f(x) = xe^x - 1$. Since $f(0) = -1$ and $f(1) = 1.718$, it follows that a root lies between 0 and 1. Thus,

$$x_0 = \frac{0+1}{2} = 0.5.$$

Since $f(0.5)$ is negative, it follows that a root lies between 0.5 and 1. Hence the new root is 0.75, i.e.,

$$x_1 = \frac{.5+1}{2} = 0.75.$$

Since $f(x_1)$ is positive, a root lies between 0.5 and 0.75. Hence

$$x_2 = \frac{.5+.75}{2} = 0.625$$

Since $f(x_2)$ is positive, a root lies between 0.5 and 0.625. Hence

$$x_3 = \frac{.5+.625}{2} = 0.5625.$$

We accept 0.5625 as an approximate root.

Merits of bisection method

- a) The iteration using bisection method always produces a root, since the method brackets the root between two values.
- b) As iterations are conducted, the length of the interval gets halved. So one can guarantee the convergence in case of the solution of the equation.
- c) the Bisection Method is simple to program in a computer.

Demerits of bisection method

- a) The convergence of the bisection method is slow as it is simply based on halving the interval.
- b) Bisection method cannot be applied over an interval where there is a discontinuity.
- c) Bisection method cannot be applied over an interval where the function takes always values of the same sign.
- d) The method fails to determine complex roots.
- e) If one of the initial guesses a_0 or b_0 is closer to the exact solution, it will take larger number of iterations to reach the root.

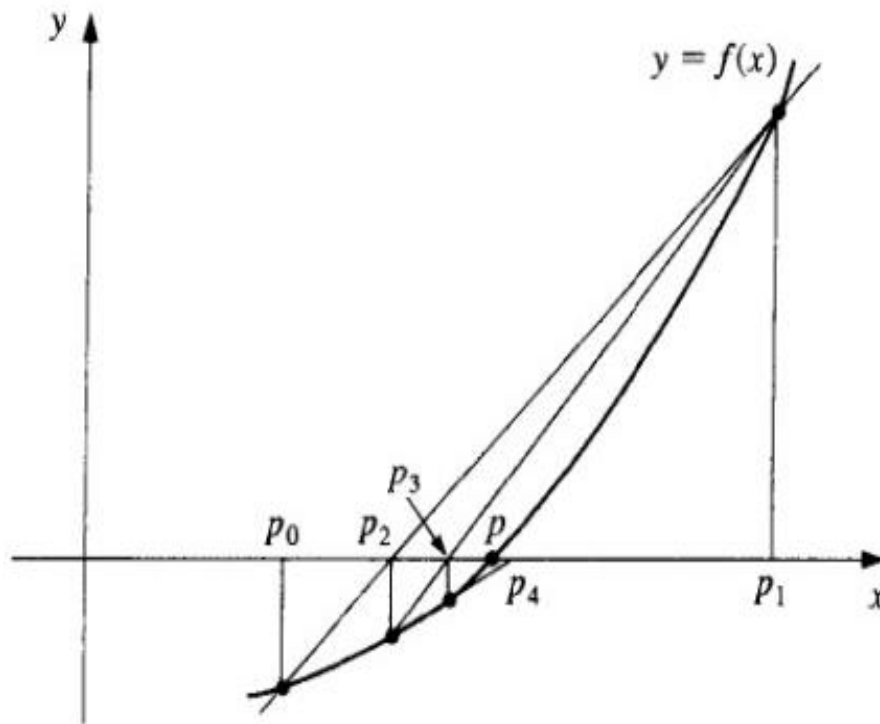
Exercises

Find a real root of the following equations by bisection method.

- | | |
|------------------------------------|------------------------------|
| 1. $3x = \sqrt{1 + \sin x}$ | 2. $x^3 + 1.2x^2 - 4x + 48$ |
| 3. $e^x = 3x$ | 4. $x^3 - 4x - 9 = 0$ |
| 5. $x^3 + 3x - 1 = 0$ | 6. $3x = \cos x + 1$ |
| 7. $x^3 + x^2 - 1 = 0$ | 8. $2x = 3 + \cos x$ |
| 9. $x^4 = 3$ | 10. $x^3 - 5x = 6$ |
| 11. $\cos x = \sqrt{x}$ | 12. $x^3 - x^2 - x - 3 = 0,$ |
| 13. $x^4 = x + 0.15$ near $x = 0.$ | |

Regula Falsi method or Method of False Position

This method is also based on the intermediate value theorem. In this method also, as in bisection method, we choose two points a_n and b_n such that $f(a_n)$ and $f(b_n)$ are of opposite signs (i.e., $f(a_n)f(b_n) < 0$). Then, intermediate value theorem suggests that a zero of f lies in between a_n and b_n , if f is a continuous function.



Algorithm: Given a function $f(x)$ continuous on an interval $[a_0, b_0]$ and satisfying $f(a_0)f(b_0) < 0$.

For $n = 0, 1, 2, \dots$ until termination do:

Compute

$$x_n = \frac{\begin{vmatrix} a_n & b_n \\ f(a_n) & f(b_n) \end{vmatrix}}{f(b_n) - f(a_n)}.$$

If $f(x_n) = 0$, accept x_n as a solution and stop.

Else continue.

If $f(a_n)f(x_n) < 0$, set $a_{n+1} = a_n, b_{n+1} = x_n$. Else set $a_{n+1} = x_n, b_{n+1} = b_n$.

Then $f(x) = 0$ for some x in $[a_{n+1}, b_{n+1}]$.

Example Using regula-falsi method, find a real root of the equation,

$$f(x) = x^3 + x - 1 = 0, \text{ near } x = 1.$$

Here note that $f(0) = -1$ and $f(1) = -1$. Hence $f(0)f(1) < 0$, so by intermediate value theorem a root lies in between 0 and 1. We search for that root by regula falsi method and we will get an approximate root.

Set $a_0 = 0$ and $b_0 = 1$. Then

$$x_0 = \frac{\begin{vmatrix} a_0 & b_0 \\ f(a_0) & f(b_0) \end{vmatrix}}{f(b_0) - f(a_0)} = \frac{\begin{vmatrix} 0 & 1 \\ -1 & -1 \end{vmatrix}}{1 - (-1)} = 0.5$$

and $f(x_0) = f(0.5) = -0.375$.

Since $f(0)f(0.5) > 0$, a root lies between 0.5 and 1. Set $a_1 = x_0 = 0.5$ and $b_1 = b_0 = 1$.

Then

$$x_1 = \frac{\begin{vmatrix} a_1 & b_1 \\ f(a_1) & f(b_1) \end{vmatrix}}{f(b_1) - f(a_1)} = \frac{\begin{vmatrix} 0.5 & 1 \\ -0.375 & -1 \end{vmatrix}}{1 - (-0.375)} = 0.6364$$

and $f(x_1) = f(0.6364) = -0.1058$.

Since $f(0.6364)f(x_1) > 0$, a root lies between x_1 and 1 and hence we set $a_2 = x_1 = 0.6364$ and $b_2 = b_1 = 1$. Then

$$x_2 = \frac{\begin{vmatrix} a_2 & b_2 \\ f(a_2) & f(b_2) \end{vmatrix}}{f(b_2) - f(a_2)} = \frac{\begin{vmatrix} 0.6364 & 1 \\ -0.1058 & -1 \end{vmatrix}}{1 - (-0.1058)} = 0.6712$$

and $f(x_2) = f(0.6712) = -0.0264$

Since $f(0.6712)f(0.6364) > 0$, a root lies between x_2 and 1, and hence we set $a_3 = x_2 = 0.6712$ and $b_3 = b_1 = 1$.

Then
$$x_3 = \frac{\begin{vmatrix} a_3 & b_3 \\ f(a_3) & f(b_3) \end{vmatrix}}{f(b_3) - f(a_3)} = \frac{\begin{vmatrix} 0.6712 & 1 \\ -0.0264 & -1 \end{vmatrix}}{1 - (-0.0264)} = 0.6796$$

and $f(x_3) = f(0.6796) = -0.0063 \approx 0$.

Since $f(0.6796) \approx 0.0000$ we accept 0.6796 as an (approximate) solution of $x^3 - x - 1 = 0$.

Example Given that the equation $x^{2.2} = 69$ has a root between 5 and 8. Use the method of regula-falsi to determine it.

Let $f(x) = x^{2.2} - 69$. We find

$$f(5) = -3450675846 \text{ and } f(8) = -28.00586026.$$

$$x_1 = \frac{\begin{vmatrix} 5 & 8 \\ f(5) & f(8) \end{vmatrix}}{f(8) - f(5)} = \frac{5(28.00586026) - 8(-34.50675846)}{28.00586026 + 34.50675846} = 6.655990062.$$

Now, $f(x_1) = -4.275625415$ and therefore, $f(5)f(x_1) > 0$ and hence the root lies between 6.655990062 and 8.0. Proceeding similarly,

$$x_2 = 6.83400179, \quad x_3 = 6.850669653,$$

The correct root is $x_3 = 6.8523651\dots$, so that x_3 is correct to these significant figures. We accept 6.850669653 as an approximate root.

Theoretical Exercises with Answers:

1. What is the difference between algebraic and transcendental equations?

Ans: An equation $f(x) = 0$ is called an algebraic equation if the corresponding $f(x)$ is a polynomial, while, $f(x) = 0$ is called transcendental equation if the $f(x)$ contains trigonometric, or exponential or logarithmic functions.

2. Why we are using numerical iterative methods for solving equations?

Ans: As analytic solutions are often either too tiresome or simply do not exist, we need to find an approximate method of solution. This is where numerical analysis comes into the picture.

3. Based on which principle, the bisection and regula-falsi method is developed?

Ans: These methods are based on the *intermediate value theorem for continuous functions*: stated as, "If f is a continuous function and $f(a)$ and $f(b)$ have opposite signs, then at least one root lies in between a and b . If the interval (a, b) is small enough, it is likely to contain a single root."

4. What are the advantages and disadvantages of the bracketing methods like bisection and regula-falsi?

Ans: (i) The bisection and regula-falsi method is always convergent. Since the method brackets the root, the method is guaranteed to converge. The main disadvantage is, if it is not possible to bracket the roots, the methods cannot be applicable. For example, if $f(x)$ is such that it always takes the values with same sign, say, always positive or always negative, then we cannot work with bisection method. Some examples of such functions are

- $f(x) = x^2$ which take only non-negative values and
- $f(x) = -x^2$, which take only non-positive values.

Exercises

Find a real root of the following equations by false position method:

- | | |
|--------------------------------|---------------------------|
| 1. $x^3 - 5x = 6$ | 2. $4x = e^x$ |
| 3. $x \log_{10} x = 1.2$ | 4. $\tan x + \tanh x = 0$ |
| 5. $e^{-x} = \sin x$ | 6. $x^3 - 5x - 7 = 0$ |
| 7. $x^3 + 2x^2 + 10x - 20 = 0$ | 8. $2x - \log_{10} x = 7$ |
| 9. $xe^x = \cos x$ | 10. $x^3 - 5x + 1 = 0$ |
| 11. $e^x = 3x$ | 12. $x^2 - \log_e x = 12$ |
| 13. $3x - \cos x = 1$ | 14. $2x - 3 \sin x = 5$ |
| 15. $2x = \cos x + 3$ | 16. $xe^x = 3$ |
| 17. $\cos x = \sqrt{x}$ | 18. $x^3 - 5x + 3 = 0$ |

Ramanujan's Method

We need the following Theorem:

Binomial Theorem: If n is any rational number and $|x| < 1$, then

$$(1+x)^n = 1 + \frac{n}{1}x + \frac{n(n-1)}{1 \cdot 2}x^2 + \dots + \frac{n(n-1) \dots (n-(r-1))}{1 \cdot 2 \dots r}x^r + \dots$$

In particular,

$$(1+x)^{-1} = 1 - x + x^2 - x^3 + \dots + (-1)^n x^n + \dots$$

and $(1-x)^{-1} = 1 + x + x^2 + x^3 + \dots + x^n + \dots$

Indian Mathematician Srinivasa Ramanujan (1887-1920) described an iterative method which can be used to determine the smallest root of the equation

$$f(x) = 0,$$

where $f(x)$ is of the form

$$f(x) = 1 - (a_1x + a_2x^2 + a_3x^3 + a_4x^4 + \dots).$$

For smaller values of x , we can write

$$[1 - (a_1x + a_2x^2 + a_3x^3 + a_4x^4 + \dots)]^{-1} = b_1 + b_2x + b_3x^2 + \dots$$

Expanding the left-hand side using binomial theorem, we obtain

$$\begin{aligned} 1 + (a_1x + a_2x^2 + a_3x^3 + \dots) + (a_1x + a_2x^2 + a_3x^3 + \dots)^2 + \dots \\ = b_1 + b_2x + b_3x^2 + \dots \end{aligned}$$

Comparing the coefficients of like powers of x on both sides we obtain

$$\left. \begin{aligned} b_1 &= 1, \\ b_2 &= a_1 = a_1b_1, \\ b_3 &= a_1^2 + a_2 = a_1b_2 + a_2b_1, \\ &\vdots \\ b_n &= a_1b_{n-1} + a_2b_{n-2} + \dots + a_{n-1}b_1 \quad n = 2, 3, \dots \end{aligned} \right\}$$

Then b_n / b_{n+1} approach a root of the equation $f(x) = 0$.

Example Find the smallest root of the equation

$$f(x) = x^3 - 6x^2 + 11x - 6 = 0.$$

Solution

The given equation can be written as $f(x)$

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

Comparing,

$$a_1 = \frac{11}{6}, \quad a_2 = -1, \quad a_3 = \frac{1}{6}, \quad a_4 = a_5 = \dots = 0$$

To apply Ramanujan's method we write

$$1 - \left(\frac{11x - 6x^2 + x^3}{6} \right)^{-1} = b_1 + b_2x + b_3x^2 + \dots$$

Hence,

$$b_1 = 1;$$

$$b_2 = a_1 = \frac{11}{6};$$

$$b_3 = a_1b_2 + a_2b_1 = \frac{121}{36} - 1 = \frac{85}{36};$$

$$b_4 = a_1b_3 + a_2b_2 + a_3b_1 = \frac{575}{216};$$

$$b_5 = a_1b_4 + a_2b_3 + a_3b_2 + a_4b_1 = \frac{3661}{1296};$$

$$b_6 = a_1b_5 + a_2b_4 + a_3b_3 + a_4b_2 + a_5b_1 = \frac{22631}{7776};$$

Therefore,

$$\frac{b_1}{b_2} = \frac{6}{11} = 0.54545; \quad \frac{b_2}{b_3} = \frac{66}{85} = 0.7764705$$

$$\frac{b_3}{b_4} = \frac{102}{115} = 0.8869565; \quad \frac{b_4}{b_5} = \frac{3450}{3661} = 0.9423654$$

$$\frac{b_5}{b_6} = \frac{3138}{3233} = 0.9706155$$

By inspection, a root of the given equation is unity and it can be seen that the successive convergents $\frac{b_n}{b_{n+1}}$ approach this root.

Example Find a root of the equation $xe^x = 1$.

Let $xe^x = 1$

Recall $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$

Hence,

$$f(x) = 1 - \left(x + x^2 + \frac{x^3}{2} + \frac{x^4}{6} + \frac{x^5}{24} + \dots \right) = 0$$

$$a_1 = 1, \quad a_2 = 1, \quad a_3 = \frac{1}{2}, \quad a_4 = \frac{1}{6}, \quad a_5 = \frac{1}{24}, \dots$$

We then have

$$b_1 = 1;$$

$$b_2 = a_2 = 1;$$

$$b_3 = a_1 b_2 + a_2 b_1 = 1 + 1 = 2;$$

$$b_4 = a_1 b_3 + a_2 b_2 + a_3 b_1 = 2 + 1 + \frac{1}{2} = \frac{7}{2};$$

$$b_5 = a_1 b_4 + a_2 b_3 + a_3 b_2 + a_4 b_1 = \frac{7}{2} + 2 + \frac{1}{2} + \frac{1}{6} = \frac{37}{6};$$

$$b_6 = a_1 b_5 + a_2 b_4 + a_3 b_3 + a_4 b_2 + a_5 b_1 = \frac{37}{6} + \frac{7}{2} + 1 + \frac{1}{6} + \frac{1}{24} = \frac{261}{24};$$

Therefore,

$$\frac{b_2}{b_3} = \frac{1}{2} = 0.5; \quad \frac{b_3}{b_4} = \frac{4}{7} = 0.5714;$$

$$\frac{b_4}{b_5} = \frac{21}{37} = 0.56756756; \quad \frac{b_5}{b_6} = \frac{148}{261} = 0.56704980.$$

Example Using Ramanujan's method, find a real root of the equation

$$1 - x + \frac{x^2}{(2!)^2} - \frac{x^3}{(3!)^2} + \frac{x^4}{(4!)^2} - \dots = 0.$$

Solution

Let
$$f(x) = 1 - \left[x - \frac{x^2}{(2!)^2} + \frac{x^3}{(3!)^2} - \frac{x^4}{(4!)^2} + \dots \right] = 0.$$

Here

$$a_1 = 1, \quad a_2 = -\frac{1}{(2!)^2}, \quad a_3 = \frac{1}{(3!)^2}, \quad a_4 = -\frac{1}{(4!)^2},$$

$$a_5 = \frac{1}{(5!)^2}, \quad a_6 = -\frac{1}{(6!)^2}, \dots$$

Writing

$$\left\{ 1 - \left[x - \frac{x^2}{(2!)} + \frac{x^3}{(3!)^2} - \frac{x^4}{(4!)^2} + \dots \right] \right\}^{-1} = b_1 + b_2x + b_3x^2 + \dots,$$

we obtain

$$b_1 = 1,$$

$$b_2 = a_1 = 1,$$

$$b_3 = a_1b_2 + a_2b_1 = 1 - \frac{1}{(2!)^2} = \frac{3}{4};$$

$$b_4 = a_1b_3 + a_2b_2 + a_3b_1 = \frac{3}{4} - \frac{1}{(2!)^2} + \frac{1}{(3!)^2} = \frac{3}{4} - \frac{1}{4} + \frac{1}{36} = \frac{19}{36},$$

$$b_5 = a_1b_4 + a_2b_3 + a_3b_2 + a_4b_1$$

$$= \frac{19}{36} - \frac{1}{4} \times \frac{3}{4} + \frac{1}{36} \times 1 - \frac{1}{576} = \frac{211}{576}.$$

It follows

$$\frac{b_1}{b_2} = 1; \quad \frac{b_2}{b_3} = \frac{4}{3} = 1.333\dots;$$

$$\frac{b_3}{b_4} = \frac{3}{4} \times \frac{36}{19} = \frac{27}{19} = 1.4210\dots, \quad \frac{b_4}{b_5} = \frac{19}{36} \times \frac{576}{211} = 1.4408\dots,$$

where the last result is correct to three significant figures.

Example Find a root of the equation $\sin x = 1 - x$.

Using the expansion of $\sin x$, the given equation may be written as

$$f(x) = 1 - \left(x + x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots \right) = 0.$$

Here

$$a_1 = 2, \quad a_2 = 0, \quad a_3 = \frac{1}{6}, \quad a_4 = 0,$$

$$a_5 = \frac{1}{120}, \quad a_6 = 0, \quad a_7 = -\frac{1}{5040}, \dots$$

we write

$$\left[1 - \left(2x - \frac{x^3}{6} + \frac{x^5}{120} - \frac{x^7}{5040} + \dots \right) \right]^{-1} = b_1 + b_2x + b_3x^2 + \dots$$

We then obtain

$$b_1 = 1;$$

$$b_2 = a_1 = 2;$$

$$b_3 = a_1b_2 + a_2b_1 = 4;$$

$$b_4 = a_1b_3 + a_2b_2 + a_3b_1 = 8 - \frac{1}{6} = \frac{47}{6};$$

$$b_5 = a_1b_4 + a_2b_3 + a_3b_2 + a_4b_1 = \frac{46}{3};$$

$$b_6 = a_1b_5 + a_2b_4 + a_3b_3 + a_4b_2 + a_5b_1 = \frac{3601}{120};$$

Therefore,

$$\frac{b_1}{b_2} = \frac{1}{2}, \quad \frac{b_2}{b_3} = \frac{1}{2},$$

$$\frac{b_3}{b_4} = \frac{24}{47} = 0.5106382 \quad \frac{b_4}{b_5} = \frac{47}{92} = 0.5108695$$

$$\frac{b_5}{b_6} = \frac{1840}{3601} = 0.5109691.$$

The root, correct to four decimal places is 0.5110

Exercises

1. Using Ramanujan's method, obtain the first-eight convergents of the equation

$$1 - x + \frac{x^2}{(2!)^2} - \frac{x^3}{(3!)^2} + \frac{x^4}{(4!)^2} - \dots = 0$$

2. Using Ramanujan's method, find the real root of the equation $x + x^3 = 1$.

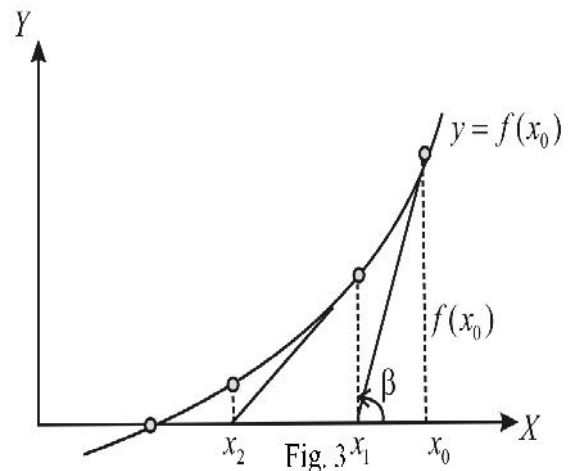
3

NEWTON RAPHSON ETC..

The Newton-Raphson method, or Newton Method, is a powerful technique for solving equations numerically. Like so much of the differential calculus, it is based on the simple idea of linear approximation.

Newton - Raphson Method

Consider $f(x)=0$, where f has continuous derivative f' . From the figure we can say that at $x=a$, $y=f(a)=0$; which means that a is a solution to the equation $f(x)=0$. In order to find the value of a , we start with any arbitrary point x_0 . From figure we can see that, the tangent to the curve f at $(x_0, f(x_0))$ (with slope $f'(x_0)$) touches the x -axis at x_1 .



$$\text{Now, } \tan S = f'(x_0) = \frac{f(x_0) - f(x_1)}{x_0 - x_1},$$

As $f(x_1)=0$, the above simplifies to

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

In the second step, we compute

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)},$$

in the third step we compute

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

and so on. More generally, we write x_{n+1} in terms of x_n , $f(x_n)$ and $f'(x_n)$ for $n=1, 2, \dots$ by means of the **Newton-Raphson** formula

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

The refinement on the value of the root x_n is terminated by any of the following conditions.

- (i) Termination after a pre-fixed number of steps
- (ii) After n iterations where, $|x_{n+1} - x_n| \leq \varepsilon$ (for a given $\varepsilon > 0$), or
- (iii) After n iterations, where $f(x_n) \leq \alpha$ (for a given $\alpha > 0$).

Termination after a fixed number of steps is not advisable, because a fine approximation cannot be ensured by a fixed number of steps.

Algorithm: The steps of the Newton-Raphson method to find the root of an equation $f(x) = 0$ are

1. Evaluate $f'(x)$
2. Use an initial guess of the root, x_i , to estimate the new value of the root, x_{i+1} , as

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

3. Find the absolute relative approximate error $|\epsilon_a|$ as

$$|\epsilon_a| = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \times 100$$

4. Compare the absolute relative approximate error with the pre-specified relative error tolerance, ϵ_s . If $|\epsilon_a| > \epsilon_s$ then go to Step 2, else stop the algorithm. Also, check if the number of iterations has exceeded the maximum number of iterations allowed. If so, one needs to terminate the algorithm and notify the user.

The method can be used for both algebraic and transcendental equations, and it also works when coefficients or roots are complex. It should be noted, however, that in the case of an algebraic equation with real coefficients, a complex root cannot be reached with a real starting value.

Example Set up a Newton iteration for computing the square root of a given positive number. Using the same find the square root of 2 exact to six decimal places.

Let c be a given positive number and let x be its positive square root, so that $x = \sqrt{c}$. Then $x^2 = c$ or

$$f(x) = x^2 - c = 0$$

$$f'(x) = 2x$$

Using the Newton's iteration formula we have

$$x_{n+1} = x_n - \frac{x_n^2 - c}{2x_n}$$

or
$$x_{n+1} = \frac{x_n}{2} + \frac{c}{2x_n}$$

or
$$x_{n+1} = \frac{1}{2} \left(x_n + \frac{c}{x_n} \right), n = 0, 1, 2, \dots,$$

Now to find the square root of 2, let $c = 2$, so that

$$x_{n+1} = \frac{1}{2} \left(x_n + \frac{2}{x_n} \right), n = 0, 1, 2, \dots$$

Choose $x_0 = 1$. Then

$$x_1 = 1.500000, x_2 = 1.416667, x_3 = 1.414216, x_4 = 1.414214, \dots$$

and accept 1.414214 as the square root of 2 exact to 6D.

Historical Note: Heron of Alexandria (60 CE?) used a pre-algebra version of the above recurrence. It is still at the heart of computer algorithms for finding square roots.

Example. Let us find an approximation to $\sqrt{5}$ to ten decimal places.

Note that $\sqrt{5}$ is an irrational number. Therefore the sequence of decimals which defines $\sqrt{5}$ will not stop. Clearly $\sqrt{5}$ is the only zero of $f(x) = x^2 - 5$ on the interval $[1, 3]$. See the Picture.



Let us start this process by taking $x_1 = 2$.

Example. Let us approximate the only solution to the equation $x = \cos x$

This solution is also the only zero of the function $f(x) = x - \cos x$. So now we see how Newton's method may be used to approximate r . Since r is between 0 and $\pi/2$, we set $x_1 = 1$. The rest of the sequence is generated through the formula

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

We have

$$\begin{aligned} x_1 &= 1. \\ x_2 &= 0.750363867840243893034942306682177 \\ x_3 &= 0.739112890911361670360585290904890 \\ x_4 &= 0.739085133385283969760125120856804 \\ x_5 &= 0.739085133215160641661702625685026 \\ x_6 &= 0.739085133215160641655312087673873 \\ x_7 &= 0.739085133215160641655312087673873 \\ x_8 &= 0.739085133215160641655312087673873 \end{aligned}$$

Example Apply Newton's method to solve the algebraic equation $f(x) = x^3 + x - 1 = 0$ correct to 6 decimal places. (Start with $x_0 = 1$)

$$f(x) = x^3 + x - 1,$$

$$f'(x) = 3x^2 + 1$$

and substituting these in Newton's iterative formula, we have

$$x_{n+1} = x_n - \frac{x_n^3 + x_n - 1}{3x_n^2 + 1} \quad \text{or} \quad x_{n+1} = \frac{2x_n^3 + 1}{3x_n^2 + 1}, \quad n = 0, 1, 2, \dots$$

Starting from $x_0 = 1.000\,000$,

$x_1 = 0.750000$, $x_2 = 0.686047$, $x_3 = 0.682340$, $x_4 = 0.682328$, \dots and we accept 0.682328 as an approximate solution of $f(x) = x^3 + x - 1 = 0$ correct to 6 decimal places.

Example Set up Newton-Raphson iterative formula for the equation

$$x \log_{10} x - 1.2 = 0.$$

Solution

Take $f(x) = x \log_{10} x - 1.2$.

Noting that $\log_{10} x = \log_e x \cdot \log_{10} e \approx 0.4343 \log_e x$,

we obtain $f(x) = 0.4343x \log_e x - 1.2$.

$$f'(x) = 0.4343 \log_e x + 0.4343x \times \frac{1}{x} = \log_{10} x + 0.4343$$

and hence the Newton's iterative formula for the given equation is

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{0.4343x_n \log_e x_n - 1.2}{\log_{10} x_n + 0.4343}.$$

Example Find the positive solution of the transcendental equation

$$2 \sin x = x.$$

Here $f(x) = x - 2 \sin x$,

so that $f'(x) = 1 - 2 \cos x$

Substituting in Newton's iterative formula, we have

$$x_{n+1} = x_n - \frac{x_n - 2 \sin x_n}{1 - 2 \cos x_n}, \quad n = 0, 1, 2, \dots \quad \text{or}$$

$$x_{n+1} = \frac{2(\sin x_n - x_n \cos x_n)}{1 - 2 \cos x_n} = \frac{N_n}{D_n}, \quad n = 0, 1, 2, \dots$$

where we take $N_n = 2(\sin x_n - x_n \cos x_n)$ and $D_n = 1 - 2 \cos x_n$, to easy our calculation. Values calculated at each step are indicated in the following table (Starting with $x_0 = 2$).

n	x_n	N_n	D_n	x_{n+1}
0	2.000	3.483	1.832	1.901
1	1.901	3.125	1.648	1.896
2	1.896	3.107	1.639	1.896

1.896 is an approximate solution to $2 \sin x = x$.

Example Use Newton-Raphson method to find a root of the equation $x^3 - 2x - 5 = 0$.

Here $f(x) = x^3 - 2x - 5$ and $f'(x) = 3x^2 - 2$. Hence Newton's iterative formula becomes

$$x_{n+1} = x_n - \frac{x_n^3 - 2x_n - 5}{3x_n^2 - 2}$$

Choosing $x_0 = 2$, we obtain $f(x_0) = -1$ and $f'(x_0) = 10$.

$$x_1 = 2 - \left(-\frac{1}{10}\right) = 2.1$$

$$f(x_1) = (2.1)^3 - 2(2.1) - 5 = 0.06,$$

and $f'(x_1) = 3(2.1)^2 - 2 = 11.23$.

$$x_2 = 2.1 - \frac{0.061}{11.23} = 2.094568.$$

2.094568 is an approximate root.

Example Find a root of the equation $x \sin x + \cos x = 0$.

We have

$$f(x) = x \sin x + \cos x \quad \text{and} \quad f'(x) = x \cos x.$$

Hence the iteration formula is

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

With $x_0 = \pi$, the successive iterates are given below:

n	x_n	$f(x_n)$	x_{n+1}
0	3.1416	-1.0	2.8233
1	2.8233	-0.0662	2.7986
2	2.7986	-0.0006	2.7984
3	2.7984	0.0	2.7984

Example Find a real root of the equation $x = e^{-x}$, using the Newton - Raphson method.

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

Let $x_0 = 1$. Then

$$x_1 = 1 - \frac{e-1}{2e} = \frac{1}{2} \left(1 + \frac{1}{e}\right) = 0.6839397$$

Now $f(x_1) = 0.3553424$, and $f'(x_1) = 3.337012$,

$$x_2 = 0.6839397 - \frac{0.3553424}{3.337012} = 0.5774545.$$

$$x_3 = 0.5672297 \text{ and } x_4 = 0.5671433.$$

Example $f(x) = x^{-2} + \ln x$ has a root near $x = 1.5$. Use the Newton-Raphson formula to obtain a better estimate.

Here $x_0 = 1.5$, $f(1.5) = -0.5 + \ln(1.5) = -0.0945$

$$f'(x) = 1 + \frac{1}{x}; \quad f'(1.5) = \frac{5}{3}; \quad x_1 = 1.5 - \frac{(-0.0945)}{1.6667} = 1.5567$$

The Newton-Raphson formula can be used again: this time beginning with 1.5567 as our initial

$$x_2 = 1.5567 - \frac{(-0.0007)}{1.6424} = 1.5571$$

This is in fact the correct value of the root to 4 d.p.

Generalized Newton's Method

If α is a root of $f(x) = 0$ with multiplicity p , then the generalized Newton's formula is

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

Since α is a root of $f(x) = 0$ with multiplicity p , it follows that α is a root of $f'(x) = 0$ with multiplicity $(p-1)$, of $f''(x) = 0$ with multiplicity $(p-2)$, and so on. Hence the expressions

$$x_0 - p \frac{f(x_0)}{f'(x_0)}, \quad x_0 - (p-1) \frac{f'(x_0)}{f''(x_0)}, \quad x_0 - (p-2) \frac{f''(x_0)}{f'''(x_0)}$$

must have the same value if there is a root with multiplicity p , provided that the initial approximation x_0 is chosen sufficiently close to the root.

Example Find a double root of the equation

$$f(x) = x^3 - x^2 - x + 1 = 0.$$

Here $f'(x) = 3x^2 - 2x - 1$, and $f''(x) = 6x - 2$. With $x_0 = 0.8$, we obtain

$$x_0 - 2 \frac{f(x_0)}{f'(x_0)} = 0.8 - 2 \frac{0.072}{-(0.68)} = 1.012,$$

and

$$x_0 - \frac{f'(x_0)}{f''(x_0)} = 0.8 - \frac{-(0.68)}{2.8} = 1.043,$$

The closeness of these values indicates that there is a double root near to unity. For the next approximation, we choose $x_1 = 1.01$ and obtain

$$x_1 - 2 \frac{f(x_1)}{f'(x_1)} = 1.01 - 0.0099 = 1.0001,$$

and

$$x_1 - \frac{f'(x_1)}{f''(x_1)} = 1.01 - 0.0099 = 1.0001,$$

Hence we conclude that there is a double root at $x = 1.0001$ which is sufficiently close to the actual root unity.

On the other hand, if we apply Newton-Raphson method with $x_0 = 0.8$, we obtain $x_1 = 0.8 + 0.106 \approx 0.91$, and $x_2 = 0.91 + 0.046 \approx 0.96$.

Exercises

1. Approximate the real root to two four decimal places of $x^3 + 5x - 3 = 0$
2. Approximate to four decimal places $\sqrt[3]{3}$
3. Find a positive root of the equation $x^4 + 2x + 1 = 0$ correct to 4 places of decimals. (Choose $x_0 = 1.3$)
4. Explain how to determine the square root of a real number by $N-R$ method and using it determine $\sqrt{3}$ correct to three decimal places.
5. Find the value of $\sqrt{2}$ correct to four decimals places using Newton Raphson method.
6. Use the Newton-Raphson method, with 3 as starting point, to find a fraction that is within 10^{-8} of $\sqrt{10}$.
7. Design Newton iteration for the cube root. Calculate $\sqrt[3]{7}$, starting from $x_0 = 2$ and performing 3 steps.
8. Calculate $\sqrt{7}$ by Newton's iteration, starting from $x_0 = 2$ and calculating x_1, x_2, x_3 . Compare the results with the value $\sqrt{7} = 2.645751$

9. Design a Newton's iteration for computing k^{th} root of a positive number c .
10. Find all real solutions of the following equations by Newton's iteration method.

$$(a) \sin x = \frac{x}{2} \quad (b) \ln x = 1 - 2x \quad (c) \cos x = \sqrt{x}$$

11. Using Newton-Raphson method, find the root of the equation $x^3 - x^2 - x - 3 = 0$, correct to three decimal places

12. Apply Newton's method to the equation

$$x^3 - 5x + 3 = 0$$

starting from the given $x_0 = 2$ and performing 3 steps.

13. Apply Newton's method to the equation

$$x^4 - x^3 - 2x - 34 = 0$$

starting from the given $x_0 = 3$ and performing 3 steps.

14. Apply Newton's method to the equation

$$x^3 - 3.9x^2 + 4.79x - 1.881 = 0$$

starting from the given $x_0 = 1$ and performing 3 steps.

Ramanujan's Method

We need the following Theorem:

Binomial Theorem: If n is any rational number and $|x| < 1$, then

$$(1+x)^n = 1 + \frac{n}{1}x + \frac{n(n-1)}{1 \cdot 2}x^2 + \dots + \frac{n(n-1) \dots (n-(r-1))}{1 \cdot 2 \dots r}x^r + \dots$$

In particular,

$$(1+x)^{-1} = 1 - x + x^2 - x^3 + \dots + (-1)^n x^n + \dots$$

and $(1-x)^{-1} = 1 + x + x^2 + x^3 + \dots + x^n + \dots$

Indian Mathematician Srinivasa Ramanujan (1887-1920) described an iterative method which can be used to determine the smallest root of the equation

$$f(x) = 0,$$

where $f(x)$ is of the form

$$f(x) = 1 - (a_1x + a_2x^2 + a_3x^3 + a_4x^4 + \dots).$$

For smaller values of x , we can write

$$[1 - (a_1x + a_2x^2 + a_3x^3 + a_4x^4 + \dots)]^{-1} = b_1 + b_2x + b_3x^2 + \dots$$

Expanding the left-hand side using binomial theorem, we obtain

$$\begin{aligned} 1 + (a_1x + a_2x^2 + a_3x^3 + \dots) + (a_1x + a_2x^2 + a_3x^3 + \dots)^2 + \dots \\ = b_1 + b_2x + b_3x^2 + \dots \end{aligned}$$

Comparing the coefficients of like powers of x on both sides we obtain

$$\left. \begin{aligned} b_1 &= 1, \\ b_2 &= a_1 = a_1b_1, \\ b_3 &= a_1^2 + a_2 = a_1b_2 + a_2b_1, \\ &\vdots \\ b_n &= a_1b_{n-1} + a_2b_{n-2} + \dots + a_{n-1}b_1 \quad n = 2, 3, \dots \end{aligned} \right\}$$

Then b_n / b_{n+1} approach a root of the equation $f(x) = 0$.

Example Find the smallest root of the equation

$$f(x) = x^3 - 6x^2 + 11x - 6 = 0.$$

Solution

The given equation can be written as $f(x)$

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

Comparing,

$$a_1 = \frac{11}{6}, \quad a_2 = -1, \quad a_3 = \frac{1}{6}, \quad a_4 = a_5 = \dots = 0$$

To apply Ramanujan's method we write

$$1 - \left(\frac{11x - 6x^2 + x^3}{6} \right)^{-1} = b_1 + b_2x + b_3x^2 + \dots$$

Hence,

$$b_1 = 1;$$

$$b_2 = a_1 = \frac{11}{6};$$

$$b_3 = a_1 b_2 + a_2 b_1 = \frac{121}{36} - 1 = \frac{85}{36};$$

$$b_4 = a_1 b_3 + a_2 b_2 + a_3 b_1 = \frac{575}{216};$$

$$b_5 = a_1 b_4 + a_2 b_3 + a_3 b_2 + a_4 b_1 = \frac{3661}{1296};$$

$$b_6 = a_1 b_5 + a_2 b_4 + a_3 b_3 + a_4 b_2 + a_5 b_1 = \frac{22631}{7776};$$

Therefore,

$$\frac{b_1}{b_2} = \frac{6}{11} = 0.54545; \quad \frac{b_2}{b_3} = \frac{66}{85} = 0.7764705$$

$$\frac{b_3}{b_4} = \frac{102}{115} = 0.8869565; \quad \frac{b_4}{b_5} = \frac{3450}{3661} = 0.9423654$$

$$\frac{b_5}{b_6} = \frac{3138}{3233} = 0.9706155$$

By inspection, a root of the given equation is unity and it can be seen that the successive convergents $\frac{b_n}{b_{n+1}}$ approach this root.

Example Find a root of the equation $xe^x = 1$.

Let $xe^x = 1$

Recall $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$

Hence,

$$f(x) = 1 - \left(x + x^2 + \frac{x^3}{2} + \frac{x^4}{6} + \frac{x^5}{24} + \dots \right) = 0$$

$$a_1 = 1, \quad a_2 = 1, \quad a_3 = \frac{1}{2}, \quad a_4 = \frac{1}{6}, \quad a_5 = \frac{1}{24}, \dots$$

We then have

$$b_1 = 1;$$

$$b_2 = a_2 = 1;$$

$$b_3 = a_1 b_2 + a_2 b_1 = 1 + 1 = 2;$$

$$b_4 = a_1 b_3 + a_2 b_2 + a_3 b_1 = 2 + 1 + \frac{1}{2} = \frac{7}{2};$$

$$b_5 = a_1 b_4 + a_2 b_3 + a_3 b_2 + a_4 b_1 = \frac{7}{2} + 2 + \frac{1}{2} + \frac{1}{6} = \frac{37}{6};$$

$$b_6 = a_1 b_5 + a_2 b_4 + a_3 b_3 + a_4 b_2 + a_5 b_1 = \frac{37}{6} + \frac{7}{2} + 1 + \frac{1}{6} + \frac{1}{24} = \frac{261}{24};$$

Therefore,

$$\frac{b_2}{b_3} = \frac{1}{2} = 0.5; \quad \frac{b_3}{b_4} = \frac{4}{7} = 0.5714;$$

$$\frac{b_4}{b_5} = \frac{21}{37} = 0.56756756; \quad \frac{b_5}{b_6} = \frac{148}{261} = 0.56704980.$$

Example Using Ramanujan's method, find a real root of the equation

$$1 - x + \frac{x^2}{(2!)^2} - \frac{x^3}{(3!)^2} + \frac{x^4}{(4!)^2} - \dots = 0.$$

Solution

Let
$$f(x) = 1 - \left[x - \frac{x^2}{(2!)^2} + \frac{x^3}{(3!)^2} - \frac{x^4}{(4!)^2} + \dots \right] = 0.$$

Here

$$a_1 = 1, \quad a_2 = -\frac{1}{(2!)^2}, \quad a_3 = \frac{1}{(3!)^2}, \quad a_4 = -\frac{1}{(4!)^2},$$

$$a_5 = \frac{1}{(5!)^2}, \quad a_6 = -\frac{1}{(6!)^2}, \dots$$

Writing

$$\left\{ 1 - \left[x - \frac{x^2}{(2!)} + \frac{x^3}{(3!)^2} - \frac{x^4}{(4!)^2} + \dots \right] \right\}^{-1} = b_1 + b_2x + b_3x^2 + \dots,$$

we obtain

$$b_1 = 1,$$

$$b_2 = a_1 = 1,$$

$$b_3 = a_1b_2 + a_2b_1 = 1 - \frac{1}{(2!)^2} = \frac{3}{4};$$

$$b_4 = a_1b_3 + a_2b_2 + a_3b_1 = \frac{3}{4} - \frac{1}{(2!)^2} + \frac{1}{(3!)^2} = \frac{3}{4} - \frac{1}{4} + \frac{1}{36} = \frac{19}{36},$$

$$\begin{aligned} b_5 &= a_1b_4 + a_2b_3 + a_3b_2 + a_4b_1 \\ &= \frac{19}{36} - \frac{1}{4} \times \frac{3}{4} + \frac{1}{36} \times 1 - \frac{1}{576} = \frac{211}{576}. \end{aligned}$$

It follows

$$\frac{b_1}{b_2} = 1; \quad \frac{b_2}{b_3} = \frac{4}{3} = 1.333\dots;$$

$$\frac{b_3}{b_4} = \frac{3}{4} \times \frac{36}{19} = \frac{27}{19} = 1.4210\dots, \quad \frac{b_4}{b_5} = \frac{19}{36} \times \frac{576}{211} = 1.4408\dots,$$

where the last result is correct to three significant figures.

Example Find a root of the equation $\sin x = 1 - x$.

Using the expansion of $\sin x$, the given equation may be written as

$$f(x) = 1 - \left(x + x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots \right) = 0.$$

Here

$$a_1 = 2, \quad a_2 = 0, \quad a_3 = \frac{1}{6}, \quad a_4 = 0,$$

$$a_5 = \frac{1}{120}, \quad a_6 = 0, \quad a_7 = -\frac{1}{5040}, \dots$$

we write

$$\left[1 - \left(2x - \frac{x^3}{6} + \frac{x^5}{120} - \frac{x^7}{5040} + \dots \right) \right]^{-1} = b_1 + b_2x + b_3x^2 + \dots$$

We then obtain

$$b_1 = 1;$$

$$b_2 = a_1 = 2;$$

$$b_3 = a_1b_2 + a_2b_1 = 4;$$

$$b_4 = a_1b_3 + a_2b_2 + a_3b_1 = 8 - \frac{1}{6} = \frac{47}{6};$$

$$b_5 = a_1b_4 + a_2b_3 + a_3b_2 + a_4b_1 = \frac{46}{3};$$

$$b_6 = a_1b_5 + a_2b_4 + a_3b_3 + a_4b_2 + a_5b_1 = \frac{3601}{120};$$

Therefore,

$$\frac{b_1}{b_2} = \frac{1}{2},$$

$$\frac{b_2}{b_3} = \frac{1}{2},$$

$$\frac{b_3}{b_4} = \frac{24}{47} = 0.5106382$$

$$\frac{b_4}{b_5} = \frac{47}{92} = 0.5108695$$

$$\frac{b_5}{b_6} = \frac{1840}{3601} = 0.5109691.$$

The root, correct to four decimal places is 0.5110

Exercises

1. Using Ramanujan's method, obtain the first-eight convergents of the equation

$$1 - x + \frac{x^2}{(2!)^2} - \frac{x^3}{(3!)^2} + \frac{x^4}{(4!)^2} - \dots = 0$$

2. Using Ramanujan's method, find the real root of the equation $x + x^3 = 1$.

The Secant Method

We have seen that the Newton-Raphson method requires the evaluation of derivatives of the function and this is not always possible, particularly in the case of functions arising in practical problems. In the secant method, the derivative at x_n is approximated by the formula

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}},$$

which can be written as

$$f'_n = \frac{f_n - f_{n-1}}{x_n - x_{n-1}},$$

where $f_n = f(x_n)$. Hence, the Newton-Raphson formula becomes

$$x_{n+1} = x_n - \frac{f_n(x_n - x_{n-1})}{f_n - f_{n-1}} = \frac{x_{n+1}f_n - x_n f_{n-1}}{f_n - f_{n-1}}.$$

It should be noted that this formula requires two initial approximations to the root.

Example Find a real root of the equation $x^3 - 2x - 5 = 0$ using secant method.

Let the two initial approximations be given by $x_{-1} = 2$ and $x_0 = 3$.

We have

$$f(x_{-1}) = f_1 = 8 - 9 = -1, \text{ and } f(x_0) = f_0 = 27 - 11 = 16.$$

$$x_1 = \frac{2(16) - 3(-1)}{17} = \frac{35}{17} = 2.058823529.$$

Also,

$$f(x_1) = f_1 = -0.390799923.$$

$$x_2 = \frac{x_0 f_1 - x_1 f_0}{f_1 - f_0} = \frac{3(-0.390799923) - 2.058823529(16)}{-16.390799923} = 2.08126366.$$

Again

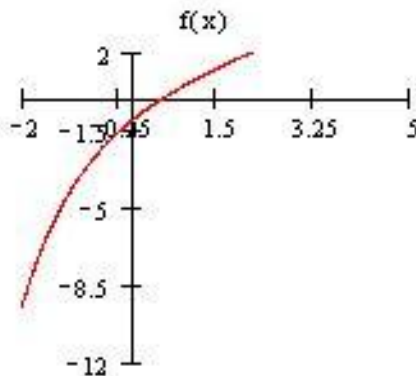
$$f(x_2) = f_2 = -0.147204057.$$

$$x_3 = 2.094824145.$$

Example: Find a real root of the equation $x - e^{-x} = 0$ using secant method.

Solution

The graph of $f(x) = x - e^{-x}$ is as shown here.



Let us assume the initial approximation to the roots as 1 and 2. That is consider $x_{-1} = 1$ and $x_0 = 2$

$$f(x_{-1}) = f_{-1} = 1 - e^{-1} = 1 - 0.367879441 = 0.632120559 \quad \text{and}$$

$$f(x_0) = f_0 = 2 - e^{-2} = 2 - 0.135335283 = 1.864664717.$$

Step 1: Putting $n = 0$, we obtain $x_1 = \frac{x_{-1}f_0 - x_0f_{-1}}{f_0 - f_{-1}}$

$$\text{Here, } x_1 = \frac{1(1.864664717) - 2(0.632120559)}{1.864664717 - 0.632120559} = \frac{0.600423599}{1.232544158} = 0.487142.$$

Also,

$$f(x_1) = f_1 = 0.487142 - e^{-0.487142} = -0.12724.$$

Step 2: Putting $n = 1$, we obtain

$$x_2 = \frac{x_0f_1 - x_1f_0}{f_1 - f_0} = \frac{2(-0.12724) - 0.487142(1.864664717)}{-0.12724 - 1.864664717} = \frac{-1.16284}{-1.99190} = 0.58378$$

Again

$$f(x_2) = f_2 = 0.58378 - e^{-0.58378} = 0.02599.$$

Step 3: Setting $n = 2$,

$$x_3 = \frac{x_1f_2 - x_2f_1}{f_2 - f_1} = \frac{0.487142(0.02599) - 0.58378(-0.12724)}{0.02599 - (-0.12724)} = \frac{0.08694}{0.15323} = 0.56738$$

$$f(x_3) = f_3 = 0.56738 - e^{-0.56738} = 0.00037.$$

Step 4: Setting $n = 3$ in (*),

$$x_4 = \frac{x_2 f_3 - x_3 f_2}{f_3 - f_2} = \frac{0.58378(0.00037) - 0.56738(0.02599)}{0.00037 - 0.02599} = \frac{-0.01453}{-0.02562} = 0.5671$$

Approximating to three digits, the root can be considered as 0.567.

Exercises

1. Determine the real root of the equation $xe^x = 1$ using the secant method. Compare your result with the true value of $x = 0.567143 \dots$.
2. Use the secant method to determine the root, lying between 5 and 8, of the equation $x^{2.2} = 69$.

Objective Type Questions

- (a) The Newton-Raphson method formula for finding the square root of a real number C from the equation $x^2 - C = 0$ is,

(i) $x_{n+1} = \frac{x_n}{2}$ (ii) $x_{n+1} = \frac{3x_n}{2}$ (iii) $x_{n+1} = \frac{1}{2} \left(x_n + \frac{C}{x_n} \right)$ (iv) None of these

- (b) The next iterative value of the root of $2x^2 - 3 = 0$ using the Newton-Raphson method, if the initial guess is 2, is

(i) 1.275 (ii) 1.375 (iii) 1.475 (iv) None of these

- (c) The next iterative value of the root of $2x^2 - 3 = 0$ using the secant method, if the initial guesses are 2 and 3, is

(i) 1 (ii) 1.25 (iii) 1.5 (iv) None of these

- (d) In secant method,

(i) $x_{n+1} = \frac{x_n f_n - x_{n-1} f_{n-1}}{f_n - f_{n-1}}$ (ii) $x_{n+1} = \frac{x_n f_n - x_{n-1} f_{n-1}}{f_n - f_{n-1}}$ (iii) $x_{n+1} = \frac{x_{n-1} f_{n-1} - x_n f_n}{f_{n-1} - f_n}$

- (iv) None of these

Answers

(a) (iii) $x_{n+1} = \frac{1}{2} \left(x_n + \frac{C}{x_n} \right)$

(b) (ii) 1.375

(c) (iii) 1.5

$$(d) (i) x_{n+1} = \frac{x_{n-1}f_n - x_nf_{n-1}}{f_n - f_{n-1}}$$

Theoretical Questions with Answers:

1. What is the difference between bracketing and open method?

Ans: For finding roots of a nonlinear equation $f(x) = 0$, bracketing method requires two guesses which contain the exact root. But in open method initial guess of the root is needed without any condition of bracketing for starting the iterative process to find the solution of an equation.

2. When the Generalized Newton's methods for solving equations is helpful?

Ans: To solve the find the oot of $f(x) = 0$ with multiplicity p , the generalized Newton's formula is required.

3. What is the importance of Secant method over Newton-Raphson method?

Ans: Newton-Raphson method requires the evaluation of derivatives of the function and this is not always possible, particularly in the case of functions arising in practical problems. In such situations Secant method helps to solve the equation with an approximation to the derivative.

4

FINITE DIFFERENCES OPERATORS

For a function $y=f(x)$, it is given that y_0, y_1, \dots, y_n are the values of the variable y corresponding to the equidistant arguments, x_0, x_1, \dots, x_n , where $x_1 = x_0 + h, x_2 = x_0 + 2h, x_3 = x_0 + 3h, \dots, x_n = x_0 + nh$. In this case, even though Lagrange and divided difference interpolation polynomials can be used for interpolation, some simpler interpolation formulas can be derived. For this, we have to be familiar with some finite difference operators and finite differences, which were introduced by Sir Isaac Newton. Finite differences deal with the changes that take place in the value of a function $f(x)$ due to finite changes in x . Finite difference operators include, forward difference operator, backward difference operator, shift operator, central difference operator and mean operator.

- **Forward difference operator (Δ) :**

For the values y_0, y_1, \dots, y_n of a function $y=f(x)$, for the equidistant values $x_0, x_1, x_2, \dots, x_n$, where $x_1 = x_0 + h, x_2 = x_0 + 2h, x_3 = x_0 + 3h, \dots, x_n = x_0 + nh$, the forward difference operator Δ is defined on the function $f(x)$ as,

$$\Delta f(x_i) = f(x_i + h) - f(x_i) = f(x_{i+1}) - f(x_i)$$

That is,

$$\Delta y_i = y_{i+1} - y_i$$

Then, in particular

$$\begin{aligned} \Delta f(x_0) &= f(x_0 + h) - f(x_0) = f(x_1) - f(x_0) \\ \Rightarrow \Delta y_0 &= y_1 - y_0 \\ \Delta f(x_1) &= f(x_1 + h) - f(x_1) = f(x_2) - f(x_1) \\ \Rightarrow \Delta y_1 &= y_2 - y_1 \end{aligned}$$

etc.,

$\Delta y_0, \Delta y_1, \dots, \Delta y_i, \dots$ are known as the **first forward differences**.

The second forward differences are defined as,

$$\begin{aligned}
 \Delta^2 f(x_i) &= \Delta[\Delta f(x_i)] = \Delta[f(x_i + h) - f(x_i)] \\
 &= \Delta f(x_i + h) - \Delta f(x_i) \\
 &= f(x_i + 2h) - f(x_i + h) - [f(x_i + h) - f(x_i)] \\
 &= f(x_i + 2h) - 2f(x_i + h) + f(x_i) \\
 &= y_{i+2} - 2y_{i+1} + y_i
 \end{aligned}$$

In particular,

$$\Delta^2 f(x_0) = y_2 - 2y_1 + y_0 \quad \text{or} \quad \Delta^2 y_0 = y_2 - 2y_1 + y_0$$

The third forward differences are,

$$\begin{aligned}
 \Delta^3 f(x_i) &= \Delta[\Delta^2 f(x_i)] \\
 &= \Delta[f(x_i + 2h) - 2f(x_i + h) + f(x_i)] \\
 &= y_{i+3} - 3y_{i+2} + 3y_{i+1} - y_i
 \end{aligned}$$

In particular,

$$\Delta^3 f(x_0) = y_3 - 3y_2 + 3y_1 - y_0 \quad \text{or} \quad \Delta^3 y_0 = y_3 - 3y_2 + 3y_1 - y_0$$

In general the n^{th} forward difference,

$$\Delta^n f(x_i) = \Delta^{n-1} f(x_i + h) - \Delta^{n-1} f(x_i)$$

The differences $\Delta y_0, \Delta^2 y_0, \Delta^3 y_0, \dots$ are called the **leading differences**.

Forward differences can be written in a tabular form as follows:

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
x_0	$y_0 = f(x_0)$	$\Delta y_0 = y_1 - y_0$		
x_1	$y_1 = f(x_1)$	$\Delta y_1 = y_2 - y_1$	$\Delta^2 y_0 = \Delta y_1 - \Delta y_0$	
x_2	$y_2 = f(x_2)$	$\Delta y_2 = y_3 - y_2$	$\Delta^2 y_1 = \Delta y_2 - \Delta y_1$	$\Delta^3 y_0 = \Delta^2 y_1 - \Delta^2 y_0$
x_3	$y_3 = f(x_3)$			

Example Construct the forward difference table for the following x values and its corresponding f values.

x	0.1	0.3	0.5	0.7	0.9	1.1	1.3
f	0.003	0.067	0.148	0.248	0.370	0.518	0.697

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$	$\Delta^5 f$
0.1	0.003					
		0.064				
0.3	0.067		0.017			
		0.081		0.002		
0.5	0.148		0.019		0.001	
		0.100		0.003		0.000
0.7	0.248		0.022		0.001	
		0.122		0.004		0.000
0.9	0.370		0.026		0.001	
		0.148		0.005		
1.1	0.518		0.031			
		0.179				
1.3	0.697					

Example Construct the forward difference table, where $f(x) = \frac{1}{x}$, $x = 1(0.2)2, 4D$.

x	$f(x) = \frac{1}{x}$	Δf first differe nce	$\Delta^2 f$ second differe nce	$\Delta^3 f$	$\Delta^4 f$	$\Delta^5 f$
1.0	1.000					
		-0.1667				
1.2	0.8333		0.0477			
		-0.1190		-0.0180		
1.4	0.7143		0.0297		0.0082	-0.0045
		-0.0893		-0.0098		
1.6	0.6250		0.0199		0.0037	
		-0.0694		-0.0061		
1.8	0.5556		0.0138			
		-0.0556				
2.0	0.5000					

Example Construct the forward difference table for the data

$$\begin{array}{cccc} x: & -2 & 0 & 2 & 4 \\ y = f(x): & 4 & 9 & 17 & 22 \end{array}$$

The forward difference table is as follows:

x	y=f(x)	Δy	$\Delta^2 y$	$\Delta^3 y$
-2	4			
0	9	$\Delta y_0 = 5$		
2	17	$\Delta y_1 = 8$	$\Delta^2 y_0 = 3$	
4	22	$\Delta y_2 = 5$	$\Delta^2 y_1 = -3$	$\Delta^3 y_0 = -6$

Properties of Forward difference operator (Δ):

(i) Forward difference of a constant function is zero.

Proof: Consider the constant function $f(x) = k$

$$\text{Then,} \quad \Delta f(x) = f(x+h) - f(x) = k - k = 0$$

(ii) For the functions $f(x)$ and $g(x)$; $\Delta(f(x) + g(x)) = \Delta f(x) + \Delta g(x)$

Proof: By definition,

$$\begin{aligned} \Delta(f(x) + g(x)) &= \Delta((f + g)(x)) \\ &= (f + g)(x+h) - (f + g)(x) \\ &= f(x+h) + g(x+h) - (f(x) + g(x)) \\ &= f(x+h) - f(x) + g(x+h) - g(x) \\ &= \Delta f(x) + \Delta g(x) \end{aligned}$$

(iii) Proceeding as in (ii), for the constants a and b ,

$$\Delta(af(x) + bg(x)) = a\Delta f(x) + b\Delta g(x).$$

(iv) Forward difference of the product of two functions is given by,

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

Proof:

$$\begin{aligned}\Delta(f(x)g(x)) &= \Delta((fg)(x)) \\ &= (fg)(x+h) - (fg)(x) \\ &= f(x+h)g(x+h) - f(x)g(x)\end{aligned}$$

Adding and subtracting $f(x+h)g(x)$, the above gives

$$\begin{aligned}\Delta(f(x)g(x)) &= f(x+h)g(x+h) - f(x+h)g(x) + f(x+h)g(x) - f(x)g(x) \\ &= f(x+h)[g(x+h) - g(x)] + g(x)[f(x+h) - f(x)] \\ &= f(x+h)\Delta g(x) + g(x)\Delta f(x)\end{aligned}$$

Note : Adding and subtracting $g(x+h)f(x)$ instead of $f(x+h)g(x)$, it can also be proved that

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

(v) Forward difference of the quotient of two functions is given by

$$\Delta\left(\frac{f(x)}{g(x)}\right) = \frac{g(x)\Delta f(x) - f(x)\Delta g(x)}{g(x+h)g(x)}$$

Proof:

$$\begin{aligned}\Delta\left(\frac{f(x)}{g(x)}\right) &= \frac{f(x+h)}{g(x+h)} - \frac{f(x)}{g(x)} \\ &= \frac{f(x+h)g(x) - f(x)g(x+h)}{g(x+h)g(x)} \\ &= \frac{f(x+h)g(x) - f(x)g(x) + f(x)g(x) - f(x)g(x+h)}{g(x+h)g(x)} \\ &= \frac{g(x)[f(x+h) - f(x)] - f(x)[g(x+h) - g(x)]}{g(x+h)g(x)} \\ &= \frac{g(x)\Delta f(x) - f(x)\Delta g(x)}{g(x+h)g(x)}\end{aligned}$$

Following are some results on forward differences:

Result 1: The n^{th} forward difference of a polynomial of degree n is constant when the values of the independent variable are at equal intervals.

Result 2: If n is an integer,

$$f(a + nh) = f(a) + {}^nC_1 \Delta f(a) + {}^nC_2 \Delta^2 f(a) + \dots + \Delta^n f(a)$$

for the polynomial $f(x)$ in x .

Forward Difference Table

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$	$\Delta^5 f$	$\Delta^6 f$
x_0	f_0						
x_1	f_1	Δf_0	$\Delta^2 f_0$	$\Delta^3 f_0$			
x_2	f_2	Δf_1	$\Delta^2 f_1$	$\Delta^3 f_1$	$\Delta^4 f_0$		
x_3	f_3	Δf_2	$\Delta^2 f_2$	$\Delta^3 f_2$	$\Delta^4 f_1$	$\Delta^5 f_0$	
x_4	f_4	Δf_3	$\Delta^2 f_3$	$\Delta^3 f_3$	$\Delta^4 f_2$	$\Delta^5 f_1$	$\Delta^6 f_0$
x_5	f_5	Δf_4	$\Delta^2 f_4$				
		Δf_5					
x_6	f_6						

Example Express $\Delta^2 f_0$ and $\Delta^3 f_0$ in terms of the values of the function f .

$$\Delta^2 f_0 = \Delta f_1 - \Delta f_0 = f_2 - f_1 - (f_1 - f_0) = f_2 - 2f_1 + f_0$$

$$\begin{aligned} \Delta^3 f_0 &= \Delta^2 f_1 - \Delta^2 f_0 = \Delta f_2 - \Delta f_1 - (\Delta f_1 - \Delta f_0) \\ &= (f_3 - f_2) - (f_2 - f_1) - (f_2 - f_1) + (f_1 - f_0) \\ &= f_3 - 3f_2 + 3f_1 - f_0 \end{aligned}$$

In general,

$$\Delta^n f_0 = f_n - {}^nC_1 f_{n-1} + {}^nC_2 f_{n-2} - {}^nC_3 f_{n-3} + \dots + (-1)^n f_0.$$

If we write y_n to denote f_n the above results takes the following forms:

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

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

$$\Delta^n y_0 = y_n - {}^nC_1 y_{n-1} + {}^nC_2 y_{n-2} - {}^nC_3 y_{n-3} + \dots + (-1)^n y_0$$

Example Show that the value of y_n can be expressed in terms of the leading value y_0 and the leading differences $\Delta y_0, \Delta^2 y_0, \dots, \Delta^n y_0$.

Solution

(For notational convenience, we treat y_n as f_n and so on.)

From the forward difference table we have

$$\left. \begin{array}{l} \Delta f_0 = f_1 - f_0 \quad \text{or} \quad f_1 = f_0 + \Delta f_0 \\ \Delta f_1 = f_2 - f_1 \quad \text{or} \quad f_2 = f_1 + \Delta f_1 \\ \Delta f_2 = f_3 - f_2 \quad \text{or} \quad f_3 = f_2 + \Delta f_2 \end{array} \right\}$$

and so on. Similarly,

$$\left. \begin{array}{l} \Delta^2 f_0 = \Delta f_1 - \Delta f_0 \quad \text{or} \quad \Delta f_1 = \Delta f_0 + \Delta^2 f_0 \\ \Delta^2 f_1 = \Delta f_2 - \Delta f_1 \quad \text{or} \quad \Delta f_2 = \Delta f_1 + \Delta^2 f_1 \end{array} \right\}$$

and so on. Similarly, we can write

$$\left. \begin{array}{l} \Delta^3 f_0 = \Delta^2 f_1 - \Delta^2 f_0 \quad \text{or} \quad \Delta^2 f_1 = \Delta^2 f_0 + \Delta^3 f_0 \\ \Delta^3 f_1 = \Delta^2 f_2 - \Delta^2 f_1 \quad \text{or} \quad \Delta^2 f_2 = \Delta^2 f_1 + \Delta^3 f_1 \end{array} \right\}$$

and so on. Also, we can write f_2 as

$$\begin{aligned} f_2 &= (f_0 + \Delta f_0) + (\Delta f_0 + \Delta^2 f_0) \\ &= f_0 + 2\Delta f_0 + \Delta^2 f_0 \\ &= (1 + \Delta)^2 f_0 \end{aligned}$$

Hence

$$\begin{aligned} f_3 &= f_2 + \Delta f_2 \\ &= (f_1 + \Delta f_1) + \Delta f_0 + 2\Delta^2 f_0 + \Delta^3 f_0 \\ &= f_0 + 3\Delta f_0 + 3\Delta^2 f_0 + \Delta^3 f_0 \\ &= (1 + \Delta)^3 f_0 \end{aligned}$$

That is, we can symbolically write

$$f_1 = (1 + \Delta)f_0, \quad f_2 = (1 + \Delta)^2 f_0, \quad f_3 = (1 + \Delta)^3 f_0.$$

Continuing this procedure, we can show, in general

$$f_n = (1 + \Delta)^n f_0.$$

Using binomial expansion, the above is

$$f_n = f_0 + {}^nC_1 \Delta f_0 + {}^nC_2 \Delta^2 f_0 + \dots + \Delta^n f_0$$

Thus

$$f_n = \sum_{i=0}^n {}^nC_i \Delta^i f_0.$$

Backward Difference Operator

For the values y_0, y_1, \dots, y_n of a function $y=f(x)$, for the equidistant values x_0, x_1, \dots, x_n , where $x_1 = x_0 + h, x_2 = x_0 + 2h, x_3 = x_0 + 3h, \dots, x_n = x_0 + nh$, the **backward difference operator** ∇ is defined on the function $f(x)$ as,

$$\nabla f(x_i) = f(x_i) - f(x_i - h) = y_i - y_{i-1},$$

which is the **first backward difference**.

In particular, we have the first backward differences,

$$\nabla f(x_1) = y_1 - y_0; \nabla f(x_2) = y_2 - y_1 \text{ etc}$$

The second backward difference is given by

$$\begin{aligned} \nabla^2 f(x_i) &= \nabla(\nabla f(x_i)) = \nabla[f(x_i) - f(x_i - h)] = \nabla f(x_i) - \nabla f(x_i - h) \\ &= [f(x_i) - f(x_i - h)] - [f(x_i - h) - f(x_i - 2h)] \\ &= (y_i - y_{i-1}) - (y_{i-1} - y_{i-2}) \\ &= y_i - 2y_{i-1} + y_{i-2} \end{aligned}$$

Similarly, the third backward difference, $\nabla^3 f(x_i) = y_i - 3y_{i-1} + 3y_{i-2} - y_{i-3}$ and so on.

Backward differences can be written in a tabular form as follows:

x	Y	∇y	$\nabla^2 y$	$\nabla^3 y$
x_0	$y_0 = f(x_0)$			
x_1	$y_1 = f(x_1)$	$\nabla y_1 = y_1 - y_0$		
x_2	$y_2 = f(x_2)$	$\nabla y_2 = y_2 - y_1$	$\nabla^2 y_2 = \nabla y_2 - \nabla y_1$	
x_3	$y_3 = f(x_3)$	$\nabla y_3 = y_3 - y_2$	$\nabla^2 y_3 = \nabla y_3 - \nabla y_2$	$\nabla^3 y_3 = \nabla^2 y_3 - \nabla^2 y_2$

Relation between backward difference and other differences:

$$1. \Delta y_0 = y_1 - y_0 = \nabla y_1; \Delta^2 y_0 = y_2 - 2y_1 + y_0 = \nabla^2 y_2 \text{ etc.}$$

2. $\Delta - \nabla = \Delta \nabla$

Proof: Consider the function $f(x)$.

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

$$\nabla f(x) = f(x) - f(x-h)$$

$$\begin{aligned} (\Delta - \nabla)(f(x)) &= \Delta f(x) - \nabla f(x) \\ &= [f(x+h) - f(x)] - [f(x) - f(x-h)] \\ &= \Delta f(x) - \Delta f(x-h) \\ &= \Delta[f(x) - f(x-h)] \\ &= \Delta[\nabla f(x)] \\ \Rightarrow \quad \Delta - \nabla &= \Delta \nabla \end{aligned}$$

3. $\nabla = \Delta E^{-1}$

Proof: Consider the function $f(x)$.

$$\nabla f(x) = f(x) - f(x-h) = \Delta f(x-h) = \Delta E^{-1} f(x) \Rightarrow \nabla = \Delta E^{-1}$$

4. $\nabla = 1 - E^{-1}$

Proof: Consider the function $f(x)$.

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

Problem: Construct the backward difference table for the data

$$\begin{array}{cccc} x: & -2 & 0 & 2 & 4 \\ y = f(x): & -8 & 3 & 1 & 12 \end{array}$$

Solution: The backward difference table is as follows:

x	Y=f(x)	∇y	$\nabla^2 y$	$\nabla^3 y$
-2	-8			
0	3	$\nabla y_1 = 3 - (-8) = 11$		
2	1	$\nabla y_2 = 1 - 3 = -2$	$\nabla^2 y_2 = -2 - 11 = -13$	
4	12	$\nabla y_3 = 12 - 1 = 11$	$\nabla^2 y_3 = 11 - (-2) = 13$	$\nabla^3 y_3 = 13 - (-13) = 26$

Backward Difference Table

x	f	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$	$\nabla^5 f$	$\nabla^6 f$
x_0	f_0						
x_1	f_1	∇f_1	$\nabla^2 f_2$				
x_2	f_2	∇f_2	$\nabla^2 f_3$	$\nabla^3 f_3$	$\nabla^4 f_4$	$\nabla^5 f$	
x_3	f_3	∇f_3	$\nabla^2 f_4$	$\nabla^3 f_4$	$\nabla^4 f_5$	$\nabla^5 f$	$\nabla^6 f_6$
x_4	f_4	∇f_4	$\nabla^2 f_5$	$\nabla^3 f_5$	$\nabla^4 f_6$	$\nabla^5 f$	
x_5	f_5	∇f_5	$\nabla^2 f_6$	$\nabla^3 f_6$			
x_6	f_6	∇f_6					

Example Show that any value of f (or y) can be expressed in terms of f_n (or y_n) and its backward differences.

Solution

$$\nabla f_n = f_n - f_{n-1} \text{ implies } f_{n-1} = f_n - \nabla f_n$$

$$\text{and } \nabla f_{n-1} = f_{n-1} - f_{n-2} \text{ implies } f_{n-2} = f_{n-1} - \nabla f_{n-1}$$

$$\nabla^2 f_n = \nabla f_n - \nabla f_{n-1} \text{ implies } \nabla f_{n-1} = \nabla f_n - \nabla^2 f_n$$

From equations (1) to (3), we obtain

$$f_{n-2} = f_n - 2\nabla f_n + \nabla^2 f_n.$$

Similarly, we can show that

$$f_{n-3} = f_n - 3\nabla f_n + 3\nabla^2 f_n - \nabla^3 f_n.$$

Symbolically, these results can be rewritten as follows:

$$f_{n-1} = (1 - \nabla)f_n, \quad f_{n-2} = (1 - \nabla)^2 f_n, \quad f_{n-3} = (1 - \nabla)^3 f_n.$$

Thus, in general, we can write

$$f_{n-r} = (1 - \nabla)^r f_n.$$

$$\text{i.e., } f_{n-r} = f_n - {}^r C_1 \nabla f_n + {}^r C_2 \nabla^2 f_n - \dots + (-1)^r \nabla^r f_n$$

If we write y_n to denote f_n the above result is:

$$y_{n-r} = y_n - {}^r C_1 \nabla y_n + {}^r C_2 \nabla^2 y_n - \dots + (-1)^r \nabla^r y_n$$

Central Differences

Central difference operator u for a function $f(x)$ at x_i is defined as,

$$u f(x_i) = f\left(x_i + \frac{h}{2}\right) - f\left(x_i - \frac{h}{2}\right), \text{ where } h \text{ being the interval of differencing.}$$

Let $y_{\frac{1}{2}} = f\left(x_0 + \frac{h}{2}\right)$. Then,

$$\begin{aligned} u y_{\frac{1}{2}} &= u f\left(x_0 + \frac{h}{2}\right) = f\left(x_0 + \frac{h}{2} + \frac{h}{2}\right) - f\left(x_0 + \frac{h}{2} - \frac{h}{2}\right) \\ &= f(x_0 + h) - f(x_0) = f(x_1) - f(x_0) = y_1 - y_0 \\ \Rightarrow u y_{\frac{1}{2}} &= \Delta y_0 \end{aligned}$$

Central differences can be written in a tabular form as follows:

x	y	$u y$	$u^2 y$	$u^3 y$
x_0	$y_0 = f(x_0)$			
x_1	$y_1 = f(x_1)$	$u y_{\frac{1}{2}} = y_1 - y_0$		
x_2	$y_2 = f(x_2)$	$u y_{\frac{3}{2}} = y_2 - y_1$	$u^2 y_1 = u y_{\frac{3}{2}} - u y_{\frac{1}{2}}$	$u^3 y_{\frac{3}{2}} = u^2 y_2 - u^2 y_1$
x_3	$y_3 = f(x_3)$	$u y_{\frac{5}{2}} = y_3 - y_2$	$u^2 y_2 = u y_{\frac{5}{2}} - u y_{\frac{3}{2}}$	

Central Difference Table

x	f	δf	$\delta^2 f$	$\delta^3 f$	$\delta^4 f$
x_0	f_0				
x_1	f_1	$\delta f_{1/2}$	$\delta^2 f_1$		
x_2	f_2	$\delta f_{3/2}$	$\delta^2 f_2$	$\delta^3 f_{3/2}$	$\delta^4 f_2$
x_3	f_3	$\delta f_{5/2}$	$\delta^2 f_3$	$\delta^3 f_{5/2}$	
x_4	f_4	$\delta f_{7/2}$			

Example Show that

$$(a) \quad u^2 f_m = f_{m+1} - 2f_m + f_{m-1}$$

$$(b) \quad u^3 f_{m+\frac{1}{2}} = f_{m+2} - 3f_{m+1} + 3f_m - f_{m-1}$$

$$\begin{aligned} (a) \quad \delta^2 f_m &= f_{m+1/2} - f_{m-1/2} = (f_{m+1} - f_m) - (f_m - f_{m-1}) \\ &= f_{m+1} - 2f_m + f_{m-1} \end{aligned}$$

$$\begin{aligned} (b) \quad \delta^3 f_{m+1/2} &= \delta^2 f_{m+1} - \delta^2 f_m = (f_{m+2} - 2f_{m+1} + f_m) - \\ &\quad (f_{m+1} - 2f_m + f_{m-1}) = f_{m+2} - 3f_{m+1} + 3f_m - f_{m-1} \end{aligned}$$

Shift operator, E

Let $y = f(x)$ be a function of x , and let x takes the consecutive values $x, x + h, x + 2h$, etc. We then define an operator E , called **the shift operator** having the property

$$E f(x) = f(x + h) \quad \dots(1)$$

Thus, when E operates on $f(x)$, the result is the next value of the function. If we apply the operator twice on $f(x)$, we get

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

Thus, in general, if we apply the shift operator n times on $f(x)$, we arrive at

$$E^n f(x) = f(x + nh) \quad \dots(2)$$

for all real values of n .

If $f_0 (= y_0), f_1 (= y_1) \dots$ are the consecutive values of the function

$y = f(x)$, then we can also write

$$E f_0 = f_1 \text{ (or } E y_0 = y_1), \quad E f_1 = f_2 \text{ (or } E y_1 = y_2) \dots$$

$$E^2 f_0 = f_2 \text{ (or } E^2 y_0 = y_2), \quad E^2 f_1 = f_3 \text{ (or } E y_1 = y_3) \dots$$

$$E^3 f_0 = f_3 \text{ (or } E^3 y_0 = y_3), \quad E^3 f_1 = f_4 \text{ (or } E y_1 = y_4) \dots$$

and so on. The **inverse operator** E^{-1} is defined as:

$$E^{>1} f(x) = f(x > h) \quad \dots(3)$$

and similarly

$$E^{>n} f(x) = f(x > nh) \quad \dots(4)$$

Average Operator ~

The **average operator** ~ is defined as

$$\sim f(x) = \frac{1}{2} \left[f\left(x + \frac{h}{2}\right) + f\left(x - \frac{h}{2}\right) \right]$$

Differential operator D

The **differential operator** D has the property

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

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

Relations between the operators:

Operators $\Delta, \nabla, \delta, \sim$ and D in terms of E

From the definition of operators Δ and E, we have

$$\Delta f(x) = f(x + h) - f(x) = E f(x) - f(x) = (E - 1) f(x).$$

Therefore,

$$\Delta = E - 1$$

From the definition of operators ∇ and E^{-1} , we have

$$\nabla f(x) = f(x) - f(x > h) = f(x) - E^{-1} f(x) = (1 - E^{-1}) f(x).$$

Therefore,

$$\nabla = 1 - E^{-1} = \frac{E - 1}{E}.$$

The definition of the operators δ and E gives

$$\begin{aligned} \delta f(x) &= f\left(x + \frac{h}{2}\right) - f\left(x - \frac{h}{2}\right) = E^{1/2} f(x) - E^{-1/2} f(x) \\ &= (E^{1/2} - E^{-1/2}) f(x). \end{aligned}$$

Therefore,

$$\delta = E^{1/2} - E^{-1/2}$$

The definition of the operators \sim and E yields

$$\mu f(x) = \frac{1}{2} \left[f\left(x + \frac{h}{2}\right) + f\left(x - \frac{h}{2}\right) \right] = \frac{1}{2} [E^{1/2} + E^{-1/2}] f(x).$$

Therefore,

$$\mu = \frac{1}{2} (E^{1/2} + E^{-1/2}).$$

It is known that

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

Using the Taylor series expansion, we have

$$\begin{aligned} E f(x) &= f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \dots \\ &= f(x) + h D f(x) + \frac{h^2}{2!} D^2 f(x) + \dots \\ &= \left(1 + \frac{hD}{1!} + \frac{h^2 D^2}{2!} + \dots \right) f(x) = e^{hD} f(x). \end{aligned}$$

Thus $E = e^{hD}$. Or,

$$hD = \log E.$$

Example If Δ , ∇ , δ denote forward, backward and central difference operators, E and \sim respectively the shift operator and average operators, in the analysis of data with equal spacing h , prove the following:

$$(i) 1 + u^2 \sim^2 = \left(1 + \frac{u^2}{2} \right)^2 \quad (ii) E^{1/2} = \sim + \frac{u}{2}$$

$$(iii) \Delta = \frac{u^2}{2} + u \sqrt{1 + (u^2/4)}$$

$$(iv) \mu \delta = \frac{\Delta E^{-1}}{2} + \frac{\Delta}{2} \quad (v) \mu \delta = \frac{\Delta + \nabla}{2}.$$

Solution

(i) From the definition of operators, we have

$$\mu\delta = \frac{1}{2}(E^{1/2} + E^{-1/2})(E^{1/2} - E^{-1/2}) = \frac{1}{2}(E - E^{-1}).$$

Therefore

$$1 + \mu^2\delta^2 = 1 + \frac{1}{4}(E^2 - 2 + E^{-2}) = \frac{1}{4}(E + E^{-1})^2$$

Also,

$$1 + \frac{\delta^2}{2} = 1 + \frac{1}{2}(E^{1/2} - E^{-1/2})^2 = \frac{1}{2}(E + E^{-1})$$

From equations (1) and (2), we get

$$1 + \delta^2\mu^2 = \left(1 + \frac{\delta^2}{2}\right)^2.$$

$$(ii) \quad \mu + \frac{\delta}{2} = \frac{1}{2}(E^{1/2} + E^{-1/2} + E^{1/2} - E^{-1/2}) = E^{1/2}.$$

(iii) We can write

$$\begin{aligned} \frac{\delta^2}{2} + \delta\sqrt{1 + (\delta^2/4)} &= \frac{(E^{1/2} - E^{-1/2})^2}{2} + (E^{1/2} - E^{-1/2})\sqrt{1 + \frac{1}{4}(E^{1/2} - E^{-1/2})^2} \\ &= \frac{E - 2 + E^{-1}}{2} + \frac{1}{2}(E^{1/2} - E^{-1/2})(E^{1/2} + E^{-1/2}) \\ &= \frac{E - 2 + E^{-1}}{2} + \frac{E - E^{-1}}{2} \\ &= E - 1 \\ &= \Delta \end{aligned}$$

(iv) We write

$$\begin{aligned} \mu\delta &= \frac{1}{2}(E^{1/2} + E^{-1/2})(E^{1/2} - E^{-1/2}) = \frac{1}{2}(E - E^{-1}) \\ &= \frac{1}{2}(1 + \Delta - E^{-1}) = \frac{\Delta}{2} + \frac{1}{2}(1 - E^{-1}) = \frac{\Delta}{2} + \frac{1}{2}\left(\frac{E - 1}{E}\right) = \frac{\Delta}{2} + \frac{\Delta}{2E}. \end{aligned}$$

(v) We can write

$$\begin{aligned} \mu\delta &= \frac{1}{2}(E^{1/2} + E^{-1/2})(E^{1/2} - E^{-1/2}) = \frac{1}{2}(E - E^{-1}) \\ &= \frac{1}{2}(1 + \Delta - (1 - \nabla)) = \frac{1}{2}(\Delta + \nabla). \end{aligned}$$

Example Prove that

$$hD = \log(1 + \Delta) = -\log(1 - \nabla) = \sinh^{-1}(\mu\delta).$$

Using the standard relations given in boxes in the last section, we have

$$hD = \log E = \log(1 + \Delta) = \log E = -\log E^{-1} = -\log(1 + \nabla)$$

Also,

$$\begin{aligned}\mu\delta &= \frac{1}{2}(E^{1/2} + E^{-1/2})(E^{1/2} - E^{-1/2}) = \frac{1}{2}(E + E^{-1}) \\ &= \frac{1}{2}(e^{hD} - e^{-hD}) = \sinh(hD)\end{aligned}$$

Therefore

$$hD = \sinh^{-1}(\mu\delta).$$

Example Show that the operations \sim and E commute.

Solution

From the definition of operators \sim and E , we have

$$\mu E f_0 = \mu f_1 = \frac{1}{2}(f_{3/2} + f_{1/2})$$

and also

$$E \mu f_0 = \frac{1}{2} E (f_{1/2} + f_{-1/2}) = \frac{1}{2} (f_{3/2} + f_{1/2})$$

Hence

$$\mu E = E \mu.$$

Therefore, the operators \sim and E commute.

Example Show that

$$\begin{aligned}e^x \left(u_0 + x \Delta u_0 + \frac{x^2}{2!} \Delta^2 u_0 + \dots \right) &= u_0 + u_1 x + u_2 \frac{x^2}{2!} + \dots \\ e^x \left(u_0 + x \Delta u_0 + \frac{x^2}{2!} \Delta^2 u_0 + \dots \right) &= e^x \left(1 + x \Delta + \frac{x^2 \Delta^2}{2!} + \dots \right) u_0 \\ &= e^x e^{x \Delta} u_0 = e^{x(1+\Delta)} u_0 \\ &= e^{xE} u_0\end{aligned}$$

$$\begin{aligned}
 &= \left(1 + xE + \frac{x^2 E^2}{2!} + \dots \right) u_0 \\
 &= u_0 + xu_1 + \frac{x^2}{2!} u_2 + \dots,
 \end{aligned}$$

as desired.

Example Using the method of separation of symbols, show that

$$\Delta^n u_{x-n} = u_x - nu_{x-1} + \frac{n(n-1)}{2} u_{x-2} + \dots + (-1)^n u_{x-n}.$$

To prove this result, we start with the right-hand side. Thus,

$$\begin{aligned}
 \text{R.H.S} &= u_x - nu_{x-1} + \frac{n(n-1)}{2} u_{x-2} + \dots + (-1)^n u_{x-n}. \\
 &= u_x - nE^{-1}u_x + \frac{n(n-1)}{2} E^{-2}u_x + \dots + (-1)^n E^{-n}u_x \\
 &= \left[1 - nE^{-1} + \frac{n(n-1)}{2} E^{-2} + \dots + (-1)^n E^{-n} \right] u_x \\
 &= (1 - E^{-1})^n u_x \\
 &= \left(1 - \frac{1}{E} \right)^n u_x \\
 &= \left(\frac{E-1}{E} \right)^n u_x \\
 &= \frac{\Delta^n}{E^n} u_x \\
 &= \Delta^n E^{-n} u_x \\
 &= \Delta^n u_{x-n}, \\
 &= \text{L.H.S}
 \end{aligned}$$

Differences of a Polynomial

Let us consider the polynomial of degree n in the form

$$f(x) = a_0 x^n + a_1 x^{n-1} + a_2 x^{n-2} + \dots + a_{n-1} x + a_n,$$

where $a_0 \neq 0$ and $a_0, a_1, a_2, \dots, a_{n-1}, a_n$ are constants. Let h be the interval of differencing. Then

$$f(x+h) = a_0(x+h)^n + a_1(x+h)^{n-1} + a_2(x+h)^{n-2} + \dots + a_{n-1}(x+h) + a_n$$

Now the difference of the polynomials is:

$$\Delta f(x) = f(x+h) - f(x) = a_0[(x+h)^n - x^n] + a_1[(x+h)^{n-1} - x^{n-1}] + \dots + a_{n-1}(x+h-x)$$

Binomial expansion yields

$$\begin{aligned} \Delta f(x) &= a_0 \left[x^n + {}^nC_1 x^{n-1} h + {}^nC_2 x^{n-2} h^2 + \dots + h^n - x^n \right] \\ &\quad + a_1 \left[x^{n-1} + {}^{(n-1)}C_1 x^{n-2} h + {}^{(n-1)}C_2 x^{n-3} h^2 \right. \\ &\quad \left. + \dots + h^{n-1} - x^{n-1} \right] + \dots + a_{n-1} h \\ &= a_0 n h x^{n-1} + \left[a_0 {}^nC_2 h^2 + a_1 {}^{(n-1)}C_1 h \right] x^{n-2} + \dots + a_{n-1} h. \end{aligned}$$

Therefore,

$$\Delta f(x) = a_0 n h x^{n-1} + b' x^{n-2} + c' x^{n-3} + \dots + k' x + l',$$

where b', c', \dots, k', l' are constants involving h but not x . Thus, the first difference of a polynomial of degree n is another polynomial of degree $(n-1)$. Similarly,

$$\begin{aligned} \Delta^2 f(x) &= \Delta(\Delta f(x)) = \Delta f(x+h) - \Delta f(x) \\ &= a_0 n h \left[(x+h)^{n-1} - x^{n-1} \right] + b' \left[(x+h)^{n-2} - x^{n-2} \right] \\ &\quad + \dots + k' (x+h-x) \end{aligned}$$

On simplification, it reduces to the form

$$\Delta^2 f(x) = a_0 n(n-1)h^2 x^{n-2} + b'' x^{n-3} + c'' x^{n-4} + \dots + q''.$$

Therefore, $\Delta^2 f(x)$ is a polynomial of degree $(n-2)$ in x . Similarly, we can form the higher order differences, and every time we observe that the degree of the polynomial is reduced by 1. After differencing n times, we are left with only the first term in form

$$\begin{aligned} \Delta^n f(x) &= a_0 n(n-1)(n-2)(n-3) \dots (2)(1)h^n \\ &= a_0 (n!)h^n = \text{constant}. \end{aligned}$$

This constant is independent of x . Since $\Delta^n f(x)$ is a constant $\Delta^{n+1} f(x) = 0$. Hence the $(n+1)th$ and higher order differences of a polynomial of degree n are 0.

Conversely, if the n th differences of a tabulated function are constant and the $(n+1)$ th, $(n+2)$ th, ..., differences all vanish, then the tabulated function represents a polynomial of degree n . It should be noted that these results hold good only if the values of x are equally spaced. The converse is important in numerical analysis since it enables us to approximate a function by a polynomial if its differences of some order become nearly constant.

Theorem (Differences of a polynomial) The n th differences of a polynomial of degree n is a constant, when the values of the independent variable are given at equal intervals.

Exercises

1. Calculate $f(x) = \frac{1}{x+1}$, $x = 0(0.2)1$ to (a) 2 decimal places, (b) 3 decimal places and (c) 4 decimal places. Then compare the effect of rounding errors in the corresponding difference tables.
2. Express $\Delta^2 y_1$ (i.e. $\Delta^2 f_1$) and $\Delta^4 y_0$ (i.e. $\Delta^4 f_0$) in terms of the values of the function $y = f(x)$.
3. Set up a difference table of $f(x) = x^2$ for $x = 0(1)10$. Do the same with the calculated value 25 of $f(5)$ replaced by 26. Observe the spread of the error.
4. Calculate $f(x) = \frac{1}{x+1}$, $x = 0(0.2)1$ to (a) 2 decimal places, (b) 3 decimal places and (c) 4 decimal places. Then compare the effect of rounding errors in the corresponding difference tables.
5. Set up a forward difference table of $f(x) = x^2$ for $x = 0(1)10$. Do the same with the calculated value 25 of $f(5)$ replaced by 26. Observe the spread of the error.
6. Construct the difference table based on the following table.

x	0.0	0.1	0.2	0.3	0.4	0.5
$\cos x$	1.000 00	0.995 00	0.980 07	0.955 34	0.921 06	0.877 58

7. Construct the difference table based on the following table.

x	0.0	0.1	0.2	0.3	0.4	0.5
$\sin x$	0.000 00	0.099 83	0.198 67	0.295 52	0.389 42	0.479

8. Construct the backward difference table, where

$$f(x) = \sin x, \quad x = 1.0(0.1)1.5, 4D.$$

9. Show that $E \nabla = \Delta = \delta E^{1/2}$.
10. Prove that
11. (i) $\delta = 2 \sinh(hD/2)$ and (ii) $\mu = 2 \cosh(hD/2)$.
12. Show that the operators δ, \sim, E, Δ and ∇ commute with each other.
13. Construct the backward difference table based on the following table.

x	0.0	0.1	0.2	0.3	0.4	0.5
$\cos x$	1.000	0.995	0.980	0.955	0.921	0.877
	00	00	07	34	06	58

Construct the difference table based on the following table.

x	0.0	0.1	0.2	0.3	0.4	0.5
$\sin x$	0.000	0.099	0.198	0.295	0.389	0.479
	00	83	67	52	42	43

6. Construct the backward difference table, where

$$f(x) = \sin x, \quad x = 1.0(0.1)1.5, 4D.$$

7. Evaluate $(2U + 3)(E + 2)(3x^2 + 2)$, interval of differencing being unity.
8. Compute the missing values of y_n and Δy_n in the following table:

y_n	Δy_n	$\Delta^2 y_n$
-		
-	-	1
-	-	4
6	5	13
-	-	18
-	-	24
-	-	

5

NUMERICAL INTERPOLATION

Consider a single valued continuous function $y = f(x)$ defined over $[a, b]$ where $f(x)$ is known explicitly. It is easy to find the values of ' y ' for a given set of values of ' x ' in $[a, b]$. i.e., it is possible to get information of all the points (x, y) where $a \leq x \leq b$.

But the converse is not so easy. That is, using only the points $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ where $a \leq x_i \leq b, i = 0, 1, 2, \dots, n$, it is not so easy to find the relation between x and y in the form $y = f(x)$ explicitly. That is one of the problem we face in numerical differentiation or integration.

Now we have first to find a simpler function, say $g(x)$, such that $f(x)$ and $g(x)$ agree at the given set of points and accept the value of $g(x)$ as the required value of $f(x)$ at some point x in between a and b . Such a process is called **interpolation**. If $g(x)$ is a polynomial, then the process is called polynomial interpolation.

When a function $f(x)$ is not given explicitly and only values of $f(x)$ are given at a set of distinct points called *nodes* or *tabular points*, using the interpolated function $g(x)$ to the function $f(x)$, the required operations intended for $f(x)$, like determination of roots, differentiation and integration etc. can be carried out. The approximating polynomial $g(x)$ can be used to predict the value of $f(x)$ at a non- tabular point. The deviation of $g(x)$ from $f(x)$, that is $|f(x) - g(x)|$ is called the *error of approximation*.

Consider a continuous single valued function $f(x)$ defined on an interval $[a, b]$. Given the values of the function for $n + 1$ distinct tabular points x_0, x_1, \dots, x_n such that $a \leq x_0 \leq x_1 \leq \dots \leq x_n \leq b$. The problem of polynomial interpolation is to find a polynomial $g(x)$ or $p_n(x)$, of degree n , which fits the given data. The interpolation polynomial fitted to a given data is unique.

If we are given two points satisfying the function such as $(x_0, y_0); (x_1, y_1)$, where $y_0 = f(x_0)$ and $y_1 = f(x_1)$ it is possible to fit a unique polynomial of degree 1. If three distinct points are given, a polynomial of degree not greater than two can be fitted uniquely. In general, if $n + 1$ distinct points are given, a polynomial of degree not greater than n can be fitted uniquely.

Interpolation fits a real function to discrete data. Given the set of tabular values $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ satisfying the relation $y = f(x)$, where the explicit nature of

$f(x)$ is not known, and it is required to find the values of $f(x)$ corresponding to certain given values of x in between x_0 and x_n . To do this we have first to find a simpler function, say $g(x)$, such that $f(x)$ and $g(x)$ agree at the set of tabulated points and accept the value of $g(x)$ as the required value of $f(x)$ at some point x in between x_0 and x_n . Such a process is called **interpolation**. If $g(x)$ is a polynomial, then the process is called **polynomial interpolation**.

In interpolation, we have to determine the function $g(x)$, in the case that $f(x)$ is difficult to be obtained, using the **pivotal values** $f_0 = f(x_0)$, $f_1 = f(x_1)$, \dots , $f_n = f(x_n)$.

Linear interpolation

In linear interpolation, we are given with two pivotal values $f_0 = f(x_0)$ and $f_1 = f(x_1)$, and we approximate the curve of f by a chord (straight line) P_1 passing through the points (x_0, f_0) and (x_1, f_1) . Hence the approximate value of f at the intermediate point $x = x_0 + rh$ is given by the **linear interpolation formula**

$$f(x) \approx P_1(x) = f_0 + r(f_1 - f_0) = f_0 + r\Delta f_0$$

where $r = \frac{x - x_0}{h}$ and $0 \leq r \leq 1$.

Example Evaluate $\ln 9.2$, given that $\ln 9.0 = 2.197$ and $\ln 9.5 = 2.251$.

Here $x_0 = 9.0$, $x_1 = 9.5$, $h = x_1 - x_0 = 9.5 - 9.0 = 0.5$, $f_0 = f(x_0) = \ln 9.0 = 2.197$ and $f_1 = f(x_1) = \ln 9.5 = 2.251$. Now to calculate $\ln 9.2 = f(9.2)$, take $x = 9.2$, so that

$$r = \frac{x - x_0}{h} = \frac{9.2 - 9.0}{0.5} = \frac{0.2}{0.5} = 0.4 \text{ and hence}$$

$$\ln 9.2 = f(9.2) \approx P_1(9.2) = f_0 + r(f_1 - f_0) = 2.197 + 0.4(2.251 - 2.197) = 2.219$$

Example Evaluate $f(15)$, given that $f(10) = 46$, $f(20) = 66$.

Here $x_0 = 10$, $x_1 = 20$, $h = x_1 - x_0 = 20 - 10 = 10$,

$$f_0 = f(x_0) = 46 \text{ and } f_1 = f(x_1) = 66.$$

Now to calculate $f(15)$, take $x = 15$, so that

$$r = \frac{x - x_0}{h} = \frac{15 - 10}{10} = \frac{5}{10} = 0.5$$

$$\text{and hence } f(15) \approx P_1(15) = f_0 + r(f_1 - f_0) = 46 + 0.5(66 - 46) = 56$$

Example Evaluate $e^{1.24}$, given that $e^{1.1} = 3.0042$ and $e^{1.4} = 4.0552$.

Here $x_0 = 1.1$, $x_1 = 1.4$, $h = x_1 - x_0 = 1.4 - 1.1 = 0.3$, $f_0 = f(x_0) = 1.1$ and $f_1 = f(x_1) = 1.24$. Now to calculate $e^{1.24} = f(1.24)$, take $x = 1.24$, so that $r = \frac{x - x_0}{h} = \frac{1.24 - 1.1}{0.3} = \frac{0.14}{0.3} = 0.4667$ and hence

$e^{1.24} \approx P_1(1.24) = f_0 + r(f_1 - f_0) = 3.0042 + 0.4667(4.0552 - 3.0042) = 3.4933$, while the exact value of $e^{1.24}$ is 3.4947.

Quadratic Interpolation

In quadratic interpolation we are given with three pivotal values $f_0 = f(x_0)$, $f_1 = f(x_1)$ and $f_2 = f(x_2)$ and we approximate the curve of the function f between x_0 and $x_2 = x_0 + 2h$ by the quadratic parabola P_2 , which passes through the points (x_0, f_0) , (x_1, f_1) , (x_2, f_2) and obtain the quadratic interpolation formula

$$f(x) \approx P_2(x) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2}\Delta^2 f_0$$

where $r = \frac{x - x_0}{h}$ and $0 \leq r \leq 2$.

Example Evaluate $\ln 9.2$, using quadratic interpolation, given that

$$\ln 9.0 = 2.197, \quad \ln 9.5 = 2.251 \quad \text{and} \quad \ln 10.0 = 2.3026.$$

Here $x_0 = 9.0$, $x_1 = 9.5$, $x_2 = 10.0$, $h = x_1 - x_0 = 9.5 - 9.0 = 0.5$, $f_0 = f(x_0) = \ln 9.0 = 2.197$, $f_1 = f(x_1) = \ln 9.5 = 2.251$ and $f_2 = f(x_2) = \ln 10.0 = 2.3026$. Now to calculate $\ln 9.2 = f(9.2)$, take $x = 9.2$, so that $r = \frac{x - x_0}{h} = \frac{9.2 - 9.0}{0.5} = \frac{0.2}{0.5} = 0.4$ and

$$\ln 9.2 = f(9.2) \approx P_2(x) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2}\Delta^2 f_0$$

To proceed further, we have to construct the following forward difference table.

x	f	Δf	$\Delta^2 f$
9.0	2.1972		
9.5	2.2513	0.0541	-
		0.0513	0.0028
10.0	2.3026		

Hence,

$\ln 9.2 = f(9.2) \approx P_2(9.2) = 2.1972 + 0.4(0.0541) + \frac{0.4(0.4-1)}{2}(-0.0028) = 2.2192$, which exact to 4D to the exact value of $\ln 9.2 = 2.2192$.

Example Using the values given in the following table, find $\cos 0.28$ by linear interpolation and by quadratic interpolation and compare the results with the value 0.96106 (exact to 5D)

x	$f(x) = \cos x$	First difference	Second difference
0.0	1.00000		
0.2	0.98007	-0.01993	
0.4	0.92106	-0.05901	-0.03908

Here $f(x)$, where $x_0 = 0.28$ is to determined. In linear interpolation, we need two consecutive x values and their corresponding f values and first difference. Here, since $x=0.28$ lies in between 0.2 and 0.4, we take $x_0 = 0.2$, $x_1 = 0.4$. (**Attention!** Choosing $x_0 = 0.2$, $x_1 = 0.4$ is very important; taking $x_0 = 0.0$ would give wrong answer). Then $h = x_1 - x_0 = 0.4 - 0.2 = 0.2$, $f_0 = f(x_0) = 0.98007$ and $f_1 = f(x_1) = 0.92106$.

Also $r = \frac{x - x_0}{h} = \frac{0.28 - 0.2}{0.2} = \frac{0.08}{0.2} = 0.4$ and

$$\begin{aligned}\cos 0.28 &= f(0.28) \approx P_1(0.28) = f_0 + r(f_1 - f_0) \\ &= 0.98007 + 0.4(0.92106 - 0.98007) \\ &= 0.95647, \text{ correct to 5 D.}\end{aligned}$$

In quadratic interpolation, we need three consecutive (equally spaced) x values and their corresponding f values, first differences and second difference. Here $x_0 = 0.0$, $x_1 = 0.2$, $x_2 = 0.4$, $h = x_1 - x_0 = 0.2 - 0.0 = 0.2$, $f_0 = 1.00000$, $f_1 = 0.98007$ and $f_2 = 0.92106$,

$\Delta f_0 = -0.01993$, $\Delta^2 f_0 = -0.03908$ $r = \frac{x - x_0}{h} = \frac{0.28 - 0.00}{0.2} = 1.4$ and

$$\begin{aligned}\cos 0.28 &\approx P_2(0.28) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2}\Delta^2 f_0 \\ &= 1.00 + 1.4(-0.01993) + \frac{1.4(1.4-1)}{2}(-0.03908) = 0.96116 \text{ to 5D.}\end{aligned}$$

From the above, it can be seen that quadratic interpolation gives more accurate value.

Newton's Forward Difference Interpolation Formula

Using Newton's forward difference interpolation formula we find the n degree polynomial P_n which approximates the function $f(x)$ in such a way that P_n and f agrees at $n+1$ equally spaced x values, so that $P_n(x_0) = f_0, P_n(x_1) = f_1, \dots, P_n(x_n) = f_n$, where $f_0 = f(x_0), f_1 = f(x_1), \dots, f_n = f(x_n)$ are the values of f in the table.

Newton's forward difference interpolation formula is

$$f(x) \approx P_n(x) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2!}\Delta^2 f_0 + \dots + \frac{r(r-1)\dots(r-n+1)}{n!}\Delta^n f_0$$

where $x = x_0 + rh, r = \frac{x - x_0}{h}, 0 \leq r \leq n$.

Derivation of Newton's forward Formulae for Interpolation

Given the set of $(n+1)$ values, viz., $(x_0, f_0), (x_1, f_1), (x_2, f_2), \dots, (x_n, f_n)$

of x and f , it is required to find $p_n(x)$, a polynomial of the n th degree such that $f(x)$ and $p_n(x)$ agree at the tabulated points. Let the values of x be equidistant, i.e., let

$$x_i = x_0 + rh, \quad r = 0, 1, 2, \dots, n$$

Since $p_n(x)$ is a polynomial of the n th degree, it may be written as

$$p_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + a_3(x - x_0)(x - x_1)(x - x_2) + \dots + a_n(x - x_0)(x - x_1)(x - x_2)\dots(x - x_{n-1})$$

Imposing now the condition that $f(x)$ and $p_n(x)$ should agree at the set of tabulated points, we obtain

$$a_0 = f_0; a_1 = \frac{f_1 - f_0}{x_1 - x_0} = \frac{\Delta f_0}{h}; a_2 = \frac{\Delta^2 f_0}{h^2 2!}; a_3 = \frac{\Delta^3 f_0}{h^3 3!}; \dots; a_n = \frac{\Delta^n f_0}{h^n n!};$$

Setting $x = x_0 + rh$ and substituting for a_0, a_1, \dots, a_n , we obtain the expression.

Remark 1:

Newton's forward difference formula has the permanence property. If we add a new set of value (x_{n+1}, y_{n+1}) , to the given set of values, then the forward difference table gets a new column of $(n+1)^{\text{th}}$ forward difference. Then the Newton's Forward difference

Interpolation Formula with the already given values will be added with a new term at the end, $(x-x_0)(x-x_1)\dots(x-x_n)\frac{1}{(n+1)!h^{n+1}}[\Delta^{n+1}y_0]$ to get the new interpolation formula with the newly added value.

Remark 2:

Newton's forward difference interpolation formula is useful for interpolation near the beginning of a set of tabular values and for extrapolating values of y a short distance backward, that is left from y_0 . The process of finding the value of y for some value of x outside the given range is called *extrapolation*.

Example Using Newton's forward difference interpolation formula and the following table evaluate $f(15)$.

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
10	46				
		20			
20	66		-5	2	
		15			
30	81		-3	-1	-3
		12			
40	93		-4		
		8			
50	101				

Here $x = 15$, $x_0 = 10$, $x_1 = 20$, $h = x_1 - x_0 = 20 - 10 = 10$, $r = (x - x_0)/h = (15-10)/10 = 0.5$, $f_0 = 46$, $\Delta f_0 = 20$, $\Delta^2 f_0 = -5$, $\Delta^3 f_0 = 2$, $\Delta^4 f_0 = -3$.

Substituting these values in the Newton's forward difference interpolation formula for $n = 4$, we obtain

$$f(x) \approx P_4(x) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2!}\Delta^2 f_0 + \dots + \frac{r(r-1)\dots(r-4+1)}{4!}\Delta^4 f_0,$$

so that

$$\begin{aligned} f(15) &\approx 46 + (0.5)(20) + \frac{(0.5)(0.5-1)}{2!}(-5) + \frac{(0.5)(0.5-1)(0.5-2)}{3!}(2) \\ &\quad + \frac{(0.5)(0.5-1)(0.5-2)(0.5-3)}{4!}(-3) \\ &= 56.8672, \text{ correct to 4 decimal places.} \end{aligned}$$

Example Find a cubic polynomial in x which takes on the values -3, 3, 11, 27, 57 and 107, when $x=0, 1, 2, 3, 4$ and 5 respectively.

x	$f(x)$	Δ	Δ^2	Δ^3
0	-3			
1	3	6		
2	11	8	2	
3	27	16	8	6
4	57	30	14	6
5	107	50	20	6

Now the required cubic polynomial (polynomial of degree 3) is obtained from Newton's forward difference interpolation formula

$$f(x) \approx P_3(x) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2!}\Delta^2 f_0 + \frac{r(r-1)(r-3+1)}{3!}\Delta^3 f_0,$$

where $r=(x - x_0)/h = (x - 0)/1 = x$, so that

$$f(x) \approx P_3(x) = -3 + x(6) + \frac{x(x-1)}{2!}(2) + \frac{x(x-1)(x-3+1)}{3!}(6)$$

$$\text{or } f(x) = x^3 - 2x^2 + 7x - 3$$

Example Using the Newton's forward difference interpolation formula evaluate $f(2.05)$ where $f(x) = \sqrt{x}$, using the values:

x	2.0	2.1	2.2	2.3	2.4
\sqrt{x}	1.414 214	1.449 138	1.483 240	1.516 575	1.549 193

The forward difference table is

x	\sqrt{x}	Δ	Δ^2	Δ^3	Δ^4
2.0	1.414 214				
2.1	1.449 138	0.034 924			
2.2	1.483 240	0.034 102	-0.000 822		
2.3	1.516 575	0.033 335	-0.000 767	0.000055	
2.4	1.549 193	0.032 618	-0.000 717	0.000050	-0.000 005

Here $r = \frac{x - x_0}{h} = (2.05 - 2.00)/0.1 = 0.5$, so by substituting the values in Newton's formula (for 4 degree polynomial), we get

$$\begin{aligned}
 f(2.05) \approx P_4(2.05) &= 1.414214 + (0.5)(0.034924) + \frac{(0.5)(0.5-1)}{2!}(-0.000822) \\
 &+ \frac{(0.5)(0.5-1)(0.5-2)}{3!}(0.000055) \\
 &+ \frac{(0.5)(0.5-1)(0.5-2)(0.5-3)}{4!}(0.000005) = 1.431783.
 \end{aligned}$$

Example Find the cubic polynomial which takes the following values; $f(1) = 24$, $f(3) = 120$, $f(5) = 336$, and $f(7) = 720$. Hence, or otherwise, obtain the value of $f(8)$.

We form the difference table:

x	y	Δ	Δ^2	Δ^3
1	24			
		96		
3	120		120	
		216		48
5	336		168	
		384		
7	720			

Here $h = 2$ with $x_0 = 1$, we have $x = 1 + 2p$ or $r = (x-1)/2$. Substituting this value of r , we obtain

$$f(x) = 24 + \frac{x-1}{2}(96) + \frac{\left(\frac{x-1}{2}\right)\left(\frac{x-1}{2}-1\right)}{2}(120)$$

$$+\frac{\left(\frac{x-1}{2}\right)\left(\frac{x-1}{2}-1\right)\left(\frac{x-1}{2}-2\right)}{6}(48)=x^3+6x^2+11x+6.$$

To determine $f(9)$, we put $x=9$ in the above and obtain $f(9)=1320$.

With $x_0=1$, $x_r=9$, and $h=2$, we have $r=\frac{x_r-x_0}{h}=\frac{9-1}{2}=4$. Hence

$$\begin{aligned} f(9) &\approx p(9) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2!}\Delta^2 f_0 + \frac{r(r-1)(r-2)}{3!}\Delta^3 f_0 \\ &= 24 + 4 \times 96 + \frac{4 \times 3}{2} \times 120 + \frac{4 \times 3 \times 2}{3 \times 2} \times 48 = 1320 \end{aligned}$$

Example Using Newton's forward difference formula, find the sum

$$S_n = 1^3 + 2^3 + 3^3 + \dots + n^3.$$

Solution

$$S_{n+1} = 1^3 + 2^3 + 3^3 + \dots + n^3 + (n+1)^3$$

and hence

$$S_{n+1} - S_n = (n+1)^3,$$

or

$$\Delta S_n = (n+1)^3.$$

it follows that

$$\Delta^2 S_n = \Delta S_{n+1} - \Delta S_n = (n+2)^3 - (n+1)^3 = 3n^2 + 9n + 7$$

$$\Delta^3 S_n = 3(n+1) + 9n + 7 - (3n^2 + 9n + 7) = 6n + 12$$

$$\Delta^4 S_n = 6(n+1) + 12 - (6n + 12) = 6$$

Since $\Delta^5 S_n = \Delta^6 S_n = \dots = 0$, S_n is a fourth-degree polynomial in the variable n .

Also,

$$S_1 = 1, \quad \Delta S_1 = (1+1)^3 = 8, \quad \Delta^2 S_1 = 3 + 9 + 7 = 19,$$

$$\Delta^3 S_1 = 6 + 12 = 18, \quad \Delta^4 S_1 = 8.$$

formula (3) gives (with $f_0 = S_1$ and $r = n-1$)

$$S_n = 1 + (n-1)(8) + \frac{(n-1)(n-2)}{2}(19) + \frac{(n-1)(n-2)(n-3)}{6}(18)$$

$$\begin{aligned}
 & + \frac{(n-1)(n-2)(n-3)(n-4)}{24}(6) \\
 & = \frac{1}{4}n^4 + \frac{1}{2}n^3 + \frac{1}{4}n^2 \\
 & = \left[\frac{n(n+1)}{2} \right]^2
 \end{aligned}$$

Problem: The population of a country for various years in millions is provided. Estimate the population for the year 1898.

Year x:	1891	1901	1911	1921	1931
Population y:	46	66	81	93	101

Solution: Here the interval of difference among the arguments $h=10$. Since 1898 is at the beginning of the table values, we use Newton's forward difference interpolation formula for finding the population of the year 1898.

The forward differences for the given values are as shown here.

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
1891	46	$\Delta y_0 = 20$			
1901	66		$\Delta^2 y_0 = -5$		
1911	81	$\Delta y_1 = 15$		$\Delta^3 y_0 = 2$	
1921	93	$\Delta y_2 = 12$	$\Delta^2 y_1 = -3$		$\Delta^4 y_0 = -3$
1931	101	$\Delta y_3 = 8$	$\Delta^2 y_2 = -4$	$\Delta^3 y_1 = -1$	

Let $x=1898$. Newton's forward difference interpolation formula is,

$$\begin{aligned}
 f(x) = & y_0 + (x-x_0)\frac{1}{h}[\Delta y_0] + (x-x_0)(x-x_1)\frac{1}{2!h^2}[\Delta^2 y_0] \\
 & + (x-x_0)(x-x_1)(x-x_2)\frac{1}{3!h^3}[\Delta^3 y_0] + \dots + \\
 & (x-x_0)(x-x_1)\dots(x-x_{n-1})\frac{1}{n!h^n}[\Delta^n y_0]
 \end{aligned}$$

Now, substituting the values, we get,

$$\begin{aligned}
 f(1898) &= 46 + (1898 - 1891) \frac{1}{10} [20] + (1898 - 1891)(1898 - 1901) \frac{1}{2!10^2} [-5] \\
 &\quad + (1898 - 1891)(1898 - 1901)(1898 - 1911) \frac{1}{3!10^3} [2] + \\
 &\quad (1898 - 1891)(1898 - 1901)(1898 - 1911)(1898 - 1921) \frac{1}{4!10^4} [-3] \\
 \Rightarrow f(1898) &= 46 + 14 + \frac{21}{40} + \frac{91}{500} + \frac{18837}{40000} = 61.178
 \end{aligned}$$

Example Values of x (in degrees) and $\sin x$ are given in the following table:

x (in degrees)	$\sin x$
15	0.2588190
20	0.3420201
25	0.4226183
30	0.5
35	0.5735764
40	0.6427876

Determine the value of $\sin 38^\circ$.

Solution

The difference table is

x	$\sin x$	Δ	Δ^2	Δ^3	Δ^4	Δ^5
15	0.2588190					
		0.0832011				
20	0.3420201		-0.0026029			
		0.0805982		-0.0006136		
25	0.4226183		-0.0032165		0.0000248	
		0.0773817		-0.0005888		0.0000041
30	0.5		-0.0038053		0.0000289	
		0.0735764		-0.0005599		
35	0.5735764		-0.0043652			
		0.0692112				
40	0.6427876					

As 38 is closer to $x_n = 40$ than $x_0 = 15$, we use Newton's backward difference formula with $x_n = 40$ and $x = 38$. This gives

$$r = \frac{x - x_n}{h} = \frac{38 - 40}{5} = -\frac{2}{5} = -0.4$$

Hence, using formula, we obtain

$$\begin{aligned} f(38) &= 0.6427876 - 0.4(0.0692112) + \frac{-0.4(-0.4-1)}{2}(-0.0043652) \\ &\quad + \frac{(-0.4)(-0.4+1)(-0.4+2)}{6}(-0.0005599) \\ &\quad + \frac{(-0.4)(-0.4+1)(-0.4+2)(-0.4+3)}{24}(0.0000289) \\ &\quad + \frac{(-0.4)(-0.4+1)(-0.4+2)(-0.4+3)(-0.4+4)}{120}(0.0000041) \\ &= 0.6427876 - 0.02768448 + 0.00052382 + 0.00003583 \\ &\quad - 0.00000120 \\ &= 0.6156614 \end{aligned}$$

Example Find the missing term in the following table:

x	$y = f(x)$
0	1
1	3
2	9
3	—
4	81

Explain why the result differs from $3^3 = 27$?

Since four points are given, the given data can be approximated by a third degree polynomial in x . Hence $\Delta^4 f_0 = 0$. Substituting $\Delta = E - 1$ we get, $(E - 1)^4 f_0 = 0$, which on simplification yields

$$E^4 f_0 - 4E^3 f_0 + 6E^2 f_0 - 4E f_0 + f_0 = 0.$$

Since $E^r f_0 = f_r$ the above equation becomes

$$f_4 - 4f_3 + 6f_2 - 4f_1 + f_0 = 0$$

Substituting for f_0, f_1, f_2 and f_4 in the above, we obtain

$$f_3 = 31$$

By inspection it can be seen that the tabulated function is 3^x and the exact value of $f(3)$ is 27. The error is due to the fact that the exponential function 3^x is approximated by means of a polynomial in x of degree 3.

Example The table below gives the values of $\tan x$ for $0.10 \leq x \leq 0.30$

x	$y = \tan x$
0.10	0.1003
0.15	0.1511
0.20	0.2027
0.25	0.2553
0.30	0.3093

Find: (a) $\tan 0.12$ (b) $\tan 0.26$. (c) $\tan 0.40$ (d) $\tan 0.50$

The table difference is

x	$y = f(x)$	Δ	Δ^2	Δ^3	Δ^4
0.10	0.1003				
		0.0508			
0.15	0.1511		0.0008		
		0.0516		0.0002	
0.20	0.2027		0.0010		0.0002
		0.0526		0.0004	
0.25	0.2553		0.0014		
		0.0540			
0.30	0.3093				

a) To find $\tan(0.12)$, we have $r = 0.4$ Hence Newton's forward difference interpolation formula gives

$$\begin{aligned}
 \tan(0.12) &= 0.1003 + 0.4(0.0508) + \frac{0.4(0.4-1)}{2}(0.0008) \\
 &\quad + \frac{0.4(0.4-1)(0.4-2)}{6}(0.0002) \\
 &\quad + \frac{0.4(0.4-1)(0.4-2)(0.4-3)}{24}(0.0002) \\
 &= 0.1205
 \end{aligned}$$

b) To find $\tan(0.26)$, we use Newton's backward difference interpolation formula with

$$\begin{aligned}
 r &= \frac{x - x_n}{n} \\
 &= \frac{0.26 - 0.3}{0.05} \\
 &= -0.8
 \end{aligned}$$

which gives

$$\begin{aligned}
 \tan(0.26) &= 0.3093 - 0.8(0.0540) + \frac{-0.8(-0.8+1)}{2}(0.0014) \\
 &\quad + \frac{-0.8(-0.8+1)(-0.8+2)}{6}(0.0004) \\
 &\quad + \frac{-0.8(-0.8+1)(-0.8+2)(-0.8+3)}{24}(0.0002) = 0.2662
 \end{aligned}$$

Proceeding as in the case (i) above, we obtain

(c) $\tan 0.40 = 0.4241$, and

(d) $\tan 0.50 = 0.5543$

The actual values, correct to four decimal places, of $\tan(0.12)$, $\tan(0.26)$ are respectively 0.1206 and 0.2660. Comparison of the computed and actual values shows that in the first two cases (i.e., of interpolation) the results obtained are fairly accurate whereas in the last-two cases (i.e., of extrapolation) the errors are quite considerable. The example therefore demonstrates the important results that if a tabulated function is other than a polynomial, then extrapolation very far from the table limits would be dangerous-although interpolation can be carried out very accurately.

Exercises

1. Using the difference table in exercise 1, compute $\cos 0.75$ by Newton's forward difference interpolating formula with $n = 1, 2, 3, 4$ and compare with the 5D-value 0.731 69.
2. Using the difference table in exercise 1, compute $\cos 0.28$ by Newton's forward difference interpolating formula with $n = 1, 2, 3, 4$ and compare with the 5D-value
3. Using the values given in the table, find $\cos 0.28$ (in radian measure) by linear interpolation and by quadratic interpolation and compare the results with the value 0.961 06 (exact to 5D).

x	$f(x)=\cos x$	First difference	Second difference
0.0	1.000 00		
0.2	0.980 07	-0.019 93	
0.4	0.921 06	-0.059 01	-0.03908
0.6	0.825 34	-0.095 72	-0.03671
0.8	0.696 71	-0.128 63	-0.03291
1.0	0.540 30	-0.156 41	-0.02778

4. Find Lagrangian interpolation polynomial for the function f having $f(4)=1, f(6)=3, f(8)=8, f(10)=16$. Also calculate $f(7)$.

5. The sales in a particular shop for the last ten years is given in the table:

Year	1996	1998	2000	2002	2004
Sales (in lakhs)	40	43	48	52	57

Estimate the sales for the year 2001 using Newton's backward difference interpolating formula.

6. Find $f(3)$, using Lagrangian interpolation formula for the function f having $f(1)=2, f(2)=11, f(4)=77$.

7. Find the cubic polynomial which takes the following values:

x	0	1	2	3
$f(x)$		1	2	10

8. Compute $\sin 0.3$ and $\sin 0.5$ by Everett formula and the following table.

	$\sin x$	δ^2
0.2	0.198 67	-0.007 92
0.4	0.389 42	-0.015 53
.6	0.564 64	-0.022 50

9. The following table gives the distances in nautical miles of the visible horizon for the given heights in feet above the earth's surface:

$x = \text{height}$:	100	150	200	250	300	350	400
$y = \text{distance}$:	10.63	13.03	15.04	16.81	18.42	19.90	21.27

Find the value of y when $x = 218$ ft (*Ans: 15.699*)

10. Using the same data as in exercise 9, find the value of y when $x = 410$ ft.

6

NEWTON'S AND LAGRANGIAN FORMULAE - PART I

Newton's Backward Difference Interpolation Formula

Newton's backward difference interpolation formula is

$$f(x) \approx P_n(x) = f_n + r\nabla f_n + \frac{r(r+1)}{2!}\nabla^2 f_n + \dots + \frac{r(r+1)\dots(r+n-1)}{n!}\nabla^n f_n$$

where $x = x_n + rh$, $r = \frac{x - x_n}{h}$, $-n \leq r \leq 0$.

Derivation of Newton's Backward Formulae for Interpolation

Given the set of $(n+1)$ values, viz., $(x_0, f_0), (x_1, f_1), (x_2, f_2), \dots, (x_n, f_n)$

of x and f , it is required to find $p_n(x)$, a polynomial of the n th degree such that $f(x)$ and $p_n(x)$ agree at the tabulated points. Let the values of x be equidistant, i.e., let

$$x_i = x_0 + rh, \quad r = 0, 1, 2, \dots, n$$

Since $p_n(x)$ is a polynomial of the n th degree, it may be written as

$$\begin{aligned} p_n(x) = & a_0 + a_1(x - x_n) + a_2(x - x_n)(x - x_{n-1}) \\ & + a_3(x - x_n)(x - x_{n-1})(x - x_{n-2}) + \dots \\ & + a_n(x - x_n)(x - x_{n-1})\dots(x - x_1) \end{aligned}$$

Imposing the condition that $f(x)$ and $p_n(x)$ should agree at the set of tabulated points we obtain (after some simplification) the above formula.

Remark 1:

If the values of the k^{th} forward/backward differences are same, then $(k+1)^{\text{th}}$ or higher differences are zero. Hence the given data represents a k^{th} degree polynomial.

Remark 2:

The Backward difference Interpolation Formula is commonly used for interpolation near the end of a set of tabular values and for extrapolating values of y a short distance forward that is right from y_n .

Problem: For the following table of values, estimate $f(7.5)$, using Newton's backward difference interpolation formula.

x	f	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$
1	1				
2	8	7			
3	27	19	12		
4	64	37	18	6	
5	125	61	24	6	0
6	216	91	30	6	0
7	343	127	36	6	0
8	512	169	42		

Solution:

Since the fourth and higher order differences are 0, the Newton's backward interpolation formula is

$$f(x_n + uh) = y_n + u[\nabla y_n] + \frac{u(u+1)}{2!}[\nabla^2 y_n] + \frac{u(u+1)(u+2)}{3!}[\nabla^3 y_n] + \dots + \frac{u(u+1)(u+2)\dots(u+n-1)}{n!}[\nabla^n y_n],$$

Where, $u = \frac{x - x_n}{h} = \frac{7.5 - 8.0}{1} = -0.5$ and

$$\nabla y_n = 169, \nabla^2 y_n = 42, \nabla^3 y_n = 6 \text{ and } \nabla^4 y_n = 0.$$

Hence,

$$\begin{aligned} f(7.5) &= 512 + (-0.5)(169) + \frac{(-0.5)(-0.5+1)}{2!}(42) + \frac{(-0.5)(-0.5+1)(-0.5+2)}{3!}6 \\ &= 421.875. \end{aligned}$$

Example For the following table of values, estimate $f(7.5)$, using Newton's backward difference interpolation formula.

x	f	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$
1	1				
2	8	7			
3	27	19	12		
4	64	37	18	6	
5	125	61	24	6	0
6	216	91	30	6	0
7	343	127	36	6	0
8	512	169	42		

Since the fourth and higher order differences are 0, the Newton's backward interpolation formula is

$$f(x) \approx P_n(x) = f_n + r\nabla f_n + \frac{r(r+1)}{2!}\nabla^2 f_n + \frac{r(r+1)(r+2)}{3!}\nabla^3 f_n, \text{ where}$$

$$r = \frac{x - x_n}{h} = \frac{7.5 - 8.0}{1} = -0.5 \text{ and } \nabla f_n = 169, \nabla^2 f_n = 42, \nabla^3 f_n = 6. \text{ Hence}$$

$$\begin{aligned} f(7.5) &\approx 512 + (-0.5)(169) + \frac{(-0.5)(-0.5+1)}{2!}(42) + \frac{(-0.5)(-0.5+1)(-0.5+2)}{3!}6 \\ &= 421.875 \end{aligned}$$

Gauss' Central Difference Formulae

We consider two central difference formulae.

(i) Gauss's forward formula

We consider the following table in which the central coordinate is taken for convenience as y_0 corresponding to $x = x_0$

Gauss's Forward formula is

$$f_p = f_0 + G_1\Delta f_0 + G_2\Delta^2 f_{-1} + G_3\Delta^3 f_{-1} + G_4\Delta^4 f_{-2} + \dots,$$

where G_1, G_2, \dots are given by

$$G_1 = p$$

$$G_2 = \frac{p(p-1)}{2!}$$

$$G_3 = \frac{(p+1)p(p-1)}{3!},$$

$$G_4 = \frac{(p+1)p(p-1)(p-2)}{4!},$$

Table: Gauss' Forward Formula

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
x_{-3}	y_{-3}						
		Δy_{-3}					
x_{-2}	y_{-2}		$\Delta^2 y_{-3}$				
		Δy_{-2}		$\Delta^3 y_{-3}$			
x_{-1}	y_{-1}		$\Delta^2 y_{-2}$		$\Delta^4 y_{-3}$		
		Δy_{-1}		$\Delta^3 y_{-2}$		$\Delta^5 y_{-3}$	
x_0	y_0		$\Delta^2 y_{-1}$		$\Delta^4 y_{-2}$		$\Delta^6 y_{-3}$
		Δy_0		$\Delta^3 y_{-1}$		$\Delta^5 y_{-2}$	
x_1	y_1		$\Delta^2 y_0$		$\Delta^4 y_{-1}$		
		Δy_1		$\Delta^3 y_0$			
x_2	y_2		$\Delta^2 y_1$				
		Δy^2					
x_3	y_3						

Derivation of Gauss's forward interpolation formula:

We have Newton's forward interpolation formula as,

$$f(x_0 + uh) = y_0 + u[\Delta y_0] + \frac{u(u-1)}{2!}[\Delta^2 y_0] + \frac{u(u-1)(u-2)}{3!}[\Delta^3 y_0] + \dots + \frac{u(u-1)(u-2)\dots(u-n+1)}{n!}[\Delta^n y_0]$$

where, $u = \frac{(x - x_0)}{h}$

we have,

$$\Delta^2 y_0 = \Delta^2 E y_{-1} = \Delta^2 (1 + \Delta) y_{-1} = \Delta^2 y_{-1} + \Delta^3 y_{-1}$$

$$\Delta^3 y_0 = \Delta^3 E y_{-1} = \Delta^3 (1 + \Delta) y_{-1} = \Delta^3 y_{-1} + \Delta^4 y_{-1},$$

In similar way, $\Delta^4 y_0 = \Delta^4 y_{-1} + \Delta^5 y_{-1}$; $\Delta^4 y_{-1} = \Delta^4 y_{-2} + \Delta^5 y_{-2}$ and so on.

Substituting these values in Newton's forward interpolation formula, we get,

$$f(x_0 + uh) = y_0 + u[\Delta y_0] + \frac{u(u-1)}{2!}[\Delta^2 y_{-1} + \Delta^3 y_{-1}] + \frac{u(u-1)(u-2)}{3!}[\Delta^3 y_{-1} + \Delta^4 y_{-1}] + \frac{u(u-1)(u-2)(u-3)}{4!}[\Delta^4 y_{-1} + \Delta^5 y_{-1}] + \dots$$

Solving the above expression, we get,

$$f(x_0 + uh) = y_0 + u[\Delta y_0] + {}^u C_2 [\Delta^2 y_{-1}] + {}^{u+1} C_3 [\Delta^3 y_{-1}] + {}^{u+1} C_4 [\Delta^4 y_{-2}] + {}^{u+2} C_5 [\Delta^5 y_{-2}] + \dots$$

This formula is known as Gauss's forward interpolation formula.

(ii) Gauss Backward Formula

Gauss backward formula is

$$f_p = f_0 + G'_1 \Delta f_{-1} + G'_2 \Delta^2 f_{-1} + G'_3 \Delta^3 f_{-2} + G'_4 \Delta^4 f_{-2} + \dots$$

where G'_1, G'_2, \dots are given by

$$G'_1 = p,$$

$$G'_2 = \frac{p(p+1)}{2!},$$

$$G'_3 = \frac{(p+1)p(p-1)}{3!},$$

$$G'_4 = \frac{(p+2)(p+1)p(p-1)}{4!},$$

Example From the following table, find the value of $e^{1.17}$ using Gauss' forward formula.

x	1.00	1.05	1.10	1.15	1.20	1.25	1.30
e^x	2.7183	2.8577	3.0042	3.1582	3.3201	3.4903	3.6693

Solution

Here we take $x_0 = 1.15$, $h = 0.05$.

Also, $x_p = x_0 + ph$

$$1.17 = 1.15 + p(0.05),$$

which gives

$$p = \frac{0.02}{0.05} = \frac{1}{4}$$

The difference table is given below:

x	e^x	Δ	Δ^2	Δ^3	Δ^4
1.00	2.7183				
		0.1394			
1.05	2.8577		0.0071		
		0.1465		0.0004	
1.10	3.0042		0.0075		0
		0.1540		0.0004	
1.15	3.1582		0.0079		0
		0.1619		0.0004	
1.20	3.3201		0.0083		0.0001
		0.1702		0.0005	
1.25	3.4903		0.0088		
		0.1790			
1.30	3.6693				

Using Gauss's forward difference formula we obtain

$$\begin{aligned}
 e^{1.17} &= 3.1582 + \frac{2}{5}(0.1619) + \frac{(2/5)(2/5-1)}{2}(0.0079) \\
 &\quad + \frac{(2/5+1)(2/5)(2/5-1)}{6}(0.0004) \\
 &= 3.1582 + 0.0648 - 0.0009 = 3.2221.
 \end{aligned}$$

Derivation of Gauss's backward interpolation formula:

Starting the substitution in Newton's forward interpolation formula with $\Delta y_0 = \Delta E y_{-1} = \Delta(1 + \Delta)y_{-1} = \Delta y_{-1} + \Delta^2 y_{-1}$ and the substitutions done in the case of Gauss's forward interpolation formula $\Delta^2 y_0 = \Delta^2 y_{-1} + \Delta^3 y_{-1}$; $\Delta^3 y_0 = \Delta^3 y_{-1} + \Delta^4 y_{-1}$ etc., we obtain

$$\begin{aligned}
 f(x_0 + uh) &= y_0 + u[\Delta y_{-1} + \Delta^2 y_{-1}] + \frac{u(u-1)}{2!}[\Delta^2 y_{-1} + \Delta^3 y_{-1}] \\
 &\quad + \frac{u(u-1)(u-2)}{3!}[\Delta^3 y_{-1} + \Delta^4 y_{-1}] + \frac{u(u-1)(u-2)(u-3)}{4!}[\Delta^4 y_{-1} + \Delta^5 y_{-1}] + \dots
 \end{aligned}$$

Solving the expression, we get,

$$f(x_0 + uh) = y_0 + u[\Delta y_{-1}] + {}^{u+1}C_2[\Delta^2 y_{-1}] + {}^{u+1}C_3[\Delta^3 y_{-2}] + {}^{u+2}C_4[\Delta^4 y_{-2}] + {}^{u+2}C_5[\Delta^5 y_{-3}] + \dots$$

This is known as Gauss's backward interpolation formula.

Central difference interpolation formulas:

Newton's forward and backward interpolation formula are applicable for interpolation near the beginning and near the end of the tabulated arguments, respectively. Now in this session we discuss interpolation near the centre of the tabulated arguments. For this purpose we use central difference interpolation formula. Gauss's forward interpolation formula, Gauss's backward interpolation formula, Sterling's formula, Bessel's formula, Laplace-Everett's formula are some of the various central difference interpolation formulas.

Let us consider some equidistant arguments with interval of difference, say; h and corresponding function values are given. Let x_0 , be the central point among the arguments.

For interpolation at the point x near the central value, let $f(x_0) = y_0$, $f(x_0 - h) = y_{-1}$, $f(x_0 + h) = y_1$, $f(x_0 - 2h) = y_{-2}$, $f(x_0 + 2h) = y_2$, $f(x_0 - 3h) = y_{-3}$, $f(x_0 + 3h) = y_3$ and so on.

For the values $y_{-3}, y_{-2}, y_{-1}, y_0, y_1, y_2, y_3$ the forward difference table is as follows:

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$	$\Delta^6 y$
$x_0 - 3h$	y_{-3}	Δy_{-3}					
$x_0 - 2h$	y_{-2}	Δy_{-2}	$\Delta^2 y_{-3}$	$\Delta^3 y_{-3}$			
	y_{-1}		$\Delta^2 y_{-2}$		$\Delta^4 y_{-3}$		
$x_0 - h$		Δy_{-1}		$\Delta^3 y_{-2}$		$\Delta^5 y_{-3}$	
	y_0		$\Delta^2 y_{-1}$		$\Delta^4 y_{-2}$		$\Delta^6 y_{-3}$
x_0		Δy_0		$\Delta^3 y_{-1}$		$\Delta^5 y_{-2}$	
	y_1		$\Delta^2 y_0$		$\Delta^4 y_{-1}$		
$x_0 + h$		Δy_1		$\Delta^3 y_0$			
	y_2		$\Delta^2 y_1$				
$x_0 + 2h$		Δy_2					
	y_3						
$x_0 + 3h$							

The above table can also be written in terms of central differences using the operator u as follows:

x	y	$u y$	$u^2 y$	$u^3 y$	$u^4 y$	$u^5 y$	$u^6 y$
$x_0 - 3h$	y_{-3}	$u y_{-\frac{5}{2}}$					
$x_0 - 2h$	y_{-2}	$u y_{-\frac{3}{2}}$	$u^2 y_{-2}$	$u^3 y_{-\frac{3}{2}}$			
	y_{-1}		$u^2 y_{-1}$		$u^4 y_{-1}$		
$x_0 - h$	y_0	$u y_{-\frac{1}{2}}$	$u^2 y_0$	$u^3 y_{-\frac{1}{2}}$	$u^4 y_0$	$u^5 y_{-\frac{1}{2}}$	$u^6 y_0$
x_0	y_1	$u y_{\frac{1}{2}}$	$u^2 y_1$	$u^3 y_{\frac{1}{2}}$	$u^4 y_1$	$u^5 y_{\frac{1}{2}}$	
$x_0 + h$	y_2	$u y_{\frac{3}{2}}$	$u^2 y_2$	$u^3 y_{\frac{3}{2}}$			
$x_0 + 2h$		$u y_{\frac{5}{2}}$					
$x_0 + 3h$	y_3						

The difference given in both the tables are same can be established as follows:

We have $u = \Delta E^{-\frac{1}{2}}$. Then, $u y_{-\frac{5}{2}} = \Delta E^{-\frac{1}{2}} \left(y_{-\frac{5}{2}} \right) = \Delta \left(y_{-\frac{5}{2}-\frac{1}{2}} \right) = \Delta y_{-3};$

$$u^2 y_{-2} = \left(\Delta E^{-\frac{1}{2}} \right)^2 (y_{-2}) = \Delta^2 (y_{-2-1}) = \Delta^2 y_{-3};$$

$$u^3 y_{-\frac{3}{2}} = \left(\Delta E^{-\frac{1}{2}} \right)^3 \left(y_{-\frac{3}{2}} \right) = \Delta^3 y_{-3} \text{ and so on.}$$

We use the central differences as found in the first table for interpolation near the central value. Among the various formulae for Central Difference Interpolation, first we consider Gauss's forward interpolation formula.

INTERPOLATION - Arbitrarily Spaced x values

In the previous sections we have discussed interpolations when the x -values are equally spaced. These interpolation formulae cannot be used when the x -values are not equally spaced. In the following sections, we consider formulae that can be used even if the x -values are not equally spaced.

Newton's Divided Difference Interpolation Formula

If x_0, x_1, \dots, x_n are *arbitrarily spaced* (i.e. if the difference between x_0 and x_1 , x_1 and x_2 etc. may not be equal), then the polynomial of degree n through $(x_0, f_0), (x_1, f_1), \dots, (x_n, f_n)$, where $f_j = f(x_j)$, is given by the **Newton's divided difference interpolation formula** (also known as Newton's general interpolation formula) given by

$$f(x) \approx f_0 + (x - x_0)f[x_0, x_1] + (x - x_0)(x - x_1)f[x_0, x_1, x_2] + \dots + (x - x_0) \dots (x - x_{n-1})f[x_0, \dots, x_n],$$

with the remainder term after $(n+1)$ terms is given by

$$(x - x_0)(x - x_1) \dots (x - x_n)f[x, x_0, x_1, \dots, x_n]$$

where $f[x_0, x_1], f[x_0, x_1, x_2], \dots$ are the **divided differences** given by

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

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

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

Also,
$$f[x, x_0, x_1, \dots, x_n] = \frac{f[x_1, x_2, \dots, x_n] - f[x_0, x_1, \dots, x_n]}{x_n - x}$$

Note If x_0, x_1, \dots, x_n are equally spaced, i.e. when $x_k = x_0 + kh$, then $f[x_0, \dots, x_k] = \frac{\Delta^k f_0}{k! h^k}$

and Newton's divided difference interpolation formula takes the form of Newton's forward difference interpolation formula.

Derivation of the formula:

For a function $y = f(x)$, let us given the set of $(n+1)$ points, $(x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2)), \dots, (x_n, f(x_n))$. The values x_1, x_2, \dots, x_n of the independent variable x are called the arguments and the corresponding values $y_1 = f(x_1), y_2 = f(x_2), \dots, y_n = f(x_n)$ of the depending variable y are called entries. We define the first divided difference of $f(x)$ between two consecutive arguments x_i and x_{i+1} as,

$$f(x_i, x_{i+1}) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \text{ for } i = 0, 1, \dots, n-1$$

The second divided difference between three consecutive arguments x_i, x_{i+1} and x_{i+2} is given by,

$$f(x_i, x_{i+1}, x_{i+2}) = \frac{f(x_{i+1}, x_{i+2}) - f(x_i, x_{i+1})}{x_{i+2} - x_i} \text{ for } i = 0, 1, \dots, n-2$$

In general the n^{th} divided difference (or divided difference of order n) between x_1, x_2, \dots, x_n is,

$$f(x_0, x_1, \dots, x_n) = \frac{f(x_1, x_2, \dots, x_n) - f(x_0, x_1, \dots, x_{n-1})}{x_n - x_0}$$

Hence, in particular, the first divided difference between x_0 and x_1 is,

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

The second divided difference between three consecutive arguments x_0, x_1 and x_2 is

$$\begin{aligned} f(x_0, x_1, x_2) &= \frac{f(x_1, x_2) - f(x_0, x_1)}{x_2 - x_0} \\ &= \frac{1}{x_2 - x_0} \left[\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0} \right] \\ &= \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)} - \frac{f(x_1)}{(x_2 - x_0)} \left[\frac{1}{(x_2 - x_1)} + \frac{1}{(x_1 - x_0)} \right] + \frac{f(x_0)}{(x_2 - x_0)(x_1 - x_0)} \\ &= \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)} - \frac{f(x_1)}{(x_2 - x_1)(x_1 - x_0)} + \frac{f(x_0)}{(x_2 - x_0)(x_1 - x_0)} \\ \Rightarrow f(x_0, x_1, x_2) &= \frac{f(x_0)}{(x_0 - x_2)(x_0 - x_1)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)} \end{aligned}$$

As above, the n^{th} divided difference between x_1, x_2, \dots, x_n , $f(x_0, x_1, \dots, x_n)$ is expressed as

$$\begin{aligned} f(x_0, x_1, \dots, x_n) &= \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2) \dots (x_0 - x_n)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2) \dots (x_1 - x_n)} + \dots \\ &\quad + \frac{f(x_n)}{(x_n - x_0)(x_n - x_1) \dots (x_n - x_{n-1})} \end{aligned}$$

Properties of divided difference:

1. The divided differences are symmetrical about their arguments.

$$\begin{aligned}\text{We have, } f(x_0, x_1) &= \frac{f(x_1) - f(x_0)}{x_1 - x_0} \\ &= \frac{f(x_0) - f(x_1)}{x_0 - x_1} = f(x_1, x_0)\end{aligned}$$

$\Rightarrow f(x_0, x_1) = f(x_1, x_0)$. Hence, the order of the arguments has no importance.

When we are considering the n^{th} divided difference also, we can write, $f(x_0, x_1, \dots, x_n)$ as

$$f(x_0, x_1, \dots, x_n) = \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2) \dots (x_0 - x_n)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2) \dots (x_1 - x_n)} + \dots + \frac{f(x_n)}{(x_n - x_0)(x_n - x_1) \dots (x_n - x_{n-1})}$$

From this expression it is clear that, whatever be the order of the arguments, the expression is same.

Hence the divided differences are symmetrical about their arguments.

2. Divided difference operator is linear.

For example, consider two polynomials $f(x)$ and $g(x)$. Let

$$h(x) = af(x) + bg(x),$$

where ' a ' and ' b ' are any two real constants. The first divided difference of $h(x)$ corresponding to the arguments x_0 and x_1 is,

$$\begin{aligned}h(x_0, x_1) &= \frac{h(x_1) - h(x_0)}{x_1 - x_0} = \frac{af(x_1) + bg(x_1) - af(x_0) - bg(x_0)}{x_1 - x_0} \\ &= \frac{a[f(x_1) - f(x_0)] + b[g(x_1) - g(x_0)]}{x_1 - x_0} \\ &= a \frac{f(x_1) - f(x_0)}{x_1 - x_0} + b \frac{g(x_1) - g(x_0)}{x_1 - x_0} \\ &= a f(x_0, x_1) + b g(x_0, x_1)\end{aligned}$$

3. The n^{th} divided difference of a polynomial of degree n is its leading coefficient.

Consider $f(x) = x^n$, where n is a positive number

$$\text{Now, } f(x_0, x_1) = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{x_1^n - x_0^n}{x_1 - x_0}$$

$$= x_1^{n-1} + x_1^{n-2}x_0 + x_1^{n-3}x_0^2 + \dots + x_0^{n-1}$$

This is a polynomial of degree (n-1) and symmetric in arguments x_0 and x_1 with leading coefficient 1.

The second divided difference,

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

$$= \frac{(x_2^{n-1} + x_2^{n-2}x_1 + \dots + x_1^{n-1}) - (x_0^{n-1} + x_0^{n-2}x_1 + \dots + x_1^{n-1})}{x_2 - x_0}, \quad \text{which}$$

can be expressed as a polynomial of degree n-2, is symmetric about x_0, x_1 and x_2 with leading coefficient 1.

Proceeding like this, we get the n^{th} divided difference of $f(x) = x^n$ is 1.

Now we consider a general polynomial of degree n as,

$$g(x) = a_0x^n + a_1x^{n-1} + a_2x^{n-2} + \dots + a_n$$

Since the divided difference operator is linear, we get n^{th} divided difference of $g(x)$ as a_0 , which is the leading coefficient of $g(x)$.

Example Using the following table find $f(x)$ as a polynomial in x

x	$f(x)$
-1	3
0	-6
3	39
6	822
7	1611

The divided difference table is

x	$f(x)$	$f[x_k, x_{k+1}]$			
-1	3				
		-9			
0	-6		6		
		15		5	
3	39		41		1
		261		13	
6	822		132		
		789			
7	1611				

Hence

$$\begin{aligned}
 f(x) &= 3 + (x+1)(-9) + x(x+1)(6) + x(x+1)(x-3)(5) \\
 &\quad + x(x+1)(x-3)(x-6) \\
 &= x^4 - 3x^3 + 5x^2 - 6.
 \end{aligned}$$

Example Find the interpolating polynomial by Newton's divided difference formula for the following table and then calculate $f(2.1)$.

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

x	$f(x)$	First divided difference $f[x_{k-1}, x_k]$	Second divided difference $f[x_{k-1}, x_k, x_{k+1}]$	Third divided difference $f[x_{k-1}, x_k, x_{k+1}, x_{k+2}]$
0	1	$f(x_0, x_1) = 0$		
1	1	$f(x_1, x_2) = 1$	$-1/2$	
2	2	$f(x_2, x_3) = 3/2$	$-1/6$	$-\frac{1}{2}$
4	5			

Now substituting the values in the formula, we get

$$\begin{aligned}
 f(x) &\approx 1 + (x-0)(0) + (x-0)(x-1)\left(\frac{1}{2}\right) + (x-0)(x-1)(x-2)\left(-\frac{1}{12}\right) \\
 &= -\frac{1}{12}x^3 + \frac{3}{4}x^2 - \frac{2}{3}x + 1
 \end{aligned}$$

Substituting $x = 2.1$ in the above polynomial, we get $f(2.1) = 2.135$,

NEWTON' S AND LAGRANGIAN FORMULAE - PART II

Problem: Obtain Newton's divided difference interpolating polynomial satisfied by $(-4,1245), (-1,33), (0,5), (2,9)$ and $(5,1335)$.

Solution: Newton's divided difference interpolating polynomial is given by,

$$f(x) = f(x_0) + (x-x_0)f(x_0, x_1) + (x-x_0)(x-x_1)f(x_0, x_1, x_2) \\ + (x-x_0)(x-x_1)(x-x_2)f(x_0, x_1, x_2, x_3) + \dots + \\ (x-x_0)(x-x_1)\dots(x-x_{n-1})f(x_0, x_1, \dots, x_n)$$

Here x values are gives as, -4, -1, 0, 2 and 9. Corresponding f(x) values are 1245, 33, 5, 9 and 1335.

Hence the divided difference as shown in the following table:

X	First divided differences	Second divided differences	Third divided differences	Fourth divided differences
-4	-404			
-1		94		
	-28		-14	
0		10		3
	2		13	
2		88		
	442			
5				

Given $f(x_0)=1245$. From the table, we can observe that

$$f(x_0, x_1) = -404; \quad f(x_0, x_1, x_2) = 94; \\ f(x_0, x_1, x_2, x_3) = -14 \text{ and } f(x_0, x_1, x_2, x_3, x_4) = 3$$

Hence the interpolating polynomial is,

$$\begin{aligned} f(x) &= 1245 + (x - (-4)) \times (-404) + (x - (-4))(x - (-1)) \times 94 \\ &\quad + (x - (-4))(x - (-1))(x - 0) \times 14 + (x - (-4))(x - (-1))(x - 0)(x - 2) \times 3 \\ \Rightarrow f(x) &= 1245 - 404(x + 4) + 94(x + 4)(x + 1) \\ &\quad + 14(x + 4)(x + 1)(x - 0) + 3(x + 4)(x + 1)(x - 0)(x - 2) \end{aligned}$$

On simplification, we get,

$$f(x) = 3x^4 - 5x^3 + 6x^2 - 14x + 5.$$

Newton's Interpolation formula with divided differences

Consider two arguments x and x_0 . The first divided difference between x and x_0 is,

$$\begin{aligned} f(x, x_0) &= \frac{f(x_0) - f(x)}{x_0 - x} = \frac{f(x) - f(x_0)}{x - x_0} \\ \Rightarrow f(x) &= f(x_0) + (x - x_0)f(x, x_0) \quad \text{---- (1)} \end{aligned}$$

Consider x , x_0 and x_1 . Then,

$$\begin{aligned} f(x, x_0, x_1) &= \frac{f(x_0, x_1) - f(x, x_0)}{x_1 - x} = \frac{f(x, x_0) - f(x_0, x_1)}{x - x_1} \\ \Rightarrow f(x, x_0) &= f(x_0, x_1) + (x - x_1)f(x, x_0, x_1) \end{aligned}$$

Put it in (1), we get,

$$f(x) = f(x_0) + (x - x_0)[f(x_0, x_1) + (x - x_1)f(x, x_0, x_1)]$$

That is,

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

Again, for x , x_0 , x_1 and x_2

$$\begin{aligned} \Rightarrow f(x, x_0, x_1, x_2) &= \frac{f(x, x_0, x_1) - f(x_0, x_1, x_2)}{x_2 - x} = \frac{f(x_0, x_1, x_2) - f(x, x_0, x_1)}{x - x_2} \\ \Rightarrow f(x, x_0, x_1) &= (x_2 - x)f(x, x_0, x_1, x_2) + f(x_0, x_1, x_2) \end{aligned}$$

Hence (2) implies,

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

Proceeding like this, we obtain for $f(x)$ as,

$$\begin{aligned} f(x) &= f(x_0) + (x-x_0)f(x_0, x_1) + (x-x_0)(x-x_1)f(x_0, x_1, x_2) \\ &\quad + (x-x_0)(x-x_1)(x-x_2)f(x_0, x_1, x_2, x_3) + \dots + \\ &\quad (x-x_0)(x-x_1)\dots(x-x_n)f(x, x_0, x_1, \dots, x_n) \end{aligned}$$

If $f(x)$ is a polynomial of degree n , then $f(x, x_0, x_1, \dots, x_n) = 0$, because it is the $(n+1)$ th difference.

Hence we get,

$$\begin{aligned} f(x) &= f(x_0) + (x-x_0)f(x_0, x_1) + (x-x_0)(x-x_1)f(x_0, x_1, x_2) \\ &\quad + (x-x_0)(x-x_1)(x-x_2)f(x_0, x_1, x_2, x_3) + \dots + \\ &\quad (x-x_0)(x-x_1)\dots(x-x_{n-1})f(x_0, x_1, \dots, x_n) \end{aligned}$$

This is known as **Newton's interpolation formula with divided difference**.

Note:

1. For the given arguments x_1, x_2, \dots, x_n , if all the k^{th} , ($k < n$) divided differences are equal, the $k+1^{\text{th}}$ divided differences are zeroes. Then Newton's interpolation formula gives a polynomial of degree k for the given data.
2. Newton's divided difference interpolation formula possesses the permanence property. Apart from the given arguments x_1, x_2, \dots, x_n along with the corresponding function values, suppose that on a later time a new argument x_{n+1} with corresponding entry $f(x_{n+1})$ are given. The new set of data values can be represented by a polynomial of degree $(n+1)$. To obtain the required polynomial we add the term $(x-x_0)(x-x_1)\dots(x-x_n)f(x_0, x_1, \dots, x_n, x_{n+1})$ to the previously obtained n^{th} degree polynomial.

Problem 2: The following table gives the relation between steam pressure and temperature. Find the pressure at temperature 375^0 .

Temp. :	361 ⁰	367 ⁰	378 ⁰	387 ⁰	399 ⁰
Pressure:	154.9	167.9	191	212.5	244.2

Solution:

To find the pressure at temperature 375⁰, it is to establish the relation giving pressure in terms of temperature. Let us consider temperature as x values and pressure as corresponding f(x) values.

The given x values are 361⁰, 367⁰, 378⁰, 387⁰ and 399⁰. Corresponding f(x) values are 154.9, 167.9, 191, 212.5 and 244.2.

f(x) is obtained by Newton's divided difference interpolating polynomial as,

$$f(x) = f(x_0) + (x-x_0)f(x_0, x_1) + (x-x_0)(x-x_1)f(x_0, x_1, x_2) + (x-x_0)(x-x_1)(x-x_2)f(x_0, x_1, x_2, x_3) + \dots + (x-x_0)(x-x_1)\dots(x-x_n)f(x, x_0, x_1, \dots, x_n)$$

Given $f(x_0) = f(361^0) = 154.9$. The divided differences for the given points are as shown in the table.

X	First divided differences	Second divided differences	Third divided differences	Fourth divided differences
361	2.01666			
367	2.18181	0.00971		
378	2.38888	0.01035	0.0000246	
387	2.64166	0.01204	0.0000528	0.00000074
399				

From the table, we can observe that

$$f(x_0, x_1) = 2.01666; \quad f(x_0, x_1, x_2) = 0.00971;$$

$$f(x_0, x_1, x_2, x_3) = 0.0000246 \quad \text{and} \quad f(x_0, x_1, x_2, x_3, x_4) = 0.00000074$$

Hence,

$$f(x) = 154.9 + (x-361) \times 2.01666 + (x-361)(x-367) \times 0.00971 + (x-361)(x-367)(x-378) \times 0.0000246 + (x-361)(x-367)(x-378)(x-387) \times 0.00000074$$

Substituting x=375 in the above expression gives, f(375)= 184.21548.

Problem 3: Obtain Newton's divided difference interpolating polynomial satisfying the following values:

x:	1	3	4	5	7	10
f(x):	3	31	69	131	351	1011

Also find $f(4.5)$, $f(8)$ and the second derivative of $f(x)$ at $x=3.2$.

Solution:

To obtain the Newton's divided difference interpolating polynomial $f(x)$, we need the divided difference using the given values.

It is calculated and listed in the following table

X	First divided differences	Second divided differences	Third divided differences	Fourth divided differences
1	14			
3	38	8		
4	62	12	1	0
5	110	16	1	0
7	220	22	1	
9				

Since the fourth divided differences are zeroes, $f(x)$ is of degree 3 and it is obtained as,

$$f(x) = f(x_0) + (x-x_0)f(x_0, x_1) + (x-x_0)(x-x_1)f(x_0, x_1, x_2) + (x-x_0)(x-x_1)(x-x_2)f(x_0, x_1, x_2, x_3)$$

$$f(x_0) = f(1) = 3; f(x_0, x_1) = 14; f(x_0, x_1, x_2) = 8 \quad \text{and} \quad f(x_0, x_1, x_2, x_3) = 1$$

$$\Rightarrow f(x) = 3 + (x-1) \times 14 + (x-1)(x-3) \times 8 + (x-1)(x-3)(x-4) \times 1$$

That is,

$$f(x) = x^3 + x + 1$$

$$\text{Hence, } f(4.5) = (4.5)^3 + 4.5 + 1 = 96.625 \quad \text{and} \quad f(8) = (8)^3 + 8 + 1 = 521$$

Second derivative of $f(x)$ is $6x$. Now second derivative of $f(x)$ at $x=3.2$ is $6 \times 3.2 = 19.2$

Lagrangian Interpolation

Another method of interpolation in the case of *arbitrarily spaced pivotal values* x_0, x_1, \dots, x_n is Lagrangian interpolation. This method is based on Lagrange's $n+1$ point interpolation formula given by

$$f(x) \approx L_n(x) = \sum_{k=0}^n \frac{l_k(x)}{l_k(x_k)} f_k,$$

where

$$l_0(x) = (x - x_1)(x - x_2) \dots (x - x_n),$$

$$l_k(x) = (x - x_0) \dots (x - x_{k-1})(x - x_{k+1}) \dots (x - x_n), \quad 0 < k < n.$$

$$l_n(x) = (x - x_0)(x - x_1) \dots (x - x_{n-1})$$

Remark: $L_k(x_k) = f_k$. For, $l_k(x_j) = 0$, when $j \neq k$, so that for $x = x_k$, the sum on the RHS of the formula reduces to the single term f_k , which indicates that f and L_k agrees at $n+1$ tabulated points.

Derivation of the formula:

Given the set of $(n+1)$ points, $(x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2)), \dots, (x_n, f(x_n))$ of x and $f(x)$, it is required to fit the unique polynomial $p_n(x)$ of maximum degree n , such that $f(x)$ and $p_n(x)$ agree at the given set of points. The values x_0, x_1, \dots, x_n may not be equidistant.

Since the interpolating polynomial must use all the ordinates $f(x_0), f(x_1), \dots, f(x_n)$, it can be written as a linear combination of these ordinates. That is, we can write the polynomial as

$$p_n(x) = l_0(x)f(x_0) + l_1(x)f(x_1) + \dots + l_n(x)f(x_n).$$

where $f(x_i)$ and $l_i(x)$, for $i = 0, 1, 2, \dots, n$ are polynomials of degree n .

This polynomial fits the given data exactly.

At $x = x_0$, as $p_n(x)$ and $f(x)$ coincide, we get,

$$f(x_0) = p_n(x_0) = l_0(x_0)f(x_0) + l_1(x_0)f(x_1) + \dots + l_n(x_0)f(x_n)$$

This equation is satisfied only when $l_0(x_0) = 1$ and $l_i(x_0) = 0, i \neq 0$

At a general point $x = x_i$, we get,

$$f(x_i) = p_n(x_i) = l_0(x_i)f(x_0) + l_1(x_i)f(x_1) + \dots + l_n(x_i)f(x_n)$$

This equation is satisfied only when $l_i(x_i) = 1$ and $l_j(x_i) = 0, i \neq j$

Therefore, $l_i(x)$, which are polynomials of degree n , satisfy the conditions

$$l_i(x_j) = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

Since, $l_i(x) = 0$ at $x = x_0, x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n$, we know that

$(x - x_0), (x - x_1), \dots, (x - x_{i-1}), (x - x_{i+1}), \dots, (x - x_n)$ are factors of $l_i(x)$. The product of these factors is a polynomial of degree n . Therefore, we can write

$$l_i(x) = C(x - x_0)(x - x_1) \dots (x - x_{i-1})(x - x_{i+1}) \dots (x - x_n), \text{ where } C \text{ is a constant.}$$

Now, since $l_i(x_i) = 1$, we get

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

$$\text{Hence, } C = \frac{1}{(x_i - x_0)(x_i - x_1) \dots (x_i - x_{i-1})(x_i - x_{i+1}) \dots (x_i - x_n)}$$

Therefore,

$$l_i(x) = \frac{(x - x_0)(x - x_1) \dots (x - x_{i-1})(x - x_{i+1}) \dots (x - x_n)}{(x_i - x_0)(x_i - x_1) \dots (x_i - x_{i-1})(x_i - x_{i+1}) \dots (x_i - x_n)}$$

Now the polynomial

$$p_n(x) = l_0(x)f(x_0) + l_1(x)f(x_1) + \dots + l_n(x)f(x_n),$$

with $l_i(x) = \frac{(x - x_0)(x - x_1) \dots (x - x_{i-1})(x - x_{i+1}) \dots (x - x_n)}{(x_i - x_0)(x_i - x_1) \dots (x_i - x_{i-1})(x_i - x_{i+1}) \dots (x_i - x_n)}$ is called Lagrange interpolating polynomial and $l_i(x)$ are called Lagrange fundamental polynomials.

To fit a polynomial of degree 1, we require at least two points. Let $(x_0, f(x_0)), (x_1, f(x_1))$ are the points. Then the Lagrange polynomial of degree one or a straight line for the given data is,

$$p_1(x) = l_0(x)f(x_0) + l_1(x)f(x_1), \text{ where, } l_0(x) = \frac{(x - x_1)}{(x_0 - x_1)} \text{ and } l_1(x) = \frac{(x - x_0)}{(x_1 - x_0)}.$$

Let $(x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2))$ are the given three points. Then the Lagrange polynomial of degree two for the data is given by

$p_2(x) = l_0(x)f(x_0) + l_1(x)f(x_1) + l_2(x)f(x_2)$, where,

$$l_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad l_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \quad \text{and} \quad l_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}.$$

For the four points $(x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2)), (x_3, f(x_3))$, the Lagrange polynomial of degree three is given by,

$$p_3(x) = l_0(x)f(x_0) + l_1(x)f(x_1) + l_2(x)f(x_2) + l_3(x)f(x_3), \quad \text{where,} \quad l_0(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}$$

$$l_1(x) = \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}, \quad l_2(x) = \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} \quad \text{and}$$

$$l_3(x) = \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} \quad \text{and so on.}$$

Problem : Given $f(2) = 9$, and $f(6) = 17$. Find an approximate value for $f(5)$ by the method of Lagrange's interpolation.

Solution:

For the given two points $(2,9)$ and $(6,17)$, the Lagrangian polynomial of degree 1 is

$$p_1(x) = l_0(x)f(x_0) + l_1(x)f(x_1), \quad \text{where,} \quad l_0(x) = \frac{(x-x_1)}{(x_0-x_1)} \quad \text{and} \quad l_1(x) = \frac{(x-x_0)}{(x_1-x_0)}. \quad \text{That is,}$$

$$p_1(x) = \frac{(x-x_1)}{(x_0-x_1)}f(x_0) + \frac{(x-x_0)}{(x_1-x_0)}f(x_1)$$

$$\Rightarrow p_1(x) = \frac{(x-6)}{(2-6)} \times 9 + \frac{(x-2)}{(6-2)} \times 17$$

Hence,

$$f(5) = P_1(5) = \frac{(5-6)}{(2-6)} \times 9 + \frac{(5-2)}{(6-2)} \times 17$$

$$= \frac{1}{4} \times 9 + \frac{3}{4} \times 17$$

$$= 15$$

Problem: Use Lagrange's formula, to find the quadratic polynomial that takes the values

$$\begin{array}{lcl} x & : & 0 \quad 1 \quad 3 \\ f(x) & : & 0 \quad 1 \quad 0 \end{array}$$

For the given three points (0,0) , (1,1) and (3,0), the quadratic polynomial by Lagrange's interpolation is $p_2(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)$

We are considering the given x values 0,1, and 3 as x_0, x_1 and x_2 . Given, $f(x_0)$ and $f(x_2)$ are zeroes. Hence the polynomial is,

$$p_2(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1)$$

Then,

$$p_2(x) = \frac{(x-0)(x-3)}{(1-0)(1-3)} \times 1$$

$$\Rightarrow p_2(x) = \frac{x(x-3)}{-2} \times 1 = \frac{1}{2}(3x - x^2).$$

Example Find Lagrange's interpolation polynomial fitting the points $f(1) = -3, f(3) = 0, f(4) = 30, f(6) = 132$. Hence find $f(5)$.

Here 4 tabulated points are given. Hence we need Lagrange's polynomial for ($n + 1 = 3 + 1 = 4$ points) and is given by

$$f(x) \approx L_3(x) = \sum_{k=0}^3 \frac{l_k(x)}{l_k(x_k)} f_k.$$

Now substituting the values, we obtain

$$L_3(x) = \frac{(x-3)(x-4)(x-6)}{(1-3)(1-4)(1-6)} (-3) + \frac{(x-1)(x-4)(x-6)}{(3-1)(3-4)(3-6)} (0)$$

$$+ \frac{(x-1)(x-3)(x-6)}{(4-1)(4-3)(4-6)} (30) + \frac{(x-1)(x-3)(x-4)}{(6-1)(6-4)(6-4)} (132)$$

$$= \frac{1}{2}(-x^3 + 27x^2 - 92x + 60), \text{ on simplification.}$$

$$\text{Now } f(5) \approx L_3(5) = \frac{1}{2}(-5^3 + 27(5)^2 - 92(5) + 60) = 75.$$

Example Find $\ln 9.2$ with $n=3$, using Lagrange's interpolation formula with the given table:

x	9.0	9.5	10.0	11.0
$\ln x$	2.197	2.251	2.302	2.397

22 29 59 90

$$\begin{aligned} \ln(9.2) &= f(9.2) \approx L_3(9.2) = \sum_{k=0}^3 \frac{l_k(9.2)}{l_k(x_k)} f_k \\ &= \frac{(9.2-9.5)(9.2-10.0)(9.2-11.0)}{(9.0-9.5)(9.0-10.0)(9.0-11.0)} (2.19722) \\ &\quad + \frac{(9.2-9.0)(9.2-10.0)(9.2-11.0)}{(9.5-9.0)(9.5-10.0)(9.5-11.0)} (2.25129) \\ &\quad + \frac{(9.2-9.0)(9.2-9.5)(9.2-11.0)}{(10.0-9.0)(10.0-9.5)(10.0-11.0)} (2.30259) \\ &\quad + \frac{(9.2-9.0)(9.2-9.5)(9.2-10.0)}{(11.0-9.0)(11.0-9.5)(11.0-10.0)} (2.39790) \end{aligned}$$

= 2.219 20, which is exact to 5D.

Example Certain corresponding values of x and $\log_{10} x$ are (300, 2.4771), (304, 2.4829), (305, 2.4843) and (307, 2.4871). Find $\log_{10} 301$.

$$\begin{aligned} \log_{10} 301 &= \frac{(-3)(-4)(-6)}{(-4)(-5)(-7)} (2.4771) + \frac{(1)(-4)(-6)}{(4)(-1)(-3)} (2.4829) \\ &\quad + \frac{(1)(-3)(-6)}{(5)(1)(-2)} (2.4843) + \frac{(1)(-3)(-4)}{(7)(3)(2)} (2.4871) \\ &= 1.2739 + 4.9658 - 4.4717 + 0.7106 \\ &= 2.4786. \end{aligned}$$

Inverse Lagrangian Interpolation Formula

Interchanging x and y in the Lagrangian Interpolation Formula, we obtain the **inverse Lagrangian interpolation formula** given by

$$x \approx L_n(y) = \sum_{k=0}^n \frac{l_k(y)}{l_k(y_k)} x_k.$$

Example If $y_1 = 4$, $y_3 = 12$, $y_4 = 19$ and $y_x = 7$, find x . Compare with the actual value.

Using the inverse interpolation formula,

$$x \approx L_n(7) = \sum_{k=0}^2 \frac{l_k(7)}{l_k(y_k)} x_k$$

where $x_0 = 1$, $y_0 = 4$, $x_1 = 3$, $y_1 = 12$, $x_2 = 4$, $y_2 = 19$ and $y = 7$

$$\text{i.e., } x \approx \frac{(7-y_1)(7-y_2)}{(y_0-y_1)(y_0-y_2)}x_0 + \frac{(7-y_0)(7-y_2)}{(y_1-y_0)(y_1-y_2)}x_1 + \frac{(7-y_0)(7-y_1)}{(y_2-y_0)(y_2-y_1)}x_2$$

$$\begin{aligned}\text{i.e., } x &= \frac{(-5)(-12)}{(-8)(-15)}(1) + \frac{(3)(-12)}{(8)(-7)}(3) + \frac{(3)(-5)}{(15)(7)}(4) \\ &= \frac{1}{2} + \frac{27}{14} - \frac{4}{7} \\ &= 1.86\end{aligned}$$

The actual value is 2.0 since the above values were obtained from the polynomial $y(x) = x^2 + 3$.

Example Find the Lagrange interpolating polynomial of degree 2 approximating the function $y = \ln x$ defined by the following table of values. Hence determine the value of $\ln 2.7$.

x	$y = \ln x$
2	0.69315
2.5	0.91629
3.0	1.09861

Similarly,

$$l_1(x) = -(4x^2 - 20x + 24) \text{ and } l_2(x) = 2x^2 - 9x + 10.$$

Hence

$$\begin{aligned}L_2(x) &= \frac{l_0(x)}{l_0(x_k)} f_0 + \frac{l_1(x)}{l_1(x_k)} f_1 + \frac{l_2(x)}{l_2(x_k)} f_2 \\ &= \frac{(x-2.5)(x-3.0)}{(-0.5)(-1.0)} \cdot f_0 + \frac{(x-2)(x-3)}{(2.5-2)(3.0-2.5)} f_1 + \frac{(x-2)(x-2.5)}{(3-2)(3-2.5)} f_2 \\ &= (2x^2 - 11x + 15)(0.69315) - (4x^2 - 20x + 24)(0.91629) \\ &\quad + (2x^2 - 9x + 10)(1.09861) \\ &= -0.08164x^2 + 0.81366x - 0.60761.\end{aligned}$$

which is the required quadratic polynomial.

Putting $x = 2.7$, in the above polynomial, we obtain

$\ln 2.7 \approx L_2(2.7) = -0.08164(2.7)^2 + 0.81366(2.7) - 0.60761 = 0.9941164$. Actual value of $\ln 2.7 = 0.9932518$, so that

$$|\text{Error}| = 0.0008646.$$

Example The function $y = \sin x$ is tabulated below

x	$y = \sin x$
0	0
$f/4$	0.70711
$f/2$	1.0

Using Lagrange's interpolation formula, find the value of $\sin(f/6)$.

Solution We have

$$\begin{aligned} \sin \frac{f}{6} &\approx \frac{(f/6-0)(f/6-f/2)}{(f/4-0)(f/4-f/2)} (0.70711) + \frac{(f/6-0)(f/6-f/4)}{(f/2-0)(f/2-f/4)} (1) = \frac{8}{9} (0.70711) - \frac{1}{9} \\ &= \frac{4.65688}{9} = 0.51743. \end{aligned}$$

Example Using Lagrange's interpolation formula, find the form of the function $y(x)$ from the following table.

x	y
0	-12
1	0
3	12
4	24

Since $y=0$ when $x=1$, it follows that $x-1$ is a factor. Let $y(x)=(x-1)R(x)$. Then $R(x)=y/(x-1)$. We now tabulate the values of x and $R(x)$: For $x=0$, $R(0)=\frac{-12}{0-1}=12$, and so on.

x	$R(x)$
0	12
3	6
4	8

Applying Lagrange's formula to the above table, we find

$$R(x) = \frac{(x-3)(x-4)}{(-3)(-4)} (12) + \frac{(x-0)(x-4)}{(3-0)(3-4)} (6) + \frac{(x-0)(x-3)}{(4-0)(4-3)} (8)$$

$$= (x-3)(x-4) - 2x(x-4) + 2x(x-3)$$

$$= x^2 - 5x + 12.$$

Hence the required polynomial approximation to $y(x)$ is given by

$$y(x) = (x-1)(x^2 - 5x + 12).$$

Example With the use of Newton's divided difference formula, find $\log 10^{301}$. Given the following divided difference table

x	$f(x) = \log_{10} x$	$f[x_{k-1}, x_k]$	$f[x_{k-2}, x_k, x_{k+1}]$
300	2.47714	0.00145	0.00001
304	2.4829		
305	2.4843		
307	2.4871	0.00140	0

$$\log_{10} 301 = 2.4771 + 0.00145 + (-3)(-0.00001) = 2.4786, \text{ as before.}$$

It is clear that the arithmetic in this method is much simpler when compare to that in Lagrange's method.

Exercises

9. Using the difference table in exercise 1, compute $\cos 0.75$ by Newton's forward difference interpolating formula with $n=1, 2, 3, 4$ and compare with the 5D-value 0.731 69.
10. Using the difference table in exercise 1, compute $\cos 0.28$ by Newton's forward difference interpolating formula with $n=1, 2, 3, 4$ and compare with the 5D-value
11. Using the values given in the table, find $\cos 0.28$ (in radian measure) by linear interpolation and by quadratic interpolation and compare the results with the value 0.961 06 (exact to 5D).

x	$f(x)=\cos x$	First difference	Second difference
0.0	1.000 00	-0.019 93	-0.03908
0.2	0.980 07	-0.059 01	-0.03671
0.4	0.921 06	-0.095 72	-0.03291

0.6	0.825 34	-0.128 63	-0.02778
0.8	0.696 71	-0.156 41	
1.0	0.540 30		

12. Find Lagrangian interpolation polynomial for the function f having $f(4)=1, f(6)=3, f(8)=8, f(10)=16$. Also calculate $f(7)$.

13. The sales in a particular shop for the last ten years is given in the table:

Year	1996	1998	2000	2002	2004
Sales (in lakhs)	40	43	48	52	57

Estimate the sales for the year 2001 using Newton's backward difference interpolating formula.

14. Find $f(3)$, using Lagrangian interpolation formula for the function f having $f(1)=2, f(2)=11, f(4)=77$.

15. Find the cubic polynomial which takes the following values:

x	0	1	2	3	
$f(x)$		1	2	1	10

16. Compute $\sin 0.3$ and $\sin 0.5$ by Everett formula and the following table.

	$\sin x$	δ^2
0.2	0.198 67	-0.007 92
0.4	0.389 42	-0.015 53
.6	0.564 64	-0.022 50

9. The following table gives the distances in nautical miles of the visible horizon for the given heights in feet above the earth's surface:

$x = \text{height} :$	100	150	200	250	300	350	400
$y = \text{distance} :$	10.63	13.03	15.04	16.81	18.42	19.90	21.27

Find the value of y when $x = 218$ ft (Ans: 15.699)

10. Using the same data as in exercise 9, find the value of y when $x = 410$ ft.

8

INTERPOLATION BY ITERATION

Interpolation by Iteration

Given the $(n+1)$ points $(x_0, f_0), (x_1, f_1), \dots, (x_n, f_n)$, where the values of x need not necessarily be equally spaced, then to find the value of f corresponding to any given value of x we proceed iteratively as follows: obtain a first approximation to f by considering the first-two points only; then obtain its second approximation by considering the first-three points, and so on. We denote the different interpolation polynomials by $\Delta(x)$, with suitable subscripts, so that at the first stage of approximation, we have

$$\Delta_{01}(x) = f_0 + (x - x_0) f[x_0, x_1] = \frac{1}{x_1 - x_0} \begin{vmatrix} f_0 & x_0 & -x \\ f_1 & x_1 & -x \end{vmatrix}.$$

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

Next we form Δ_{012} by considering the first-three points:

$$\Delta_{012}(x) = \frac{1}{x_2 - x_1} \begin{vmatrix} \Delta_{01}(x) & x_1 & -x \\ \Delta_{02}(x) & x_2 & -x \end{vmatrix}.$$

Similarly we obtain $\Delta_{013}(x), \Delta_{014}(x)$, etc. At the n th stage of approximation, we obtain

$$\Delta_{012 \dots n}(x) = \frac{1}{x_n - x_{n-1}} \begin{vmatrix} \Delta_{012 \dots n-1}(x) & x_{n-1} & -x \\ \Delta_{012 \dots n-2n}(x) & x_n & -x \end{vmatrix}.$$

The computations is arranged as in the following Table

Table 1 Aitken's Scheme

x	f				
x_0	f_0				
		$\Delta_{01}(x)$			
x_1	f_1		$\Delta_{012}(x)$		
		$\Delta_{02}(x)$		$\Delta_{0123}(x)$	
x_2	f_2		$\Delta_{013}(x)$		$\Delta_{01234}(x)$
		$\Delta_{03}(x)$		$\Delta_{0124}(x)$	
x_3	f_3		$\Delta_{014}(x)$		
		$\Delta_{04}(x)$			
x_4	f_4				

A modification of this scheme, due to Neville, is given in the following Table. Neville's scheme is particularly suited for iterated inverse interpolation.

Table 2 Neville's Scheme

x	f				
x_0	f_0	$\Delta_{01}(x)$			
x_1	f_1	$\Delta_{12}(x)$	$\Delta_{012}(x)$		
x_2	f_2	$\Delta_{23}(x)$	$\Delta_{123}(x)$	$\Delta_{0123}(x)$	
x_3	f_3	$\Delta_{34}(x)$	$\Delta_{234}(x)$	$\Delta_{1234}(x)$	$\Delta_{01234}(x)$
x_4	f_4				

Example 26 Using Aitken's scheme and the following values evaluate $\log_{10} 301$.

x	$\log_{10} x$			
300	2.4771			
		2.47855		
304	2.4829		2.47858	
		2.47854		2.47860
305	2.4843		2.47857	
		2.47853		
307	2.4871			

Solution

$$\log_{10} 301 = 2.4786.$$

Inverse Interpolation

Given a set of values of x and y , the process of finding the value of x for a certain value of y is called *inverse interpolation*. When the values of x are at unequal intervals, the most obvious way of performing this process is by interchanging x and y in Lagrange's or Aitken's methods.

Example If $y_1 = 4$, $y_3 = 12$, $y_4 = 19$ and $y_x = 7$, find x . Compare with the actual value.

Solution

Aitken's scheme (see Table 1) is

y	x		
4	1	1.750	
12	3	1.600	1.857
19	4		

whereas Neville's scheme (see Table 2) gives

y	x		
4	1		
		1.750	
12	3		1.857
		2.286	
19	4		

In this examples both the schemes give the same result.

Method of Successive Approximations

We start with Newton's forward difference formula which is written as

$$y_u = y_0 + u\Delta y_0 + \frac{u(u-1)}{2}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{6}\Delta^3 y_0 + \dots$$

From this we obtain

$$u = \frac{1}{\Delta y_0} \left[y_u - y_0 - \frac{u(u-1)}{2}\Delta^2 y_0 - \frac{u(u-1)(u-2)}{6}\Delta^3 y_0 - \dots \right].$$

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

$$u_1 = \frac{1}{\Delta y_0} (y_u - y_0).$$

Next, we obtain the second approximation to u by including the term containing the second differences. Thus,

$$u_2 = \frac{1}{\Delta y_0} \left[y_u - y_0 - \frac{u_1(u_1-1)}{2}\Delta^2 y_0 \right]$$

where we have used the value of u_1 for u in the coefficient of $\Delta^2 y_0$. Similarly, we obtain

$$u_3 = \frac{1}{\Delta y_0} \left[y_u - y_0 - \frac{u_2(u_2-1)}{2}\Delta^2 y_0 - \frac{u_2(u_2-1)(u_2-2)}{6}\Delta^3 y_0 \right]$$

and so on. This process should be continued till two successive approximations to u agree with each other to the required accuracy. The method is illustrated in the following example.

Example Tabulate $y = x^3$ for $x = 2, 3, 4$ and 5 , and calculate the cube root of 10 correct to three decimal places.

Solution

x	$y = x^3$	Δ	Δ^2	Δ^3
2	8			
3	27	19		
4	64	37	18	
5	125	61	24	6

Here $y_u = 10$, $y_0 = 8$, $\Delta y_0 = 19$, $\Delta^2 y_0 = 18$ and $\Delta^3 y_0 = 6$. The successive approximations to u are therefore

$$u_1 = \frac{1}{19}(2) - 0.1$$

$$u_2 = \frac{1}{19} \left[2 - \frac{0.1(0.1-1)}{2}(18) \right] = 0.15$$

$$u_3 = \frac{1}{19} \left[2 - \frac{0.15(0.15-1)}{2}(18) - \frac{0.15(0.15-1)(0.15-2)}{6}(6) \right] = 0.1532$$

$$u_4 = \frac{1}{19} \left[2 - \frac{0.1541(0.1541-1)}{2}(18) - \frac{0.1541(0.1541-1)(0.1541-2)}{6}(6) \right]$$

$$= 0.1542.$$

We take $u = 0.154$ correct to three decimal places. Hence the value of x (which corresponds to $y = 10$), i.e., the cube root of 10 is given by $x_0 + uh = 2 + (0.154)1 = 2.154$.

Exercises

1. The values of x and u_x are given in the following Table.

x	2	3	5
u_x	113	286	613

Find the value of x for which $u_x = 1001$.

2. Using Lagrange inverse formula, find the value of x corresponding to $y = 100$ from the following Table.

x	3	5	7	9	11
y	6	24	58	108	174

3. The values of x and $f(x)$ are given in the following Table.

x	5	6	9	11
$f(x)$	12	13	14	16

Find the value of x for which $f(x) = 15$.

4. The values of x and u_x are given in the following Table.

x	0	5	10	15
u_x	16.35	14.88	13.59	12.46

Find correct to one decimal place the value of x for which $u_x = 14$.

9

NUMERICAL DIFFERENTIATION AND INTEGRATION

Numerical differentiation

The problem of **numerical differentiation** is the determination of approximate value of the derivative of a function f at a given point.

Differentiation using Difference Operators

We assume that the function $y = f(x)$ is given for the equally spaced x values $x_n = x_0 + nh$, for $n = 0, 1, 2, \dots$. To find the derivatives of such a tabular function, we proceed as follows:

- **Using Forward Difference Operator**

Since $\Delta = E - 1$ and $hD = \log E$, where D is a differential operator, E a shift operator, we have seen earlier that

$$hD = \log E = \log(1 + \Delta)$$

Hence

$$D = \frac{1}{h} \log(1 + \Delta) = \frac{1}{h} \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \frac{\Delta^5}{5} - \dots \right)$$

Also,

$$\begin{aligned} D^2 &= \frac{1}{h^2} \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \frac{\Delta^5}{5} - \dots \right)^2 \\ &= \frac{1}{h^2} \left(\Delta^2 - \Delta^3 + \frac{11}{12} \Delta^4 - \frac{5}{6} \Delta^5 + \dots \right) \end{aligned}$$

Therefore,

$$\begin{aligned} f'(x) = \frac{d}{dx} f(x) = Df(x) &= \frac{1}{h} \left(\Delta f(x) - \frac{\Delta^2 f(x)}{2} + \frac{\Delta^3 f(x)}{3} - \frac{\Delta^4 f(x)}{4} + \frac{\Delta^5 f(x)}{5} - \dots \right) \\ f''(x) = D^2 f(x) &= \frac{1}{h^2} \left(\Delta^2 f(x) - \Delta^3 f(x) + \frac{11}{12} \Delta^4 f(x) - \frac{5}{6} \Delta^5 f(x) + \dots \right) \end{aligned}$$

- **Using Backward Difference Operator ∇ .**

Recall that

$$hD = -\log(1 - \nabla).$$

On expansion, we have

$$D = \frac{1}{h} \left(\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \dots \right)$$

Also,

$$\begin{aligned} D^2 &= \frac{1}{h^2} \left(\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \dots \right)^2 \\ &= \frac{1}{h^2} \left(\nabla^2 + \nabla^3 + \frac{11}{12} \nabla^4 + \frac{5}{6} \nabla^5 + \dots \right) \end{aligned}$$

Hence,

$$\begin{aligned} f'(x) &= \frac{d}{dx} f(x) = Df(x) \\ &= \frac{1}{h} \left(\nabla f(x) + \frac{\nabla^2 f(x)}{2} + \frac{\nabla^3 f(x)}{3} + \frac{\nabla^4 f(x)}{4} + \dots \right) \\ f''(x) &= D^2 f(x) = \frac{1}{h^2} \left(\nabla^2 f(x) + \nabla^3 f(x) + \frac{11}{12} \nabla^4 f(x) + \frac{5}{6} \nabla^5 f(x) + \dots \right) \end{aligned}$$

Example Compute $f'(0.2)$ and $f''(0)$ from the following tabular data.

x	0.0	0.2	0.4	0.6	0.8	1.0
$f(x)$	1.00	1.16	3.56	13.96	41.96	101.00

Since $x = 0$ and 0.2 appear at and near beginning of the table, it is appropriate to use formulae based on forward differences to find the derivatives. The forward difference table for the given data is:

x	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$	$\Delta^5 f(x)$
0.0	1.00					
		0.16				
0.2	1.16		2.24			
		2.40		5.76		
0.4	3.56		8.00		3.84	
		10.40		9.60		0.00
0.6	13.96		17.60		3.84	
		28.00		13.44		
0.8	41.96		31.04			
		59.04				
1.0	101.00					

Using $f'(x) = Df(x) = \frac{1}{h} \left(\Delta f(x) - \frac{\Delta^2 f(x)}{2} + \frac{\Delta^3 f(x)}{3} - \frac{\Delta^4 f(x)}{4} + \dots \right)$

we obtain

$$f'(0.2) = \frac{1}{0.2} \left[2.40 - \frac{8.00}{2} + \frac{9.60}{3} - \frac{3.84}{4} \right] = 3.2$$

Using

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

we obtain

$$f''(0) = \frac{1}{(0.2)^2} \left[2.24 - 5.76 + \frac{11}{12} (3.84) - \frac{5}{6} (0) \right] = 0.0$$

Example Compute $f'(2.2)$ and $f''(2.2)$ from the following tabular data.

x	1.4	1.6	1.8	2.0	2.2
$f(x)$	4.0552	4.9530	6.0496	7.3981	9.0250

Since $x = 2.2$ appears at the end of the table, it is appropriate to use formulae based on backward differences to find the derivatives. The backward difference table for the given data is:

x	$f(x)$	$\nabla f(x)$	$\nabla^2 f(x)$	$\nabla^3 f(x)$	$\nabla^4 f(x)$
1.4	4.0552				
1.6	4.9530	0.8978			
1.8	6.0496	1.0966	0.1988		
2.0	7.3891	1.3395	0.2429	0.0441	
2.2	9.0250	1.6359	0.2964	0.0535	0.0094

Using the backward difference formula

$$f'(x) = Df(x) = \frac{1}{h} \left(\nabla f(x) + \frac{\nabla^2 f(x)}{2} + \frac{\nabla^3 f(x)}{3} + \frac{\nabla^4 f(x)}{4} + \dots \right)$$

we obtain

$$f'(2.2) = \frac{1}{0.2} \left[1.6359 + \frac{0.2964}{2} + \frac{0.0535}{3} + \frac{0.0094}{4} \right] = 9.0215$$

Also, using backward difference formula for $D^2 f(x)$, i.e.

$$f''(x) = D^2 f(x) = \frac{1}{h^2} \left(\nabla^2 f(x) + \nabla^3 f(x) + \frac{11}{12} \nabla^4 f(x) + \dots \right)$$

we obtain

$$f''(2.2) = \frac{1}{(0.2)^2} \left[0.2964 + 0.0535 + \frac{11}{12} (0.0094) \right] = 8.9629$$

Example From the following table of values of x and y , obtain $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ for $x = 1.2$:

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

The difference table is

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
1.0	2.7183						
1.2	3.3201	0.6018					
1.4	4.0552	0.7351	0.133				
1.6	4.9530	0.8978	0.1627	0.0294			
1.8	6.0496	1.0966	0.1988	0.0361	0.0067		
2.0	7.3891	1.3395	0.2429	0.0441	0.0080	0.0013	0.001
2.2	9.0250	1.6359	0.2964	0.0535	0.0094	0.0014	

Here $x = 1.2$, $f(x) = 3.3201$ and $h = 0.2$. Hence

$$\begin{aligned} \left[\frac{dy}{dx} \right]_{x=1.2} &= f'(1.2) \\ &= \frac{1}{0.2} \left[0.7351 - \frac{1}{2} (0.1627) + \frac{1}{3} (0.0361) - \frac{1}{4} (0.0080) + \frac{1}{5} (0.0014) \right] \\ &= 3.3205. \end{aligned}$$

$$\text{Similarly, } \left[\frac{d^2y}{dx^2} \right]_{x=1.2} = \frac{1}{0.04} \left[0.1627 - 0.0361 + \frac{11}{12} (0.0080) - \frac{5}{6} (0.0014) \right] = 3.318.$$

Example Calculate the first and second derivatives of the function tabulated in the preceding example at the point $x = 2.2$ and also $\frac{dy}{dx}$ at $x = 2.0$.

We use the table of differences of Example 1. Here $x_n = 2.2$, $y_n = 9.0250$ and $h = 0.2$. Hence backward difference for derivative gives

$$\left[\frac{dy}{dx} \right]_{x=2.2} = f'(2.2) = \frac{1}{0.2}$$

$$\left[1.6359 + \frac{1}{2}(0.2964) + \frac{1}{3}(0.0535) + \frac{1}{4}(0.0094) + \frac{1}{5}(0.0014) \right]$$

$$= 9.0228.$$

$$\left[\frac{d^2y}{dx^2} \right]_{x=2.2} = f''(2.2) = \frac{1}{0.04}$$

$$\left[0.2964 + 0.0535 + \frac{11}{12}(0.0094) + \frac{5}{6}(0.0014) \right] = 8.992.$$

Also,

$$\left[\frac{dy}{dx} \right]_{x=2.0} = f'(2.2) = \frac{1}{0.2}$$

$$\left[1.3395 + \frac{1}{2}(0.2429) + \frac{1}{3}(0.0441) + \frac{1}{4}(0.0080) + \frac{1}{5}(0.0013) + \frac{1}{6}(0.0001) \right]$$

$$= 7.3896.$$

- **Derivative using Newton's Forward difference Formula**

For finding the derivative at a point near to the beginning of the tabular values, Newton's Forward difference Formula is used. For the values y_0, y_1, \dots, y_n of a function $y=f(x)$, corresponding to the equidistant values $x_0, x_1, x_2, \dots, x_n$, where $x_1 = x_0 + h, x_2 = x_0 + 2h, x_3 = x_0 + 3h, \dots, x_n = x_0 + nh$, Newton's Forward difference Formula is,

$$f(x) = f(x_0 + uh) = y_0 + u[\Delta y_0] + \frac{u(u-1)}{2!}[\Delta^2 y_0]$$

$$+ \frac{u(u-1)(u-2)}{3!}[\Delta^3 y_0] + \dots + \frac{u(u-1)(u-2)\dots(u-n+1)}{n!}[\Delta^n y_0]$$

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

The derivative of $f(x)$ with respect to x , where x is any point in the interval $[x_0, x_n]$ is obtained as follows:

$$\frac{d}{dx} f(x) = \frac{d}{du} f(x) \times \frac{du}{dx}, \text{ by chain rule}$$

$$= \frac{d}{du} f(x) \times \frac{d}{dx} \left(\frac{(x - x_0)}{h} \right) = \frac{d}{du} f(x) \times \frac{1}{h}$$

$$\Rightarrow \frac{d}{dx} f(x) = \frac{1}{h} \left[\Delta y_0 + \frac{2u-1}{2!} [\Delta^2 y_0] + \frac{3u^2-6u+2}{3!} [\Delta^3 y_0] + \frac{4u^3-18u^2+22u-6}{24} [\Delta^4 y_0] + \dots \right]$$

When $x = x_0$, we get $u=0$. Thus,

$$\frac{d}{dx} f(x) = \frac{1}{h} \left[\Delta y_0 - \frac{1}{2} \Delta^2 y_0 + \frac{2}{6} \Delta^3 y_0 - \frac{6}{24} \Delta^4 y_0 + \dots \right]$$

The second derivative of $f(x)$ is

$$\begin{aligned} \frac{d^2}{dx^2} f(x) &= \frac{d}{du} \left(\frac{d}{dx} f(x) \right) \times \frac{du}{dx} \\ &= \frac{d}{du} \left(\frac{1}{h} \left[\Delta y_0 + \frac{2u-1}{2!} [\Delta^2 y_0] + \frac{3u^2-6u+2}{3!} [\Delta^3 y_0] + \frac{4u^3-18u^2+22u-6}{24} [\Delta^4 y_0] + \dots \right] \right) \times \frac{1}{h} \\ &= \frac{1}{h^2} \left[\frac{2}{2!} [\Delta^2 y_0] + \frac{6u-6}{3!} [\Delta^3 y_0] + \frac{12u^2-36u+22}{24} [\Delta^4 y_0] + \dots \right] \\ &= \frac{1}{h^2} \left[\Delta^2 y_0 + (u-1) [\Delta^3 y_0] + \frac{6u^2-18u+11}{12} [\Delta^4 y_0] + \dots \right] \end{aligned}$$

In similar way,

$$\frac{d^3}{dx^3} f(x) = \frac{d}{du} \left[\frac{d^2}{dx^2} f(x) \right] \times \frac{du}{dx} = \frac{1}{h^3} \left[\Delta^3 y_0 + \frac{12u-18}{12} [\Delta^4 y_0] + \dots \right]$$

When $x = x_0$, and $u = 0$, we have

$$\frac{d^2}{dx^2} f(x) = \frac{1}{h^2} \left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \dots \right] \quad \text{and}$$

$$\frac{d^3}{dx^3} f(x) = \frac{1}{h^3} \left[\Delta^3 y_0 - \frac{3}{2} \Delta^4 y_0 + \dots \right]$$

• Derivative using Newton's Backward difference Formula

To find the derivative at a point near to the end of the tabular values, Newton's backward difference Formula is used. For the equidistant arguments, Newton's backward difference Formula is,

$$\begin{aligned} f(x) = f(x_n + uh) &= y_n + u [\nabla y_n] + \frac{u(u+1)}{2!} [\nabla^2 y_n] \\ &\quad + \frac{u(u+1)(u+2)}{3!} [\nabla^3 y_n] + \dots + \frac{u(u+1)(u+2)\dots(u+n-1)}{n!} [\nabla^n y_n] \end{aligned}$$

where $u = \frac{x - x_n}{h}$

$$\begin{aligned}\frac{d}{dx} f(x) &= \frac{d}{du} f(x) \times \frac{du}{dx} \\ &= \frac{d}{du} f(x) \times \frac{d}{dx} \left(\frac{(x - x_n)}{h} \right) = \frac{d}{du} f(x) \times \frac{1}{h}\end{aligned}$$

$$\Rightarrow \frac{d}{dx} f(x) = \frac{1}{h} \left[\nabla y_n + \frac{2u+1}{2!} [\nabla^2 y_n] + \frac{3u^2+6u+2}{3!} [\nabla^3 y_n] + \frac{4u^3+18u^2+22u+6}{24} [\nabla^4 y_n] + \dots \right]$$

$$\frac{d^2}{dx^2} f(x) = \frac{d}{du} \left[\frac{d}{dx} f(x) \right] \times \frac{du}{dx} = \frac{1}{h^2} \left[\nabla^2 y_n + (u+1) [\nabla^3 y_n] + \frac{6u^2+18u+11}{12} [\nabla^4 y_n] + \dots \right], \text{ and}$$

$$\frac{d^3}{dx^3} f(x) = \frac{d}{du} \left[\frac{d^2}{dx^2} f(x) \right] \times \frac{du}{dx} = \frac{1}{h^3} \left[\nabla^3 y_n + \frac{12u+18}{12} \nabla^4 y_n + \dots \right]$$

At $x = x_n$, $u = 0$. The above gives,

$$\frac{d}{dx} f(x) = \frac{1}{h} \left[\nabla y_n + \frac{1}{2} \nabla^2 y_n + \frac{1}{3} \nabla^3 y_n + \frac{1}{4} \nabla^4 y_n + \dots \right]$$

$$\frac{d^2}{dx^2} f(x) = \frac{1}{h^2} \left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12} \nabla^4 y_n + \dots \right] \text{ and}$$

$$\frac{d^3}{dx^3} f(x) = \frac{1}{h^3} \left[\nabla^3 y_n + \frac{3}{2} \nabla^4 y_n + \dots \right].$$

Problem: Compute $f''(0)$ and $f'(0.2)$ from the following tabular data.

x	0.0	0.2	0.4	0.6	0.8	1.0
$f(x)$	1.00	1.16	3.56	13.96	41.96	101.00

Solution:

Since $x = 0.0$ and 0.2 appear at and near beginning of the table, it is appropriate to use formulae based on forward differences to find the derivatives. The forward difference table for the given data is:

x	$y=f(x)$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
0.0	1.00					
0.2	1.16	0.16				
0.4	3.56	2.40	2.24	5.76		
0.6	13.96	10.40	8.00	9.60	3.84	
0.8	41.96	28.00	17.60	13.44	3.84	0.00
1.0	101.00	59.04	31.04			

Here $x_0 = 0$, and $h=0.2$. At $x=0$, $u = \frac{(x-x_0)}{h} = 0$,

The second derivative at $x=0$ is given by Newton's forward formula:

$$\frac{d^2}{dx^2} f(x) = \frac{1}{h^2} \left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \dots \right]$$

$$f''(0) = \frac{1}{(0.2)^2} \left[2.24 - 5.76 + \frac{11}{24} (3.84) - \frac{5}{6} (0) \right] = 0.$$

For $x=0.2$, $u = \frac{(0.2-0.0)}{0.2} = 1$.

By Newton's forward formula, we have the derivative of $f(x)$ at a point x is,

$$\frac{d}{dx} f(x) = \frac{1}{h} \left[\Delta y_0 + \frac{2u-1}{2!} [\Delta^2 y_0] + \frac{3u^2-6u+2}{3!} [\Delta^3 y_0] + \frac{4u^3-18u^2+22u-6}{24} [\Delta^4 y_0] + \dots \right]$$

Hence,

$$\left. \frac{d}{dx} f(x) \right|_{x=0.2} = \frac{1}{0.2} \left[0.16 + \frac{2 \times 1 - 1}{2!} [2.24] + \frac{3 \times 1^2 - 6 \times 1 + 2}{3!} [5.76] + \frac{4 \times 1^3 - 18 \times 1^2 + 22 \times 1 - 6}{24} [3.84] \right]$$

= 3.2, on simplification.

If the arguments are not equidistant, the approximating polynomial for the given tabular points is found by Newton's divided difference formula or Lagrange's interpolation formula. Then the derivative of the function can get at any x in the range.

For example: We find the first derivative of a function at 0, using the points $(-4,1245)$, $(-1,33)$, $(0,5)$, $(2,9)$ and $(5,1335)$ where x values are not equidistant. We can get the approximating polynomial by Newton's divided difference formula.

The table of divided differences is,

x	y	First divided differences	Second divided differences	Third divided differences	Fourth divided differences
-4	1245				
-1	33	-404			
0	5	-28	94		
2	9	2		-14	
5	1335	442	10		3
			88	13	

Given $f(x_0) = 1245$. From the table, we can observe that

$$\begin{aligned} f(x_0, x_1) &= -404; \quad f(x_0, x_1, x_2) = 94; \\ f(x_0, x_1, x_2, x_3) &= -14 \quad \text{and} \quad f(x_0, x_1, x_2, x_3, x_4) = 3 \end{aligned}$$

Hence the interpolating polynomial is

$$\begin{aligned} f(x) &= 1245 + (x - (-4)) \times (-404) + (x - (-4))(x - (-1)) \times 94 \\ &\quad + (x - (-4))(x - (-1))(x - 0) \times (-14) + (x - (-4))(x - (-1))(x - 0)(x - 2) \times 3 \end{aligned}$$

On simplification, we get

$$f(x) = 3x^4 - 5x^3 + 6x^2 - 14x + 5.$$

Then,

$$f'(x) = 12x^3 - 15x^2 + 12x - 14$$

Hence,

$$f'(0) = -14.$$

Exercises

1. From the following table of values, estimate $f'''(1.10)$ and $f''(1.10)$:

x	1.00	1.05	1.10	1.15	1.20	1.25	1.30
$f(x)$	1.0000	1.0247	1.0488	1.0724	1.0954	1.1180	1.1402

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

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

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

t	0.0	0.1	0.2	0.3	0.4	0.5	0.6
x	3.013	3.162	3.287	3.364	3.395	3.381	3.324

Use both the forward difference formula and the central difference formula to find the velocity and compare the results.

4. Using the values in the table, estimate $y''(1.3)$:

x	1.3	1.5	1.7	1.9	2.1	2.3
y	2.9648	2.6599	2.3333	1.9922	1.6442	1.2969

10

NUMERICAL INTEGRATION

THE TRAPEZOIDAL RULE

In this method to evaluate $\int_a^b f(x)dx$, we partition the interval of integration $[a, b]$ and replace f by a straight line segment on each subinterval. The vertical lines from the ends of the segments to the partition points create a collection of trapezoids that approximate the region between the curve and the x -axis. We add the areas of the trapezoids counting area above the x -axis as positive and area below the axis as negative and denote the sum by T . Then

$$\begin{aligned} T &= \frac{1}{2}(y_0 + y_1)h + \frac{1}{2}(y_1 + y_2)h + \cdots + \frac{1}{2}(y_{n-2} + y_{n-1})h + \frac{1}{2}(y_{n-1} + y_n)h \\ &= h \left(\frac{1}{2}y_0 + y_1 + y_2 + \cdots + y_{n-1} + \frac{1}{2}y_n \right) \\ &= \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n) \end{aligned}$$

where

$$y_0 = f(a), \quad y_1 = f(x_1), \quad \dots, \quad y_{n-1} = f(x_{n-1}), \quad y_n = f(b).$$

The Trapezoidal Rule

To approximate $\int_a^b f(x)dx$,

$$\text{(for } n \text{ subintervals of length } h = \frac{b-a}{n} \text{ and } y_j = f(x_j)).$$

use

$$T = \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n)$$

or

$$T = \frac{h}{2}[y_0 + y_n + 2(y_1 + y_2 + \cdots + y_{n-1})]$$

Example Use the trapezoidal rule with $n = 4$ to estimate

$$\int_1^2 x^2 dx.$$

Compare the estimate with the exact value of the integral.

To find the trapezoidal approximation, we divide the interval of integration into four subintervals of equal length and list the values of $y=x^2$ at the endpoints and partition points.

j	x_j	$y_j = x_j^2$	
0	1.0	1.0000	
1	1.25		1.5625
2	1.50		2.2500
3	1.75		3.0625
4	2.00	4.0000	
	Sum	5.0000	6.8750

With $n = 4$ and $h = \frac{b-a}{n} = \frac{2-1}{4} = \frac{1}{4}$:

$$\begin{aligned}
 T &= \frac{h}{2} [y_0 + y_4 + 2(y_1 + y_2 + y_3)] \\
 &= \frac{1}{8} [1.4 + 2(6.875)] \\
 &= 2.34375
 \end{aligned}$$

The exact value of the integral is

$$\int_1^2 x^2 dx = \left[\frac{x^3}{3} \right]_1^2 = \frac{8}{3} - \frac{1}{3} = \frac{7}{3} = 2.33334$$

The approximation is a slight overestimate. Each trapezoid contains slightly more than the corresponding strip under the curve.

Problem: Using Trapezoidal rule solve the integral, $\int_0^1 \frac{1}{x^2 + 6x + 10} dx$ with four subintervals.

Solution:

For n subintervals, the trapezoidal rule for the integral of a function in the range $[a,b]$ is,

$$\int_a^b f(x) dx = \frac{h}{2} [y_0 + 2y_1 + 2y_2 + \dots + 2y_{n-1} + y_n]$$

Here to consider $n=4$.

Now,
$$\int_a^b f(x)dx = \frac{h}{2}[y_0 + 2y_1 + 2y_2 + 2y_3 + y_4]$$

In our integral, $\int_0^1 \frac{1}{x^2 + 6x + 10} dx$, the range of integral $[0,1]$ is divided into four equal subinterval of width $h=0.25$, by the points, 0.0,0.25,0.50,0.75 and 1 .

Considering them as the x values, corresponding values of the integrand $\frac{1}{x^2 + 6x + 10}$ denoted by y_0, y_1, y_2, y_3, y_4 are 0.10, 0.08649, 0.07547, 0.06639 and 0.05882 respectively.

Hence,

$$\begin{aligned} \int_0^1 \frac{1}{x^2 + 6x + 10} dx &= \frac{0.25}{2}[0.10 + 2 \times 0.08649 + 2 \times 0.07547 + 2 \times 0.06639 + 0.05882] \\ &= 0.07694. \end{aligned}$$

Example Use the trapezoidal rule with $n=4$ to estimate

$$\int_1^2 \frac{1}{x} dx.$$

Compare the estimate with the exact value of the integral.

To find the trapezoidal approximation, we divide the interval of integration into four subintervals of equal length and list the values (correct to five decimal places) of $y = \frac{1}{x}$ at the endpoints and partition points.

j	x_j	$y_j = \frac{1}{x_j}$	
0	1.0	1.00000	
1	1.25		0.80000
2	1.50		0.66667
3	1.75		0.57143
4	2.00	0.50000	
	Sum	1.50000	2.0381

With $n=4$ and $h = \frac{b-a}{n} = \frac{2-1}{4} = \frac{1}{4} = 0.25$:

$$T = \frac{h}{2}[y_0 + y_4 + 2(y_1 + y_2 + y_3)]$$

$$= \frac{1}{8}[1.5 + 2(2.0381)] = 0.69702.$$

The exact value of the integral is

$$\int_1^2 \frac{1}{x} dx = \ln x \Big|_1^2 = \ln 2 - \ln 1 = 0.69315$$

The approximation is a slight overestimate.

Example Evaluate $\int_0^1 e^{-x^2} dx$ by means of Trapezoidal rule with $n=10$.

Here $h = \frac{b-a}{n} = \frac{1-0}{10} = 0.1$ and

$$\int_0^1 e^{-x^2} dx \approx T = \frac{0.1}{2}[y_0 + y_{10} + 2(y_1 + y_2 + \dots + y_9)]$$

j	x_j	x_j^2	$f(x_j) = e^{-x_j^2}$	
0	0.0	0.00	1.000 000	0.990 050
1	0.1	0.01		0.960 789
2	0.2	0.04		0.913 931
3	0.3	0.09		0.852 144
4	0.4	0.16		0.778 801
5	0.5	0.25		0.697 676
6	0.6	0.36		0.612 626
7	0.7	0.49		0.612 626
8	0.8	0.64		0.527 292
9	0.9	0.81		0.444 858
10	1.0	1.00	0.367 879	
Sums			1.367 879	6.778 167

Hence $\int_0^1 e^{-x^2} dx \approx T = \frac{0.1}{2}[1.367879 + 2(6.778167)] = 0.746211$

SIMPSON'S 1/3 RULE

Simpson's rule for approximating $\int_a^b f(x)dx$ is based on approximating f with quadratic polynomials instead of linear polynomials. We approximate the graph with parabolic arcs instead of line segments.

The integral of the quadratic polynomial $y = Ax^2 + Bx + C$ in Fig.3 from $x = -h$ to $x = h$ is

$$\int_{-h}^h (Ax^2 + Bx + C) dx = \frac{h}{3}(y_0 + 4y_1 + y_2)$$

Simpson's rule follows from partitioning $[a, b]$ into an even number of subintervals of equal length h , applying Eq. to successive interval pairs, and adding the results.

Algorithm: Simpson's 1/3 Rule

To approximate $\int_a^b f(x)dx$, use

$$S = \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + \dots + 2y_{n-2} + 4y_{n-1} + y_n).$$

The y 's are the values of f at this partition points

$$x_0 = a, x_1 = a+h, x_2 = a+2h, \dots, x_{n-1} = a+(n-1)h, x_n = b$$

The number n is **even**, $h = \frac{b-a}{n}$ and $y_j = f(x_j)$.

Simpson's 1/3 Rule given by (5) can be simplified as below:

$$S = \frac{h}{3}(s_0 + 4s_1 + 2s_2), \quad \dots(5A)$$

where $s_0 = y_0 + y_n$, $s_1 = y_1 + y_3 + \dots + y_{n-1}$, $s_2 = y_2 + y_4 + \dots + y_{n-2}$.

Example Find an approximate value of $\log_e 5$ by calculating $\int_0^5 \frac{dx}{4x+5}$, by Simpson's 1/3 rule of integration.

We note that

$$\int_0^5 \frac{dx}{4x+5} = \left[\frac{1}{4} \log(4x+5) \right]_0^5 = \frac{1}{4} [\log 25 - \log 5] = \frac{1}{4} \log \frac{25}{5} = \frac{1}{4} \log 5.$$

Now to calculate the value of $\int_0^5 \frac{dx}{4x+5}$, by Simpson's rule of integration, divide the interval $[0, 5]$ into $n = 10$ equal subintervals, each of length $h = \frac{b-a}{n} = \frac{5-0}{10} = 0.5$.

j	x_j	$4x_j+5$	$f_j = f(x_j) = \frac{1}{4x_j+5}$		
0	0.0	5	0.20		
1	0.5	7		0.1429	
2	1.0	9			0.1111
3	1.5	11		0.0909	
4	2.0	13			0.0769
5	2.5	15		0.6666	
6	3.0	17			0.0588
7	3.5	19		0.0526	
8	4.0	21			0.0476
9	4.5	23		0.0434	
10	5.0	25	0.04		
Sums			$s_0=0.24$	$s_1=0.3963$	$s_2=0.2944$

Hence,

$$\int_0^5 \frac{dx}{4x+5} \approx S = \frac{0.5}{3} [0.24 + 4(0.3963) + 2(0.2944)] = 0.4023.$$

and $\log_e 5 = 4(0.4023) = 1.6092.$

Problem: Find $\int_0^{10} \frac{1}{1+x^2} dx$ using Simpson's one third rule.

Solution:

By Simpson's one third rule, $\int_a^b f(x)dx = \frac{h}{3} [y_0 + 4(y_1 + y_3 + \dots) + 2(y_2 + y_4 + \dots) + y_n]$

In our integral, $\int_0^{10} \frac{1}{1+x^2} dx$, let the range $[0,10]$ is subdivided into 10 equal interval of width $h=1$, by the x values 0,1,2,3,4,5,6,7,8,9 and 10. Corresponding y values of the function $\frac{1}{1+x^2}$ are listed below:

x	0	1	2	3	4	5	6	7	8	9	10
y	1	0.5	0.2	0.1	0.0588	0.0385	0.0270	0.02	0.0154	0.0122	0.0099

Thus,

$$\begin{aligned}
 \int_0^{10} \frac{1}{1+x^2} dx &= \frac{1}{3} [1 + 4(0.5 + 0.1 + 0.0385 + 0.02 + 0.0122) + 2(0.2 + 0.0588 + 0.027 + 0.0154) + 0.0099] \\
 &= \frac{1}{3} [1.0099 + 4(0.6707) + 2(0.3012)] \\
 &= \frac{1}{3} [4.2951] = 1.4317.
 \end{aligned}$$

Problem: Evaluate $\int_0^6 \frac{1}{3+x^2} dx$ using Simpson's three eight rule.

Solution:

By Simpson's three eight rule,

$$\int_a^b f(x) dx = \frac{3h}{8} [y_0 + 3(y_1 + y_2 + y_4 + \dots + y_{n-1}) + 2(y_3 + y_6 + y_9 + \dots) + y_n]$$

Let the limit of integral $[0,6]$ be divided into six equal parts with interval $h=1$, using the x values 0,1,2,3,4,5 and 6. Corresponding y values of the given integrand function $\frac{1}{3+x^2}$ are,

x	0	1	2	3	4	5	6
y	0.333	0.25	0.1429	0.1	0.0526	0.0357	0.0256

Thus,

$$\int_0^6 \frac{1}{3+x^2} dx = \frac{3 \times 1}{8} [y_0 + 3(y_1 + y_2 + y_4 + \dots + y_{n-1}) + 2(y_3 + y_6 + y_9 + \dots) + y_n]$$

For $n=6$,

$$\int_0^6 \frac{1}{3+x^2} dx = \frac{3 \times 1}{8} [y_0 + 3(y_1 + y_2 + y_4 + y_5) + 2y_3 + y_6]$$

$$\int_0^6 \frac{1}{3+x^2} dx = \frac{3 \times 1}{8} [0.333 + 3(0.25 + 0.1429 + 0.0526 + 0.0357) + 2(0.1) + 0.0256]$$

$$= \frac{3}{8} [0.333 + 1.4436 + 0.2 + 0.0256] = \frac{3}{8} [2.0022]$$

$$\Rightarrow \int_0^6 \frac{1}{3+x^2} dx = 0.7508.$$

Example Find an approximation value of $\int_0^1 x^2 dx$ by Simpson's 1/3 rule with $n = 10$.

Here $h = \frac{b-a}{n} = \frac{1-0}{10} = 0.1$

j	x_j	$y_j = f(x_j) = x_j^2$		
0	0.0	0.00		
1	0.1		0.01	
2	0.2			0.04
3	0.3		0.09	
4	0.4			0.16
5	0.5		0.25	
6	0.6			0.36
7	0.7		0.49	
8	0.8			0.64
9	0.9		0.81	
10	1.0	1.00		
Sums		$s_0=1.00$	$s_1=1.65$	$s_2=1.20$

Hence ,

$$\int_0^1 x^2 dx \approx S = \frac{0.1}{3} [1.00 + 4(1.65) + 2(1.20)] = 0.3333.$$

Also, the exact value is given by

$$\int_0^1 x^2 dx = \left[\frac{x^3}{3} \right]_0^1 = \frac{1-0}{3} = 0.3333.$$

Example 11 A town wants to drain and fill a small-polluted swamp (See the adjacent figure). The swamp averages 5 ft deep. About how many cubic yards of dirt will it take to fill the area after the swamp is drained?

Solution To calculate the volume of the swamp, we estimate the surface area and multiply by 5. To estimate the area, we use Simpson's rule with $h=20$ ft and the y 's equal to the distances measured across the swamp, as shown in the adjacent figure.

$$S = \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + 4y_5 + y_6)$$

$$= \frac{20}{3}(146 + 488 + 152 + 216 + 80 + 120 + 13) = 8100$$

The volume is about $(8100)(5) = 40,500 \text{ ft}^3$ or 1500 yd^3 .

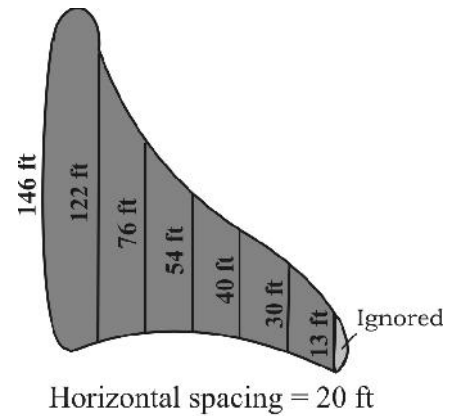


Fig.4

Example Compute the integral $I = \sqrt{\frac{2}{\pi}} \int_0^1 e^{-x^2/2} dx$ using Simpson's 1/3 rule, taking $h = 0.125$.

j	x_j	$f_j = f(x_j) = \sqrt{\frac{2}{\pi}} e^{-x_j^2/2}$		
0	0.000	0.7979		
1	0.125		0.7917	
2	0.250			0.7733
3	0.375		0.7437	
4	0.500			0.7041
5	0.625		0.6563	
6	0.750			0.6023
7	0.875		0.5441	
8	1.000	0.4839		
Sums		$s_0=1.2818$	$s_1=2.7358$	$s_2=2.0797$

Hence $I = \sqrt{\frac{2}{\pi}} \int_0^1 e^{-x^2/2} dx \approx S = \frac{0.125}{3} [1.2818 + 4(2.7358) + 2(2.0797)]$

$$= 0.6827$$

Derivation of Trapezoidal and Simpson's 1/3 rules of integration from Lagrangian Interpolation

Integrating the formula in Lagrangian interpolation, we obtain

$$\int_a^b f(x) dx \approx \int_a^b L_n(x) dx = \sum_{k=0}^n \frac{f_k}{l_k(x_k)} \int_a^b l_k(x) dx$$

For $n = 1$, we have only one interval $[x_0, x_1]$ such that $a = x_0$ and $b = x_1$ and then the above integration formula gives trapezoidal rule.

For $n = 2$, we have two subintervals $[x_0, x_1]$ and $[x_1, x_2]$ of equal width h such that $a = x_0$ and $b = x_2$ and then the above integration formula becomes

$$\int_a^b f(x) dx = \int_{x_0}^{x_2} f(x) dx \approx \frac{h}{3} (f_0 + 4f_1 + f_2),$$

and is the Simpson's 1/3 rule of integration.

For $n = 3$ the above integration formula (4) becomes

$$\int_a^b f(x) dx = \int_{x_0}^{x_3} f(x) dx \approx \frac{3h}{8} (f_0 + 3f_1 + 3f_2 + f_3),$$

and is known as Simpson's 3/8 rule of integration.

Simpson's three eight (3/8) rule

When $n=3$, all the differences of order four or higher becomes zero.

Hence,

$$\begin{aligned} \int_{x_0}^{x_3=x_0+3h} f(x) dx &= h \left[3 \times y_0 + \frac{3^2}{2} [\Delta y_0] + \frac{1}{2} \left[\frac{3^3}{3} - \frac{3^2}{2} \right] \Delta^2 y_0 + \frac{1}{6} \left[\frac{3^4}{4} - 3^3 + 3^2 \right] \Delta^3 y_0 + 0 \right] \\ &= h \left[3y_0 + \frac{9}{2} [y_1 - y_0] + \frac{1}{2} \left[\frac{27}{3} - \frac{9}{2} \right] [y_2 - 2y_1 + y_0] + \frac{1}{6} \left[\frac{81}{4} - 27 + 9 \right] [y_3 - 3y_2 + 3y_1 - y_0] \right] \\ &= \frac{h}{24} [72y_0 + 108[y_1 - y_0] + 54[y_2 - 2y_1 + y_0] + 9[y_3 - 3y_2 + 3y_1 - y_0]] \\ &= \frac{h}{24} [9y_0 + 27y_1 + 27y_2 + 9y_3] \\ \Rightarrow \int_{x_0}^{x_3=x_0+3h} f(x) dx &= \frac{3h}{8} [y_0 + 3y_1 + 3y_2 + y_3] \end{aligned}$$

Similarly,
$$\int_{x_3}^{x_6=x_0+6h} f(x) dx = \frac{3h}{8} [y_3 + 3y_4 + 3y_5 + y_6]$$

Finally, under the assumption that n is a multiple of three,

$$\int_{x_{n-3}}^{x_n=x_0+nh} f(x)dx = \frac{3h}{8} [y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n]$$

Adding these integrals, we get,

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

That is,

$$\int_a^b f(x)dx = \frac{3h}{8} [(y_0 + 3y_1 + 3y_2 + y_3) + (y_3 + 3y_4 + 3y_5 + y_6) + \dots + (y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n)]$$

$$\int_a^b f(x)dx = \frac{3h}{8} [y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + 3y_7 + \dots + 3y_{n-1} + y_n]$$

$$\Rightarrow \int_a^b f(x)dx = \frac{3h}{8} [y_0 + 3(y_1 + y_2 + y_4 + \dots + y_{n-1}) + 2(y_3 + y_6 + y_9 + \dots) + y_n]$$

Exercises

Estimate the integral using

(a) trapezoidal rule and (b) Simpson's 1/3 rule.

1. $\int_1^2 \frac{1}{s^2} ds$

2. $\int_0^f \sin t \, dt$

3. $\int_0^2 x^3 dx$

4. $\int_1^2 x \, dx$

5. $\int_{-1}^1 (x^2 + 1) dx$

6. $\int_0^{-2} (t^3 + t) dt$

7. $\int_0^1 \frac{\sin x}{x} dx$

8. $\int_0^1 \frac{1}{1+x} dx$

9. $\int_0^6 \frac{1}{1+x^2} dx$

10. $\ln 2 = \int_0^1 \frac{dx}{x}$

11. $\int_1^7 \frac{1}{x} dx$

12. $\int_1^3 (2x - 1) dx$

13. $\int_0^1 x\sqrt{1-x^2} dx$

x	$x\sqrt{1-x^2}$
0	0.0
0.125	0.12402
0.25	0.24206
0.375	0.34763
0.5	0.43301
0.625	0.48789
0.75	0.49608
0.875	0.42361
1.0	0

14. $\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{3\cos u}{(2+\sin u)^2} du$

u	$\frac{3\cos u}{(2+\sin u)^2}$
-1.57080	0.0
-1.17810	0.99138
-0.78540	1.26906
-0.39270	1.05961
0	0.75
0.39270	0.48821
0.78540	0.28946
1.17810	0.13429
1.57080	0

15. $\int_{-2}^0 (x^2 - 1) dx$ 16. $\int_{-1}^1 (t^3 + 1) dt$ 17. $\int_2^4 \frac{1}{(s-1)^2} ds$

18. $\int_0^1 \sin f t dt$

19. The following table gives values of x and $f(x)$. Find the area bounded by the curve $y = f(x)$, the x -axis and the ordinates $x = 7.47$ and 7.52 .

x	7.47	7.48	7.49	7.50	7.51	7.52
$F(x)$	1.93	1.95	1.98	2.01	2.03	2.06

20. Find the approximate value of $\int_{1.2}^{1.6} e^{-x^2} dx$ from the following table:

x	1.2	1.3	1.4	1.5	1.6
$f(x) = e^{-x^2}$	0.237	0.185	0.141	0.106	0.077

21. Estimate the errors in the results obtained by evaluating the integral $\int_0^1 \frac{dx}{1+x}$ by trapezoidal and Simpson's rule.

11

SOLUTION OF SYSTEMS OF LINEAR EQUATIONS

Solution of system of linear equations

A system of m linear equations in n unknowns x_1, x_2, \dots, x_n is a set of equations of the form

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n &= b_2 \\ &\dots\dots\dots \\ a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n &= b_m \end{aligned}$$

where the coefficients a_{jk} and the b_j are given numbers. The system is said to be **homogeneous** if all the b_j are zero; otherwise, it is said to be **non-homogeneous**.

The system of linear equations is equivalent to the matrix equation (or the single vector equation)

$$Ax = b$$

where the **coefficient matrix** $A = [a_{ij}]$ is the $m \times n$ matrix and \mathbf{x} and \mathbf{b} are the column matrices (vectors) given by:

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \dots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

A **solution** of the system is a set of numbers x_1, x_2, \dots, x_n which satisfy all the m equations, and a **solution vector** of (1) is a column matrix whose components constitute a solution of system. The method of solving such a system using methods like Cramer's rule is impracticable for large systems. Hence, we use other methods like Gauss elimination.

Gauss Elimination Method

In the Gauss elimination method, the solution to the system of equations is obtained in two stages. In the first stage, the given system of equations is reduced to an equivalent upper triangular form using elementary transformations. In the second stage, the upper triangular system is solved using back substitution procedure by which we obtain the solution in the order $x_n, x_{n-1}, x_{n-2}, \dots, x_2, x_1$.

Example Solve the system

$$2x_1 + x_2 + 2x_3 + x_4 = 6 \quad \dots(1)$$

$$6x_1 - 6x_2 + 6x_3 + 12x_4 = 36 \quad \dots(2)$$

$$4x_1 + 3x_2 + 3x_3 - 3x_4 = -1 \quad \dots(3)$$

$$2x_1 + 2x_2 - x_3 + x_4 = 10 \quad \dots(4)$$

To eliminate x_1 from equations (2), (3) and (4), we subtract suitable multiples of equation (1) and we get the following system of equations:

$$(2) - 3 \cdot (1) \rightarrow -9x_2 + 0x_3 + 9x_4 = 18 \quad \dots(5)$$

$$(3) - 2 \cdot (1) \rightarrow x_2 - x_3 - 5x_4 = -13 \quad \dots(6)$$

$$(4) - 1 \cdot (1) \rightarrow x_2 - 3x_3 + 0x_4 = 4 \quad \dots(7)$$

To eliminate x_2 from equations (6) and (7), subtract suitable multiples of equation (5) and get the following system of equations:

$$(6) - (-1/9)(5) \rightarrow -x_3 - 4x_4 = -11 \quad \dots(8)$$

$$(7) - (-1/9)(5) \rightarrow -3x_3 + x_4 = 6 \quad \dots(9)$$

To eliminate x_3 from equation (9), subtract $3 \times (8)$ and get the following equation:

$$13x_4 = 39 \quad \dots(10)$$

From equation (10), $x_4 = 39/13 = 3$; using this value of x_4 , (9) gives $x_3 = -1$; using these values of x_4 and x_3 , (7) gives $x_2 = 1$; using all these values (1) gives $x_1 = 2$. Hence the solution to the system is $x_1 = 2, x_2 = 1, x_3 = -1, x_4 = 3$.

Note: The above method can be simplified using the matrix notation. The given system of equations can be written as

$$Ax=b$$

and the augmented matrix is

$$\begin{bmatrix} 2 & 1 & 2 & 1 & 6 \\ 6 & -6 & 6 & 12 & 36 \\ 4 & 3 & 3 & -3 & -1 \\ 2 & 2 & -1 & 1 & 10 \end{bmatrix}$$

which on successive row transformations give

$$\begin{bmatrix} 2 & 1 & 2 & 1 & 6 \\ 0 & -9 & 0 & 9 & 18 \\ 0 & 0 & -1 & -4 & -11 \\ 0 & 0 & 0 & 13 & 39 \end{bmatrix}.$$

Hence

$$\begin{bmatrix} 2 & 1 & 2 & 1 \\ 0 & -9 & 0 & 9 \\ 0 & 0 & -1 & -4 \\ 0 & 0 & 0 & 13 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 6 \\ 18 \\ -11 \\ 39 \end{bmatrix}$$

Back substitution gives

$$x_1 = 2, \quad x_2 = 1, \quad x_3 = -1, \quad x_4 = 3$$

In the example, we had $a_{11} \neq 0$. Otherwise we would not have been able to eliminate x_1 by using the equations in the given order. Hence if $a_{11} \neq 0$ in the system of equations we have to reorder the equations (and perhaps even the unknowns in each equation) in a suitable fashion; similarly, in the further steps. Such a situation can be seen in the following Example.

Example Using Gauss elimination solve:

$$\begin{aligned} y + 3z &= 9 \\ 2x + 2y - z &= 8 \\ -x + 5z &= 8 \end{aligned}$$

Here the leading coefficient (i.e., coefficient of x) is 0. Hence to proceed further we have to interchange rows 1 and 2, so that

$$\begin{aligned} 2x + 2y - z &= 8 & \dots(1) \\ y + 3z &= 9 & \dots(2) \\ -x + 5z &= 8 & \dots(3) \end{aligned}$$

Elimination of x from last two equations:

$$\begin{aligned} 2x + 2y - z &= 8 \\ y + 3z &= 9 \\ (3) + \frac{1}{2} (1) \rightarrow y + \frac{9}{2} z &= 12 & \dots(4) \end{aligned}$$

Elimination of y from last equation:

$$\begin{aligned} 2x + 2y - z &= 8 \\ y + 3z &= 9 \end{aligned}$$

$$(4) - (2) \rightarrow \frac{3}{2} z = 3 \quad \dots(5)$$

Hence $z = 2, y = 9 - 6 = 3, x = 2.$

Hence

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 2 \end{bmatrix}.$$

Partial and Full Pivoting

In each step in the Gauss elimination method, the coefficient of the first unknown in the first equation is called **pivotal coefficient**. By the above Example, the Gauss elimination method fails if any one of the pivotal coefficients becomes zero. In such a situation, we rewrite the equations in a different order to avoid zero pivotal coefficient. Changing the order of equations is called **pivoting**.

In **partial pivoting**, if the pivotal coefficient a_{ii} happens to be zero or near to zero, the i^{th} column elements are searched for the numerically largest element. Let the j^{th} row ($j > i$) contains this element, then we interchange the i^{th} equation with the j^{th} equation and proceed for elimination. This process is continued whenever pivotal coefficients become zero during elimination.

In **total pivoting**, we look for an absolutely largest coefficient in the entire system and start the elimination with the corresponding variable, using this coefficient as the pivotal coefficient (for this we have to interchange *rows* and *columns*, if necessary); similarly in the further steps. Total pivoting, in fact, is more complicated than the partial pivoting. Partial pivoting is preferred for hand calculation.

Example Solve the system

$$0.0004x_1 + 1.402x_2 = 1.406 \quad \dots(1)$$

$$0.4003x_1 - 1.502x_2 = 2.501 \quad \dots(2)$$

by Gauss elimination (a) without pivoting (b) with partial pivoting.

(a) without pivoting (choosing the first equation as the pivotal equation)

$$0.0004x_1 + 1.402x_2 = 1.406 \quad \dots(1a)$$

$$(2) - \frac{0.40031}{0.0001} \times (1a) \rightarrow -1405x_2 = -1404 \quad \dots(2a)$$

and so
$$x_2 = \frac{1404}{1405} = 0.9993$$

and hence from (1a),

$$x_1 = \frac{1}{0.0004}(1.406 - 1.402 \times 0.9993) = \frac{0.005}{0.0004} = 12.5.$$

(b) (with partial pivoting)

Since $|a_{11}|$ is small and is nearer to zero as compared with $|a_{21}|$, we accept a_{21} as the pivotal coefficient (i.e. second equation becomes the pivotal equation). To start with we rearrange the given system as follows:

$$0.4003x_1 - 1.502x_2 = 2.501 \quad \dots(3)$$

$$0.0004x_1 + 1.402x_2 = 1.406 \quad \dots(4)$$

Now by Gauss elimination the system becomes,

$$0.4003x_1 - 1.502x_2 = 2.501 \quad \dots(3a)$$

$$(4) - \frac{.0004}{.4003} (3) \quad 1.404x_2 = 1.404 \quad \dots(4a)$$

and so
$$x_2 = \frac{1.404}{1.404} = 1$$

and from (3a)
$$x_1 = \frac{1}{0.4003}(2.501 + 1.502 \times 1) = 10.$$

Example Solve the following system (i) without pivoting (ii) with pivoting

$$0.0002x + 0.3003y = 0.1002 \quad \dots (1)$$

$$2.0000x + 3.0000y = 2.0000. \quad \dots (2)$$

(i) without pivoting

$$0.0002x + 0.3003y = 0.1002$$

$$(2) - \frac{2}{.0002} (1) \rightarrow \left(3.000 - \frac{0.3003 \times 2}{0.0002} \right) y = 2.0000 - \frac{0.1002 \times 2}{0.0002}$$

i.e.,
$$1498.5y = 499.$$

Now by back substitution, the solution to the system is given by $y = 0.3330$ and $x = 0.5005$;

(ii) With pivoting:

Since $|a_{11}|$ is small and is nearer to zero as compared with $|a_{21}|$, we accept a_{21} as the pivotal coefficient (i.e. second equation becomes the pivotal equation). To start with we rearrange the given system as follows:

$$2.0000x + 3.0000y = 2.0000 \quad \dots (3)$$

$$0.0002x + 0.3003y = 0.1002 \quad \dots (4)$$

$$(4) - \frac{.0002}{2}(3) \rightarrow \left(0.3003 - \frac{3.0000 \times 0.0002}{2}\right)y = 0.1002 - \frac{2 \times 0.0002}{2}$$

which simplifies to

$$0.3000y = 0.1000.$$

Hence by back substitution, the solution is

$$y = \frac{1}{3} \quad \text{and} \quad x = \frac{1}{2}.$$

Cholesky Method (Modification of the Gauss method)

Cholesky method, which is a modification of the Gauss method, is based on the result that any positive definite square matrix \mathbf{A} can be represented in the form $\mathbf{A} = \mathbf{LU}$, where \mathbf{L} and \mathbf{U} are the unique lower and upper triangular matrices. The method is illustrated through the following examples.

Example Using Cholesky's method, solve the system:

$$x_1 + 2x_2 + 3x_3 = 14$$

$$2x_1 + 3x_2 + 4x_3 = 20$$

$$3x_1 + 4x_2 + x_3 = 14$$

(LU decomposition of the coefficient matrix \mathbf{A})

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 1 \end{bmatrix} \quad \begin{array}{ll} R_2 \rightarrow R_2 + (-2)R_1 & m_{21} = -2 \\ R_3 \rightarrow R_3 + (-3)R_1 & m_{31} = -3 \end{array}$$

$$\sim \begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & -2 \\ 0 & -2 & -8 \end{bmatrix}$$

$$\sim \begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & -2 \\ 0 & 0 & -4 \end{bmatrix} \quad R_3 \rightarrow R_3 + (-2)R_2 \quad m_{32} = -3$$

We take $\mathbf{U} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & -2 \\ 0 & 0 & -4 \end{bmatrix}$ as the upper triangular matrix.

Using the multipliers $m_{21} = -2$, $m_{31} = -3$, $m_{32} = -2$, we get the lower triangular matrix as follows:

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ -m_{21} & 1 & 0 \\ -m_{31} & -m_{32} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 2 & 1 \end{bmatrix}.$$

(Solution of the system)

The given system of equations can be written as

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & -2 \\ 0 & 0 & -4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 14 \\ 20 \\ 14 \end{bmatrix} \quad \dots (1)$$

The above can be written as

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 14 \\ 20 \\ 14 \end{bmatrix} \quad \dots (2)$$

where

$$\begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & -2 \\ 0 & 0 & -4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \quad \dots (3)$$

Solving the system in (2) by forward substitution, we get

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 14 \\ -8 \\ -12 \end{bmatrix}$$

With these values of y_1, y_2, y_3 , Eq. (3) can now be solved by back substitution and we obtain

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

Example Solve the equations

$$2x + 3y + z = 9$$

$$x + 2y + 3z = 6$$

$$3x + y + 2z = 8$$

by LU decomposition.

(**LU** decomposition of the coefficient matrix **A**)

Proceeding as in the above example,

$$U = \begin{bmatrix} 2 & 3 & 1 \\ 0 & \frac{1}{2} & \frac{5}{2} \\ 0 & 0 & 18 \end{bmatrix} \text{ and } L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{3}{2} & -7 & 1 \end{bmatrix}$$

(Solution of the system)

The given system of equations can be written as

$$\begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/2 & -7 & 1 \end{bmatrix} \begin{bmatrix} 2 & 3 & 1 \\ 0 & 1/2 & 5/2 \\ 0 & 0 & 18 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 9 \\ 6 \\ 8 \end{bmatrix} \quad \dots \text{(iv)}$$

or, as
$$\begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/2 & -7 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 9 \\ 6 \\ 8 \end{bmatrix}, \quad \dots \text{(v)}$$

where
$$\begin{bmatrix} 2 & 3 & 1 \\ 0 & 1/2 & 5/2 \\ 0 & 0 & 18 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}. \quad \dots \text{(vi)}$$

Solving the system in (v) by forward substitution, we get

$$y_1 = 9, \quad y_2 = \frac{3}{2}, \quad y_3 = 5.$$

With these values of y_1, y_2, y_3 , eq. (vi) can now be solved by the back substitution process and we obtain

$$x = \frac{35}{18}, \quad y = \frac{29}{18}, \quad z = \frac{5}{18}.$$

Gauss Jordan Method

The method is based on the idea of reducing the given system of equations $\mathbf{Ax} = \mathbf{b}$, to a diagonal system of equations $\mathbf{Ix} = \mathbf{d}$, where \mathbf{I} is the identity matrix, using elementary row operations. We know that the solutions of both the systems are identical. This reduced system gives the solution vector \mathbf{x} . This reduction is equivalent to finding the solution as $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$.

In this case, a system of 3 equations in 3 unknowns

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 &= b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= b_3 \end{aligned}$$

is written as

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \quad \dots (*)$$

After some linear transformations, we obtain the 3×3 system as

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix} \quad \text{--- (**)}$$

To obtain the system as given in (**), first we augment the matrices given in (*) as,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \end{bmatrix} \text{ and after some elementary operations, it}$$

is written as,

$$\begin{bmatrix} 1 & 0 & 0 & d_1 \\ 0 & 1 & 0 & d_2 \\ 0 & 0 & 1 & d_3 \end{bmatrix} \text{--- (***)}, \text{ this helps us to write the given}$$

system as given in (**). Then it is easy to get the solution of the system as $x_1 = d_1, x_2 = d_2$ and $x_3 = d_3$.

Elimination procedure: The first step is same as in Gauss elimination method, which is, we make the elements below the first pivot in the augmented matrix as zeros, using the elementary row transformations. From the second step onwards, we make the elements below and above the pivots as zeros using the elementary row transformations. Lastly, we divide each row by its pivot so that the final matrix is of the form (***). Partial pivoting can also be used in the solution. We may also make the pivots as 1 before performing the elimination.

Problem: Solve the following system of equations

$$\begin{aligned} x_1 + x_2 + x_3 &= 1 \\ 4x_1 + 3x_2 - x_3 &= 6 \\ 3x_1 + 5x_2 + 3x_3 &= 4 \end{aligned}$$

using the Gauss-Jordan method without partial pivoting

Solution:

We have the matrix form as

$$\begin{bmatrix} 1 & 1 & 1 \\ 4 & 3 & -1 \\ 3 & 5 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 6 \\ 4 \end{bmatrix}. \text{ Then the augmented matrix is,}$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 4 & 3 & -1 & 6 \\ 3 & 5 & 3 & 4 \end{bmatrix}$$

(i) To do the eliminations follow the operations,

$R2 = R2 - 4R1$, and $R3 = R3 - 3R1$. This gives,

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & -1 & -5 & 2 \\ 0 & 2 & 0 & 1 \end{bmatrix}$$

Then, $R1 = R1 + R2$ and $R3 = R3 + 2R2$ gives,

$$\begin{bmatrix} 1 & 0 & -4 & 3 \\ 0 & -1 & -5 & 2 \\ 0 & 0 & -10 & 5 \end{bmatrix}$$

$R1 = R1 - (4/10) R3$, $R2 = R2 - (5/10) R3$ gives,

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & -1 & 0 & -\frac{1}{2} \\ 0 & 0 & -10 & 5 \end{bmatrix}$$

Now, making the pivots as 1, $R2 = (-R2)$ and $R3 = (R3/(-10))$, we get

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & -\frac{1}{2} \end{bmatrix}$$

Hence,
$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ \frac{1}{2} \\ -\frac{1}{2} \end{bmatrix}$$

Therefore, the solution of the system is,

$$x_1 = 1, x_2 = \frac{1}{2}, x_3 = -\frac{1}{2}.$$

Note: The Gauss-Jordan method looks very elegant as the solution is obtained directly. However, it is computationally more expensive than Gauss elimination. For large n , the total number of divisions and multiplications for Gauss-Jordan method is almost 1.5 times the total number of divisions and multiplications required for Gauss elimination. Hence, we do not normally use this method for the solution of the system of equations.

The most important application of this method is to find the inverse of a non-singular matrix. To obtain inverse of a matrix, we start with the augmented matrix of A with the identity matrix I of the same order.

When the Gauss-Jordan procedure is completed, we obtain, the matrix A augmented with I , $[A|I]$ in the form $[I|A^{-1}]$, since $AA^{-1} = I$.

Example Using Gauss Jordan method solve the system of equations:

$$x + 2y + z = 8 \quad \dots (1)$$

$$2x + 3y + 4z = 20 \quad \dots (2)$$

$$4x + 3y + 2z = 16 \quad \dots (3)$$

[Elimination of x from Eqs. (2) and (3), using (1)]

$$x + 2y + z = 8 \quad \dots (1a)$$

$$-y + 2z = 4 \quad \dots (2a)$$

$$-5y + 2z = -16 \quad \dots (3a)$$

[Elimination of y from (1a) and (3a), using (2a)]

$$x + 5z = 16 \quad \dots (1b)$$

$$-y + 2z = 4 \quad \dots (2b)$$

$$-12z = -36 \quad \dots (3b)$$

[Elimination of z from (1b) and (2b), using (3b)]

$$x = 1 \quad \dots (1c)$$

$$-y = -2 \quad \dots (2c)$$

$$-12z = -36 \quad \dots (3c)$$

Hence, $x = 1, y = 2, z = 3$.

Assignments

1. Apply Gauss elimination method to solve the equations:

$$2x + 3y - z = 5$$

$$4x + 4y - 3z = 3$$

$$-2x + 3y - z = 1$$

2. Apply Gauss elimination method to solve the equations:

$$3x_1 + 6x_2 + x_3 = 16$$

$$2x_1 + 4x_2 + 3x_3 = 13$$

$$x_1 + 3x_2 + 2x_3 = 9$$

3. Apply Gauss elimination method to solve the equations:

$$10x + 2y + z = 9$$

$$2x + 20y - 2z = -44$$

$$-2x + 3y + 10z = 22$$

4. Apply Gauss elimination method to solve the equations:

$$x + y + z = 10$$

$$2x + y + 2z = 17$$

$$3x + 2y + z = 17$$

5. Solve the system, using Gauss elimination method:

$$5x_1 + x_2 + x_3 + x_4 = 4$$

$$x_1 + 7x_2 + x_3 + x_4 = 12$$

$$x_1 + x_2 + 6x_3 + x_4 = -5$$

$$x_1 + x_2 + x_3 + 4x_4 = -6$$

6. Apply Gauss elimination method to solve the equations:

$$x + 4y - z = -5$$

$$x + y - 6z = -12$$

$$3x + y - z = 4$$

7. Solve the following system, using Cholesky method

$$10x + y + z = 12$$

$$2x + 10y + z = 13$$

$$2x + 2y - 10z = 14$$

8. Solve the following system, using Cholesky method

$$2x + 3y - z = 5$$

$$4x + 4y - 3z = 3$$

$$-2x + 3y - z = 1$$

9. Solve the following system, using Cholesky method

$$2x + 3y + z = 9$$

$$x + 2y + 3z = 6$$

$$3x + y + 2z = 8$$

10. Solve the following using Cholesky method:

$$\begin{bmatrix} 3 & 1 & 1 \\ 1 & 2 & 2 \\ 2 & 1 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 3 \\ 4 \end{bmatrix}.$$

11. Find the inverse of the following matrix using Cholesky method:

$$\begin{bmatrix} 1 & -1 & 1 \\ 1 & -2 & 4 \\ 1 & 2 & 2 \end{bmatrix}.$$

12. Solve the following system using Gauss Jordan method:

$$2x - 3y + z = -1$$

$$x + 4y + 5z = 25$$

$$3x - 4y + z = 2$$

13. Solve the following system using Gauss Jordan method:

$$2x - 3y + 4z = 7$$

$$5x - 2y + 2z = 7$$

$$6x - 3y + 10z = 23$$

MATRIX INVERSION USING GAUSS ELIMINATION

We know that X will be the inverse of an n -square non-singular matrix A if

$$AX = I, \quad \dots (1)$$

where I is the $n \times n$ identity matrix.

Every square non-singular matrix will have an inverse. Gauss elimination and Gauss-Jordan methods are popular among many methods available for finding the inverse of a non-singular matrix.

For the third order matrices, (1) may be written as

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Clearly the above equation is equivalent to the three equations

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{21} \\ x_{31} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_{12} \\ x_{22} \\ x_{32} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_{13} \\ x_{23} \\ x_{33} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

We can therefore solve each of these systems using Gaussian elimination method and the result in each case will be the corresponding column of $X = A^{-1}$. We solve all the three equations simultaneously as illustrated in the following examples.

Example Using Gaussian elimination, find the inverse of the matrix $A = \begin{bmatrix} 2 & 1 & 1 \\ 3 & 2 & 3 \\ 1 & 4 & 9 \end{bmatrix}$.

In this method, we place an identity matrix, whose order is same as that of A , adjacent to A which we call *augmented matrix*. Then the inverse of A is computed in two stages. In the first stage, A is converted into an upper triangular form, using Gaussian elimination method.

We write the augmented system first and then apply row transformations:

$$\begin{bmatrix} 2 & 1 & 1 & | & 1 & 0 & 0 \\ 3 & 2 & 3 & | & 0 & 1 & 0 \\ 1 & 4 & 9 & | & 0 & 0 & 1 \end{bmatrix} \sqcup \begin{bmatrix} 2 & 1 & 1 & | & 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{3}{2} & | & -\frac{3}{2} & 1 & 0 \\ 0 & \frac{7}{2} & \frac{17}{2} & | & -\frac{1}{2} & 0 & 1 \end{bmatrix} \begin{array}{l} \text{by } R_2 \rightarrow R_2 - \frac{3}{2}R_1 \\ \text{by } R_3 \rightarrow R_3 - \frac{1}{2}R_1 \end{array}$$

$$\sqcup \begin{bmatrix} 2 & 1 & 1 & | & 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{3}{2} & | & -\frac{3}{2} & 1 & 0 \\ 0 & 0 & -2 & | & 10 & -7 & 1 \end{bmatrix} \text{ by } R_3 \rightarrow R_3 - 7R_{21}$$

The above is equivalent to the following three systems:

$$\begin{bmatrix} 2 & 1 & 1 & | & 1 \\ 0 & \frac{1}{2} & \frac{3}{2} & | & -\frac{3}{2} \\ 0 & 0 & -2 & | & 10 \end{bmatrix} \quad \dots (1)$$

$$\begin{bmatrix} 2 & 1 & 1 & | & 0 \\ 0 & \frac{1}{2} & \frac{3}{2} & | & 1 \\ 0 & 0 & -2 & | & -7 \end{bmatrix} \quad \dots (2)$$

$$\begin{bmatrix} 2 & 1 & 1 & | & 0 \\ 0 & \frac{1}{2} & \frac{3}{2} & | & 1 \\ 0 & 0 & -2 & | & 1 \end{bmatrix} \quad \dots (3)$$

Now the matrix equation of the system of equations corresponding to (1) is

$$\begin{bmatrix} 2 & 1 & 1 \\ 0 & \frac{1}{2} & \frac{3}{2} \\ 0 & 0 & -2 \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{21} \\ x_{31} \end{bmatrix} = \begin{bmatrix} 1 \\ -\frac{3}{2} \\ 10 \end{bmatrix}$$

which on back substitution gives $x_{31} = -5$, $x_{21} = 12$, $x_{11} = -3$.

Similarly using the other two systems other x values are determined and hence the inverse is given by

$$A^{-1} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix} = \begin{bmatrix} -3 & \frac{5}{2} & -\frac{1}{2} \\ 12 & -\frac{17}{2} & \frac{3}{2} \\ -5 & \frac{7}{2} & -\frac{1}{2} \end{bmatrix}.$$

All these operations are also performed on the adjacently placed identity matrix.

Example Use the Gaussian elimination method to find the inverse of the matrix

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 4 & 3 & -1 \\ 3 & 5 & 3 \end{bmatrix}.$$

At first, we place an identity matrix of the same order adjacent to the given matrix. Thus, the augmented matrix can be written as

$$\left[\begin{array}{ccc|ccc} 1 & 1 & 1 & 1 & 0 & 0 \\ 4 & 3 & -1 & 0 & 1 & 0 \\ 3 & 5 & 3 & 0 & 0 & 1 \end{array} \right] \quad \dots (1)$$

In order to increase the accuracy of the result, it is essential to employ partial pivoting. We look for an absolutely largest coefficient *in the first column* and we use this coefficient as the pivotal coefficient (for this we have to interchange *rows* if necessary)

In first column of matrix (1), 4 is the largest element, and hence is the pivotal element. In order to bring 4 in the first row we interchange the first and second rows and obtain the augmented matrix in the form

$$\begin{aligned} & \left[\begin{array}{ccc|ccc} 4 & 3 & -1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 3 & 5 & 3 & 0 & 0 & 1 \end{array} \right] \quad \dots (2) \\ & \square \left[\begin{array}{ccc|ccc} 1 & \frac{3}{4} & -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 3 & 5 & 3 & 0 & 0 & 1 \end{array} \right] \text{ by } R_1 \rightarrow \frac{1}{4}R_1 \\ & \sim \left[\begin{array}{ccc|ccc} 1 & \frac{3}{4} & -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & \frac{5}{4} & 1 & -\frac{1}{4} & 0 \\ 0 & \frac{11}{4} & \frac{15}{4} & 0 & -\frac{3}{4} & 1 \end{array} \right] \begin{array}{l} \text{by } R_2 \rightarrow R_2 - R_1 \\ \text{by } R_3 \rightarrow R_3 - 3R_1 \end{array} \end{aligned}$$

We now search for an absolutely largest coefficient *in the second column* (and not in the first row) and we use this coefficient as the pivotal coefficient. The pivot element is the max $(1/4, 11/4)$ and is $11/4$. Therefore, we interchange second and third rows of the above.

$$\left[\begin{array}{ccc|ccc} 1 & \frac{3}{4} & -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & \frac{11}{4} & \frac{15}{4} & 0 & -\frac{3}{4} & 1 \\ 0 & \frac{1}{4} & \frac{5}{4} & 1 & -\frac{1}{4} & 0 \end{array} \right]$$

Now, divide R_2 by the pivot element $a_{22} = 11/4$, and obtain

$$\left[\begin{array}{ccc|ccc} 1 & \frac{3}{4} & -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & 1 & \frac{15}{11} & 0 & -\frac{3}{11} & \frac{4}{11} \\ 0 & \frac{1}{4} & \frac{5}{4} & 1 & -\frac{1}{4} & 0 \end{array} \right]$$

In order to make the entries below 1 in the second column we perform

$R_3 \rightarrow R_3 - (1/4)R_2$ in the above matrix and obtain

$$\left[\begin{array}{ccc|ccc} 1 & \frac{3}{4} & -\frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & 1 & \frac{15}{11} & 0 & -\frac{3}{11} & \frac{4}{11} \\ 0 & 0 & \frac{10}{11} & 1 & -\frac{2}{11} & -\frac{1}{11} \end{array} \right]$$

This is equivalent to the following three matrices

$$\left[\begin{array}{ccc|c} 1 & \frac{3}{4} & -\frac{1}{4} & 0 \\ 0 & 1 & \frac{15}{11} & 0 \\ 0 & 0 & \frac{10}{11} & 1 \end{array} \right]; \quad \left[\begin{array}{ccc|c} 1 & \frac{3}{4} & -\frac{1}{4} & \frac{1}{4} \\ 0 & 1 & \frac{15}{11} & -\frac{3}{11} \\ 0 & 0 & \frac{10}{11} & -\frac{2}{11} \end{array} \right]; \quad \left[\begin{array}{ccc|c} 1 & \frac{3}{4} & -\frac{1}{4} & 0 \\ 0 & 1 & \frac{15}{11} & \frac{4}{11} \\ 0 & 0 & \frac{10}{11} & -\frac{1}{11} \end{array} \right]$$

Thus we have

$$A^{-1} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix} = \begin{bmatrix} \frac{7}{5} & \frac{1}{5} & -\frac{2}{5} \\ -\frac{3}{2} & 0 & \frac{1}{2} \\ \frac{11}{10} & -\frac{1}{5} & -\frac{1}{10} \end{bmatrix}$$

Matrix Inversion using Gauss-Jordan method

This method is similar to Gaussian elimination method for matrix inversion, starting with the augmented matrix $[A|I]$ and reducing A to the identity matrix using elementary row transformations. The method is illustrated in the following example.

Example Find the inverse of the following matrix A by Gauss-Jordan method.

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 4 & 3 & -1 \\ 3 & 5 & 3 \end{bmatrix}.$$

The augmented matrix is given by

$$\begin{aligned}
 & \left[\begin{array}{ccc|ccc} 1 & 1 & 1 & 1 & 0 & 0 \\ 4 & 3 & -1 & 0 & 1 & 0 \\ 3 & 5 & 3 & 0 & 0 & 1 \end{array} \right] \\
 & \sim \left[\begin{array}{ccc|ccc} 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & -1 & -5 & -4 & 1 & 0 \\ 0 & 2 & 0 & -3 & 0 & 1 \end{array} \right] \begin{array}{l} \text{by } R_2 \rightarrow R_2 - 4R_1 \\ \text{by } R_3 \rightarrow R_3 - 3R_1 \end{array} \\
 & \sim \left[\begin{array}{ccc|ccc} 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 5 & 4 & -1 & 0 \\ 0 & 2 & 0 & -3 & 0 & 1 \end{array} \right] \text{by } R_2 \rightarrow -R_2 \\
 & \sim \left[\begin{array}{ccc|ccc} 1 & 0 & -4 & -3 & 1 & 0 \\ 0 & 1 & 5 & 4 & -1 & 0 \\ 0 & 0 & -10 & -11 & 2 & 1 \end{array} \right] \begin{array}{l} \text{by } R_1 \rightarrow R_1 - R_2 \\ \text{by } R_3 \rightarrow R_3 - 2R_2 \end{array} \\
 & \sim \left[\begin{array}{ccc|ccc} 1 & 0 & -4 & -3 & 1 & 0 \\ 0 & 1 & 5 & 4 & -1 & 0 \\ 0 & 0 & 1 & 11/10 & -1/5 & -1/10 \end{array} \right] \text{by } R_3 \rightarrow -\frac{1}{10}R_3 \\
 & \sim \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 7/5 & 1/5 & -2/5 \\ 0 & 1 & 0 & -3/2 & 0 & 1/2 \\ 0 & 0 & 1 & 11/10 & -1/5 & -1/10 \end{array} \right] \begin{array}{l} \text{by } R_1 \rightarrow R_1 + 4R_3 \\ \text{by } R_2 \rightarrow R_2 - 5R_1 \end{array}
 \end{aligned}$$

Thus we have

$$A^{-1} = \begin{bmatrix} \frac{7}{5} & \frac{1}{5} & -\frac{2}{5} \\ -\frac{3}{2} & 0 & \frac{1}{2} \\ \frac{11}{10} & -\frac{1}{5} & -\frac{1}{10} \end{bmatrix}.$$

- **Triangulation Method (LU Decomposition Method):**

In linear algebra, **LU decomposition** (also called **LU factorization**) factorizes a matrix as the product of a lower triangular matrix and an upper triangular matrix

Let A be a non-singular square matrix. **LU decomposition** is a decomposition of the form

$$A = LU$$

where L is a lower triangular matrix and U is an upper triangular matrix. This means that L has only zeros above the diagonal and U has only zeros below the diagonal. For example, for a 3-by-3 matrix A , its LU decomposition looks like this:

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

Consider a system of linear equations,

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

This can be written in the form,

$$Ax=b,$$

$$\text{where } A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ x_n \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \cdot \\ b_m \end{bmatrix}$$

To solve the system of equations by LU decomposition, first we decompose A as LU, where,

$$L = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

This gives,

$$LUx = b.$$

Let $Ux=y$. This implies, $Ly=b$.

That is,

$$\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

Thus,

$$y_1 = b_1$$

$$l_{21}y_1 + y_2 = b_2$$

$$l_{31}y_1 + l_{32}y_2 + y_3 = b_3$$

This gives the y values by forward substitution, which means, substitute the value of y_1 given by the first equation in the second and solve y_2 , then use these values of y_1 and y_2 in the third and solve y_3 .

Then the system of equations

$$Ux = y; \text{ that is } \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

gives the required values of x_1, x_2 and x_3 as the solution of the original system of linear equations by backward substitution.

To decompose a matrix $A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$, in the form

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}, \text{ we proceed as follows.}$$

On multiplying $\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix}$ and $\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$, we get,

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} & l_{21}u_{13} + u_{23} \\ l_{31}u_{11} & l_{31}u_{12} + l_{32}u_{22} & l_{31}u_{13} + l_{32}u_{23} + u_{33} \end{bmatrix}$$

Equating it with the corresponding terms of A , we get,

$$u_{11} = a_{11}; \quad u_{12} = a_{12}; \quad u_{13} = a_{13}$$

$$l_{21}u_{11} = a_{21} \Rightarrow l_{21} = \frac{a_{21}}{u_{11}}; \quad l_{31}u_{11} = a_{31} \Rightarrow l_{31} = \frac{a_{31}}{u_{11}}$$

$$l_{21}u_{12} + u_{22} = a_{22} \Rightarrow u_{22} = a_{22} - l_{21}u_{12};$$

$$l_{21}u_{13} + u_{23} = a_{23} \Rightarrow u_{23} = a_{23} - l_{21}u_{13};$$

similarly,

$$l_{31}u_{12} + l_{32}u_{22} = a_{32}, \quad l_{31}u_{13} + l_{32}u_{23} + u_{33} = a_{33} \text{ gives } l_{32} \text{ and } u_{33}$$

Example: Solve the following system of equations by LU decomposition.

$$2x+3y+z=9$$

$$x+2y+3z=6$$

$$3x+y+2z=8.$$

Solution:

The above system of equations is written as,

$$\begin{bmatrix} 2 & 3 & 1 \\ 1 & 2 & 3 \\ 3 & 1 & 2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 9 \\ 6 \\ 8 \end{bmatrix}$$

To decompose the matrix $\begin{bmatrix} 2 & 3 & 1 \\ 1 & 2 & 3 \\ 3 & 1 & 2 \end{bmatrix}$ in the form of LU, we equate the corresponding

terms of A and LU as already illustrated, and obtain

$$u_{11} = 2; \quad u_{12} = 3; \quad u_{13} = 1$$

$$l_{21} = \frac{a_{21}}{u_{11}} = \frac{1}{2}; \quad l_{31} = \frac{a_{31}}{u_{11}} = \frac{3}{2}$$

$$u_{22} = a_{22} - l_{21}u_{12} = 2 - \frac{1}{2} \times 3 = \frac{1}{2};$$

$$u_{23} = a_{23} - l_{21}u_{13} = 3 - \frac{1}{2} \times 1 = \frac{5}{2};$$

$$l_{32} = \frac{a_{32} - l_{31}u_{12}}{u_{22}} = \frac{1 - \frac{3}{2} \times 3}{\frac{1}{2}} = -7 \quad \text{and}$$

$$u_{33} = a_{33} - (l_{31}u_{13} + l_{32}u_{23}) = 2 - \left(\frac{3}{2} \times 1 + (-7) \times \frac{5}{2} \right) = 2 - \left(\frac{3}{2} - \frac{35}{2} \right) = 18$$

Hence,

$$\begin{bmatrix} 2 & 3 & 1 \\ 1 & 2 & 3 \\ 3 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{3}{2} & -7 & 1 \end{bmatrix} \begin{bmatrix} 2 & 3 & 1 \\ 0 & \frac{1}{2} & \frac{5}{2} \\ 0 & 0 & 18 \end{bmatrix}$$

This implies,

$$\begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{3}{2} & -7 & 1 \end{bmatrix} \begin{bmatrix} 2 & 3 & 1 \\ 0 & \frac{1}{2} & \frac{5}{2} \\ 0 & 0 & 18 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 9 \\ 6 \\ 8 \end{bmatrix}$$

Consider

$$\begin{bmatrix} 2 & 3 & 1 \\ 0 & \frac{1}{2} & \frac{5}{2} \\ 0 & 0 & 18 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}, \text{ then } \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{3}{2} & -7 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 9 \\ 6 \\ 8 \end{bmatrix},$$

Solving these, we get,
$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 9 \\ \frac{3}{2} \\ 5 \end{bmatrix}$$

That is,

$$\begin{bmatrix} 2 & 3 & 1 \\ 0 & \frac{1}{2} & \frac{5}{2} \\ 0 & 0 & 18 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 9 \\ \frac{3}{2} \\ 5 \end{bmatrix}$$

Now, solving the above expression we obtain the values of x, y and z as a solution of the given system of equations as,

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \frac{35}{18} \\ \frac{29}{18} \\ \frac{5}{18} \end{bmatrix}.$$

Assignments

- Using Gauss-Jordan method, find the inverse of the following matrices:

$$(i) A = \begin{bmatrix} 1 & 1 & 3 \\ 1 & 3 & -3 \\ -2 & -4 & -4 \end{bmatrix} \quad (ii) B = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 4 \\ 2 & 4 & 7 \end{bmatrix}$$

- Using Gaussian elimination method, find the inverse of the following matrices:

$$(i) A = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 3 \\ 3 & 1 & 1 \end{bmatrix} \quad (ii) B = \begin{bmatrix} 2 & 0 & 1 \\ 3 & 2 & 5 \\ 1 & -1 & 0 \end{bmatrix}$$

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SOLUTION BY ITERATIONS

SOLUTION BY ITERATION: Jacobi's iteration method and Gauss Seidel iteration method

The methods discussed in the previous section belong to the **direct methods** for solving systems of linear equations; these are methods that yield solutions after an amount of computations that can be specified in advance.

In this section, we discuss **indirect** or **iterative methods** in which we start from an initial value and obtain better and better approximations from a computational cycle repeated as often as may be necessary, for achieving a required accuracy, so that the amount of arithmetic depends upon the accuracy required.

Jacobi's iteration method and Gauss Seidel iteration method

Consider a linear system of n linear equations in n unknowns x_1, x_2, \dots, x_n of the form

$$\left. \begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \dots + a_{2n}x_n &= b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \dots + a_{3n}x_n &= b_3 \\ &\vdots \\ a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \dots + a_{nn}x_n &= b_n \end{aligned} \right\} \dots (1)$$

in which the diagonal elements a_{ii} do not vanish.

Now the system (1) can be written as

$$\left. \begin{aligned} x_1 &= \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}}x_2 - \frac{a_{13}}{a_{11}}x_3 - \dots - \frac{a_{1n}}{a_{11}}x_n \\ x_2 &= \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}}x_1 - \frac{a_{23}}{a_{22}}x_3 - \dots - \frac{a_{2n}}{a_{22}}x_n \\ x_3 &= \frac{b_3}{a_{33}} - \frac{a_{31}}{a_{33}}x_1 - \frac{a_{32}}{a_{33}}x_2 - \dots - \frac{a_{3n}}{a_{33}}x_n \\ &\vdots \\ x_n &= \frac{b_n}{a_{nn}} - \frac{a_{n1}}{a_{nn}}x_1 - \frac{a_{n2}}{a_{nn}}x_2 - \dots - \frac{a_{n,n-1}}{a_{nn}}x_{n-1} \end{aligned} \right\} \dots (2)$$

Suppose we start with $x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}$ as initial values to the variables x_1, x_2, \dots, x_n . Then we can find better approximations to x_1, x_2, \dots, x_n using the following two iterative methods:

(i) Jacobi's iteration method

Jacobi's iteration method, also called the *method of simultaneous displacements*, is as follows:

Step 1: Determination of first approximation $x_1^{(1)}, x_2^{(1)}, \dots, x_n^{(1)}$ using $x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}$.

$$\left. \begin{aligned} x_1^{(1)} &= \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}} x_2^{(0)} - \frac{a_{13}}{a_{11}} x_3^{(0)} - \dots - \frac{a_{1n}}{a_{11}} x_n^{(0)} \\ x_2^{(1)} &= \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}} x_1^{(0)} - \frac{a_{23}}{a_{22}} x_3^{(0)} - \dots - \frac{a_{2n}}{a_{22}} x_n^{(0)} \\ x_3^{(1)} &= \frac{b_3}{a_{33}} - \frac{a_{31}}{a_{33}} x_1^{(0)} - \frac{a_{32}}{a_{33}} x_2^{(0)} - \dots - \frac{a_{3n}}{a_{33}} x_n^{(0)} \\ &\vdots \\ x_n^{(1)} &= \frac{b_n}{a_{nn}} - \frac{a_{n1}}{a_{nn}} x_1^{(0)} - \frac{a_{n2}}{a_{nn}} x_2^{(0)} - \dots - \frac{a_{n,n-1}}{a_{nn}} x_{n-1}^{(0)} \end{aligned} \right\} \dots (3)$$

Step 2: Similarly, $x_1^{(2)}, x_2^{(2)}, \dots, x_n^{(2)}$ are evaluated by just replacing $x_r^{(0)}$ in the right hand sides equations in (3) by $x_r^{(1)}$.

Step $n+1$: In general, if $x_1^{(n)}, x_2^{(n)}, \dots, x_n^{(n)}$ are a system of n th approximations, then the next approximation is given by the formula

$$\left. \begin{aligned} x_1^{(n+1)} &= \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}} x_2^{(n)} - \frac{a_{13}}{a_{11}} x_3^{(n)} - \dots - \frac{a_{1n}}{a_{11}} x_n^{(n)} \\ x_2^{(n+1)} &= \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}} x_1^{(n)} - \frac{a_{23}}{a_{22}} x_3^{(n)} - \dots - \frac{a_{2n}}{a_{22}} x_n^{(n)} \\ x_3^{(n+1)} &= \frac{b_3}{a_{33}} - \frac{a_{31}}{a_{33}} x_1^{(n)} - \frac{a_{32}}{a_{33}} x_2^{(n)} - \dots - \frac{a_{3n}}{a_{33}} x_n^{(n)} \\ &\vdots \\ x_n^{(n+1)} &= \frac{b_n}{a_{nn}} - \frac{a_{n1}}{a_{nn}} x_1^{(n)} - \frac{a_{n2}}{a_{nn}} x_2^{(n)} - \dots - \frac{a_{n,n-1}}{a_{nn}} x_{n-1}^{(n)} \end{aligned} \right\} \dots (4)$$

The system in (4) can also be briefly described as follows:

$$x_i^{(r+1)} = \frac{b_i}{a_{ii}} - \sum_{\substack{j=1 \\ j \neq i}}^n \frac{a_{ij}}{a_{ii}} x_j^{(r)} \quad (r=0,1,2,\dots, \quad i=1, 2, \dots, n)$$

A sufficient condition for obtaining a solution by Jacobi's iteration method is the diagonal dominance,

$$\text{i.e.,} \quad \left| a_{ii} \right| > \sum_{\substack{j=1 \\ j \neq i}}^n a_{ij}, \quad i=1, 2, \dots, n.$$

i.e., in each row of \mathbf{A} the modulus of the diagonal element exceeds the sum of the off diagonal elements and also the diagonal elements $a_{ii} \neq 0$. If any diagonal element is 0, the equations can always be re-arranged to satisfy this condition.

(ii) Gauss Seidel iteration method

A simple modification to Jacobi's iteration method is given by *Gauss-Seidel* method.

Step 1 (*Gauss-Seidel method*): Determination of first approximation $x_1^{(1)}, x_2^{(1)}, \dots, x_n^{(1)}$ using $x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}$.

$$\left. \begin{aligned} x_1^{(1)} &= \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}}x_2^{(0)} - \frac{a_{13}}{a_{11}}x_3^{(0)} - \dots - \frac{a_{1n}}{a_{11}}x_n^{(0)} \\ x_2^{(1)} &= \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}}x_1^{(1)} - \frac{a_{23}}{a_{22}}x_3^{(0)} - \dots - \frac{a_{2n}}{a_{22}}x_n^{(0)} \\ x_3^{(1)} &= \frac{b_3}{a_{33}} - \frac{a_{31}}{a_{33}}x_1^{(1)} - \frac{a_{32}}{a_{33}}x_2^{(1)} - \dots - \frac{a_{3n}}{a_{33}}x_n^{(0)} \\ &\vdots \\ x_n^{(1)} &= \frac{b_n}{a_{nn}} - \frac{a_{n1}}{a_{nn}}x_1^{(1)} - \frac{a_{n2}}{a_{nn}}x_2^{(1)} - \dots - \frac{a_{n,n-1}}{a_{nn}}x_{n-1}^{(1)} \end{aligned} \right\} \dots (5)$$

Step $n+1$: In general, if $x_1^{(n)}, x_2^{(n)}, \dots, x_n^{(n)}$ are a system of n th approximations, then the next approximation is given by the formula

$$\left. \begin{aligned} x_1^{(n+1)} &= \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}}x_2^{(n)} - \frac{a_{13}}{a_{11}}x_3^{(n)} - \dots - \frac{a_{1n}}{a_{11}}x_n^{(n)} \\ x_2^{(n+1)} &= \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}}x_1^{(n+1)} - \frac{a_{23}}{a_{22}}x_3^{(n)} - \dots - \frac{a_{2n}}{a_{22}}x_n^{(n)} \\ x_3^{(n+1)} &= \frac{b_3}{a_{33}} - \frac{a_{31}}{a_{33}}x_1^{(n+1)} - \frac{a_{32}}{a_{33}}x_2^{(n+1)} - \dots - \frac{a_{3n}}{a_{33}}x_n^{(n)} \\ &\vdots \\ x_n^{(n+1)} &= \frac{b_n}{a_{nn}} - \frac{a_{n1}}{a_{nn}}x_1^{(n+1)} - \frac{a_{n2}}{a_{nn}}x_2^{(n+1)} - \dots - \frac{a_{n,n-1}}{a_{nn}}x_{n-1}^{(n+1)} \end{aligned} \right\} \dots (6)$$

(6) can be briefly described as follows:

$$x_i^{(r+1)} = \frac{b_i}{a_{ii}} - \sum_{j=1}^{i-1} \frac{a_{ij}}{a_{ii}}x_j^{(r+1)} - \sum_{j=i+1}^n \frac{a_{ij}}{a_{ii}}x_j^{(r)} \quad (r=0,1,2,\dots, \quad i=1,2,\dots,n).$$

Remark We note the difference between Jacobi's method and *Gauss-Seidel* method.

(Attention!) In the following the bold face letters must be carefully noted):

Jacobi's method: In the first equation of (3), we substitute the initial approximations $x_2^{(0)}, x_3^{(0)}, \dots, x_n^{(0)}$ into the right-hand side and denote the result as $x_1^{(1)}$. In the second equation, we substitute $x_1^{(0)}, x_3^{(0)}, \dots, x_n^{(0)}$ and denote the result as $x_2^{(1)}$. In third, we substitute $x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}$ and call the result as $x_3^{(1)}$. The process is repeated in this manner.

Gauss-Seidel method: In the first equation of (3), we substitute the initial approximation $x_2^{(0)}, \dots, x_n^{(0)}$ into the right-hand side and denote the result as $x_1^{(1)}$. In the second equation, we substitute $x_1^{(1)}, x_3^{(0)}, \dots, x_n^{(0)}$ and denote the result as $x_2^{(1)}$. In third, we substitute $x_1^{(1)}, x_2^{(1)}, \dots, x_n^{(0)}$ and call the result as $x_3^{(1)}$. The process is repeated in this manner and illustrated below:

Example 11 Solve the following system of equations using (a) Jacobi's iteration method and (b) Gauss-Seidel iteration method.

$$\begin{aligned} 10x_1 - 2x_2 - x_3 - x_4 &= 3 \\ -2x_1 + 10x_2 - x_3 - x_4 &= 15 \\ -x_1 - x_2 + 10x_3 - 2x_4 &= 27 \\ -x_1 - x_2 - 2x_3 + 10x_4 &= -9. \end{aligned}$$

Solution

To solve these equations by the iterative methods, we re-write them as follows:

$$\begin{aligned} x_1 &= 0.3 + 0.2x_2 + 0.1x_3 + 0.1x_4 \\ x_2 &= 1.5 + 0.2x_1 + 0.1x_3 + 0.1x_4 \\ x_3 &= 2.7 + 0.1x_1 + 0.1x_2 + 0.2x_4 \\ x_4 &= -0.9 + 0.1x_1 + 0.1x_2 + 0.2x_3 \end{aligned}$$

It can be verified that these equations satisfy the diagonal dominance condition. The process and given in the following Tables.

Table 1. Jacobi's Method

n	x_1	x_2	x_3	x_4
1	0.3	1.56	2.886	-0.1368
2	0.8869	1.9523	2.9566	-0.0248
3	0.9836	1.9899	2.9924	-0.0042
4	0.9968	1.9982	2.9987	-0.0008
5	0.9994	1.9997	2.9998	-0.0001
6	0.9999	1.9999	3.0	0.0
7	1.0	2.0	3.0	0.0

Table 2. Gauss-Seidel method

n	x_1	x_2	x_3	x_4
1	0 . 3	1 . 5	2 . 7	– 0 . 9
2	0 . 7 8	1 . 7 4	2 . 7	– 0 . 1 8
3	0 . 9	1 . 9 0 8	2 . 9 1 6	– 0 . 1 0 8
4	0 . 9 6 2 4	1 . 9 6 0 8	2 . 9 5 9 2	– 0 . 0 3 6
5	0 . 9 8 4 5	1 . 9 8 4 8	2 . 9 8 5 1	– 0 . 0 1 5 8
6	0 . 9 9 3 9	1 . 9 9 3 8	2 . 9 9 3 8	– 0 . 0 0 6
7	0 . 9 9 7 5	1 . 9 9 7 5	2 . 9 9 7 6	– 0 . 0 0 2 5
8	0 . 9 9 9 0	1 . 9 9 9 0	2 . 9 9 9 0	– 0 . 0 0 1 0
9	0 . 9 9 9 6	1 . 9 9 9 6	2 . 9 9 9 6	– 0 . 0 0 0 4
1 0	0 . 9 9 9 8	1 . 9 9 9 8	2 . 9 9 9 8	– 0 . 0 0 0 2
1 1	0 . 9 9 9 9	1 . 9 9 9 9	2 . 9 9 9 9	– 0 . 0 0 0 1
1 2	1 . 0	2 . 0	3 . 0	0 . 0

From Tables 1 and 2, it is clear that twelve iterations are required by Jacobi's method to achieve the same accuracy as seven Gauss-Seidel iterations.

Example 12 Solve by Jacobi's iteration method, the system of equations

$$20x_1 + x_2 - 7x_3 = 17$$

$$3x_1 + 20x_2 - x_3 = -18$$

$$2x_1 - 3x_2 + 20x_3 = 25$$

Solution The given system of equations can be written as

$$\left. \begin{aligned} x_1 &= \frac{17}{20} - \frac{1}{20}x_2 + \frac{7}{20}x_3 \\ x_2 &= -\frac{18}{20} - \frac{3}{20}x_1 + \frac{1}{20}x_3 \\ x_3 &= \frac{25}{20} - \frac{2}{20}x_1 + \frac{3}{20}x_2 \end{aligned} \right\} (3)$$

We start from an approximation $x_1^{(0)} = x_2^{(0)} = x_3^{(0)} = 0$ to x_1, x_2, x_3 respectively. Substituting these values on the right sides of equations in (3), we get the first approximation values $x_1^{(1)} = \frac{17}{20} = 0.85$, $x_2^{(1)} = -\frac{18}{20} = -0.90$ and $x_3^{(1)} = \frac{25}{20} = 1.25$

Putting these values on the right side of the equations in (2), we obtain the second approximation values, $x_1^{(2)} = 1.02$, $x_2^{(2)} = -0.965$ and $x_3^{(2)} = 1.03$. Similarly, third approximation values are $x_1^{(3)} = 1.00125$, $x_2^{(3)} = -1.0015$ and $x_3^{(3)} = 1.004$ and fourth approximation values are $x_1^{(4)} = 1.000475$, $x_2^{(4)} = -0.9999875$ and $x_3^{(4)} = 0.99965$. It can be seen that the values approach the exact solution $x_1 = 1$, $x_2 = -1$, $x_3 = 1$.

Example 13 Solve, using Gauss-Seidel iteration method, the system:

$$\begin{aligned} x_1 - 0.25x_2 - 0.25x_3 &= 50 \\ -0.25x_1 + x_2 - 0.25x_4 &= 50 \\ -0.25x_1 + x_3 - 0.25x_4 &= 25 \\ -0.25x_2 - 0.25x_3 + x_4 &= 25 \end{aligned}$$

Solution

The given system of equations can be written as

$$\left. \begin{aligned} x_1 &= 50 + 0.25x_2 + 0.25x_3 \\ x_2 &= 50 + 0.25x_1 + 0.25x_4 \\ x_3 &= 25 + 0.25x_1 + 0.25x_4 \\ x_4 &= 25 + 0.25x_2 + 0.25x_3 \end{aligned} \right\} \dots(2)$$

We start from an approximation $x_1^{(0)} = x_2^{(0)} = x_3^{(0)} = 100$ to x_1, x_2, x_3 respectively. Then we get approximation values as follows:

$$\begin{aligned} x_1^{(1)} &= 50 + 0.25x_2^{(0)} + 0.25x_3^{(0)} = 100.00 \\ x_2^{(1)} &= 50 + 0.25x_1^{(1)} + 0.25x_4^{(0)} = 100.00 & x_3^{(1)} &= 50 + 0.25x_1^{(1)} + 0.25x_4^{(0)} = 75.00 \\ x_4^{(1)} &= 25 + 0.25x_2^{(1)} + 0.25x_3^{(1)} = 68.75 \end{aligned}$$

Now second approximation values are given by:

$$\begin{aligned} x_1^{(2)} &= 50 + 0.25x_2^{(1)} + 0.25x_3^{(1)} = 93.75 \\ x_2^{(2)} &= 50 + 0.25x_1^{(2)} + 0.25x_4^{(1)} = 90.62 & x_3^{(2)} &= 50 + 0.25x_1^{(2)} + 0.25x_4^{(1)} = 65.62 \\ x_4^{(2)} &= 25 + 0.25x_2^{(2)} + 0.25x_3^{(2)} = 64.06. \end{aligned}$$

Note that the exact solution to the system is

$$x_1 = x_2 = 87.5, \quad x_3 = x_4 = 62.5$$

Example 14 Using Gauss Siedel iteration solve the following system of equations, in three steps starting from 1, 1, 1.

$$10x + y + z = 6$$

$$x + 10y + z = 6$$

$$x + y + 10z = 6$$

Solution

$$x = 0.6 - 0.1y - 0.1z$$

$$y = 0.6 - 0.1x - 0.1z$$

$$z = 0.6 - 0.1x - 0.1y$$

Step 1 Using $x^{(0)} = y^{(0)} = z^{(0)} = 1$, we have

$$x^{(1)} = 0.6 - 0.1 y^{(0)} - 0.1 z^{(0)} = 0.6 - 0.1 - 0.1 = 0.4$$

$$y^{(1)} = 0.6 - 0.1 x^{(1)} - 0.1 z^{(0)} = 0.6 - 0.1 \times 0.4 - 0.1 = 0.46$$

$$z^{(1)} = 0.6 - 0.1 x^{(1)} - 0.1 y^{(1)} = 0.6 - 0.1 \times 0.4 - 0.1 \times 0.46 = 0.514$$

Step 2 Using $x^{(1)} = 0.4$, $y^{(1)} = 0.46$, $z^{(1)} = 0.514$, we have

$$x^{(2)} = 0.6 - 0.1 y^{(1)} - 0.1 z^{(1)} = 0.6 - 0.1 \times 0.46 - 0.1 \times 0.514 = 0.5026$$

$$y^{(2)} = 0.6 - 0.1 x^{(2)} - 0.1 z^{(1)} = 0.6 - 0.1 \times 0.5026 - 0.1 \times 0.514 = 0.49834$$

$$z^{(2)} = 0.6 - 0.1 x^{(2)} - 0.1 y^{(2)}$$

$$= 0.6 - 0.1 \times 0.5026 - 0.1 \times 0.49834 = 0.499906$$

Step 3 Using $x^{(2)} = 0.5026$, $y^{(2)} = 0.49834$, $z^{(2)} = 0.499906$, we have

$$x^{(3)} = 0.6 - 0.1 y^{(2)} - 0.1 z^{(2)} = 0.6 - 0.1 \times 0.49834 - 0.1 \times 0.499906 = 0.5001754$$

$$y^{(3)} = 0.6 - 0.1 x^{(3)} - 0.1 z^{(2)}$$

$$= 0.6 - 0.1 \times 0.5001754 - 0.1 \times 0.499906 = 0.49999186$$

$$z^{(3)} = 0.6 - 0.1 x^{(3)} - 0.1 y^{(3)}$$

$$= 0.6 - 0.1 \times 0.5001754 - 0.1 \times 0.49999186 = 0.49996492$$

We take $x \approx 0.5$, $y \approx 0.5$, $z \approx 0.5$ as the solution of the given system of equations.

Exercises

1. Apply Gauss Seidel iteration method to solve:

$$10x + 2y + z = 9$$

$$2x + 20y - 2z = -44$$

$$-2x + 3y + 10z = 22$$

2. Apply Gauss Seidel iteration method to solve:

$$1.2x + 2.1y + 4.2z = 9.9$$

$$5.3x + 6.1y + 4.7z = 21.6$$

$$9.2x + 8.3y + z = 15.2$$

3. Apply Jacobi's iteration method to solve:

$$5x - y + z = 10$$

$$2x - y + z = 10$$

$$x + y + 5z = -1$$

4. Apply Jacobi's iteration method to solve:

$$5x + 2y + z = 12$$

$$x + 4y + 2z = 15$$

$$x + 2y + 5z = 20$$

Answers

1. $x = 1.013, y = -1.996, z = 3.001$
2. $x = 2, y = 3, z = 4$ (Approximately)
3. $x = -13.223, y = 16.766, z = -2.306$
4. $x = 2.556, y = 1.722, z = -1.005$
5. $x = 1.08, y = 1.95, z = 3.16$

13

EIGEN VALUES

Eigen Values

Definitions Suppose λ be an indeterminate. Consider the $n \times n$ matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \cdot & \cdot & \dots & \cdot \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} = [a_{ij}]_{n \times n} \quad \dots (1)$$

Then the matrix $A - \lambda I$, where I is the identity matrix of order n , is called the **characteristic matrix of A** and is given by

$$A - \lambda I = \begin{bmatrix} a_{11} - \lambda & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} - \lambda & \dots & a_{2n} \\ \cdot & \cdot & \dots & \cdot \\ a_{n1} & a_{n2} & \dots & a_{nn} - \lambda \end{bmatrix} \quad \dots (2)$$

The determinant $|A - \lambda I|$ of the characteristic matrix of A given in (2) can be found out to be

$$b_0 + b_1 \lambda + b_2 \lambda^2 + \dots + b_{n-1} \lambda^{n-1} + b_n \lambda^n \quad \dots (3)$$

where b_i are scalars. Now (3) is a non-zero polynomial of degree n in the indeterminate λ . This polynomial is called the **characteristic polynomial** of A . That is the *characteristic polynomial* of the matrix A is given by

$$|A - \lambda I| = 0 \quad \dots (3')$$

The equation

$$|A - \lambda I| = 0 \quad \dots (4)$$

i.e., the equation

$$\begin{vmatrix} a_{11} - \lambda & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} - \lambda & \dots & a_{2n} \\ \cdot & \cdot & \dots & \cdot \\ a_{n1} & a_{n2} & \dots & a_{nn} - \lambda \end{vmatrix} = 0 \quad \dots (4')$$

is called the **characteristic equation of the matrix A** .

The roots of the characteristic equation (4) are called the **characteristic roots** or **latent roots** or **eigen values** of the matrix A . If λ is an eigen value, then column vector X such that $AX = \lambda X$ is called an **eigen vector** associated with the eigen value λ .

Example Find the eigen values and the corresponding eigen vectors of the matrix

$$A = \begin{bmatrix} 8 & -6 & 2 \\ -6 & 7 & -4 \\ 2 & -4 & 3 \end{bmatrix}.$$

Solution

The characteristic equation of A is $|A - \lambda I| = 0$.

$$\text{i.e., } \begin{vmatrix} 8-\lambda & -6 & 2 \\ -6 & 7-\lambda & -4 \\ 2 & -4 & 3-\lambda \end{vmatrix} = 0$$

On simplification we get

$$-\lambda^3 + 18\lambda^2 - 45\lambda = 0,$$

which gives the eigen values $\lambda = 0$; $\lambda = 3$; $\lambda = 15$.

(Determination of eigen vector corresponding to the eigen value $\lambda = 0$)

Let $X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ be the eigen vector corresponding to $\lambda = 0$ is obtained by solving $AX = 0X$

i.e., by solving

$$\begin{bmatrix} 8 & -6 & 2 \\ -6 & 7 & -4 \\ 2 & -4 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 0 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

i.e., by solving

$$\begin{bmatrix} 8 & -6 & 2 \\ -6 & 7 & -4 \\ 2 & -4 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

The corresponding system of linear equations is

$$8x_1 - 6x_2 + 2x_3 = 0 \quad \dots(1)$$

$$-6x_1 + 7x_2 - 4x_3 = 0 \quad \dots(2)$$

$$2x_1 - 4x_2 + 3x_3 = 0 \quad \dots(3)$$

Now (1) and (3) can be written as

$$4x_1 - 3x_2 + x_3 = 0$$

and $2x_1 - 4x_2 + 3x_3 = 0.$

Now by the method of cross multiplication

$$\frac{x_1}{-3 \cdot 3 - 1 \cdot (-4)} = \frac{x_2}{1 \cdot 2 - 4 \cdot 3} = \frac{x_3}{4 \cdot (-4) - 3 \cdot 2}$$

or $\frac{x_1}{-5} = \frac{x_2}{-10} = \frac{x_3}{-10}.$

or $\frac{x_1}{1} = \frac{x_2}{2} = \frac{x_3}{2}.$

Hence $\frac{x_1}{1} = \frac{x_2}{2} = \frac{x_3}{2} = k,$

where k is arbitrary.

$\therefore x_1 = k, x_2 = 2k, x_3 = 2k. \quad \dots (4)$

The solution given in (4) also satisfies the equation (2).

\therefore eigen vector corresponding to $\lambda = 0$ is given by $X = \begin{bmatrix} k \\ 2k \\ 2k \end{bmatrix}.$

A particular eigen value is (with $k=1$) is $X = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}.$

(Determination of eigen vector corresponding to the eigen value $\lambda = 3$)

The eigen vector X corresponding to $\lambda = 3$ is obtained by solving $AX = 3X$ or by solving $(A - 3I)X = 0$

i.e., by solving

$$\begin{bmatrix} 5 & -6 & 2 \\ -6 & 4 & -4 \\ 2 & -4 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

By elementary row transformations, the above matrix equation is equivalent to the matrix equation

$$\begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Choosing $x_3 = k$, arbitrary, we have $x_1 + x_3 = 0, x_2 + \frac{1}{2}x_3 = 0.$

Hence
$$X = \begin{bmatrix} -k \\ -\frac{1}{2}k \\ k \end{bmatrix}$$

is an eigen vector corresponding to the eigen value $\lambda = 3$.

A particular eigen value is (with $k = 2$) is
$$X = \begin{bmatrix} -2 \\ -1 \\ 2 \end{bmatrix}.$$

(Determination of eigen vector corresponding to the eigen value $\lambda = 15$)

The eigen vector X corresponding to $\lambda = 15$ is obtained by solving $AX = 15X$

i.e., by solving $(A - 15I)X = 0$

i.e., by solving

$$\begin{bmatrix} -7 & -6 & 2 \\ -6 & -8 & -4 \\ 2 & -4 & -12 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Hence
$$X = \begin{bmatrix} 2a \\ -2a \\ a \end{bmatrix}$$

is an eigen vector corresponding to the eigen value $\lambda = 15$.

Example Find the eigen values and the eigen vector corresponding to the largest eigen value of the matrix

$$A = \begin{bmatrix} 6 & -2 & 2 \\ -2 & 3 & -1 \\ 2 & -1 & 3 \end{bmatrix}.$$

Solution

It can be seen that the eigen values are 2, 2 and 8.

Now we determine the eigen vector corresponding to the largest eigen value 8:

The eigen vector X corresponding to $\lambda = 8$ is obtained by solving $AX = 8X$ i.e., by solving $[A - 8I]X = 0$

i.e., by solving

$$\begin{bmatrix} 6-8 & -2 & 2 \\ -2 & 3-8 & -1 \\ 2 & -1 & 3-8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

i.e., by solving

$$\begin{bmatrix} 2 & -2 & 2 \\ -2 & -4 & -1 \\ 2 & -1 & -5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

The corresponding system of linear equations is

$$2x_1 - 2x_2 + 2x_3 = 0 \quad \dots(1)$$

$$-2x_1 - 5x_2 - x_3 = 0 \quad \dots(2)$$

$$2x_1 - x_2 - 5x_3 = 0 \quad \dots(3)$$

Now (1) and (3) can be written as

$$x_1 - x_2 + x_3 = 0$$

and $2x_1 - x_2 - 5x_3 = 0.$

Now by the method of cross multiplication

$$\frac{x_1}{-1 \cdot (-5) - 1 \cdot (-1)} = \frac{x_2}{1 \cdot 2 - (1) \cdot (-5)} = \frac{x_3}{(-1) \cdot (-1) - (-1) \cdot 2}$$

or $\frac{x_1}{6} = \frac{x_2}{-3} = \frac{x_3}{3}.$

or $\frac{x_1}{2} = \frac{x_2}{-1} = \frac{x_3}{1}.$

Hence $\frac{x_1}{2} = \frac{x_2}{-1} = \frac{x_3}{1} = k.$

$\therefore x_1 = 2k, \quad x_2 = -k, \quad x_3 = k. \quad \dots (4)$

The solution given in (4) also satisfies the equation (2).

\therefore the eigen vector corresponding to $\lambda = 8$ is

$$X = \begin{bmatrix} 2k \\ -k \\ k \end{bmatrix}.$$

A particular eigen value is (with $k=1$) is $X = \begin{bmatrix} 2 \\ -1 \\ 1 \end{bmatrix}.$

Example Find the eigenvalues and eigenvectors of the matrix:

$$A = \begin{bmatrix} 5 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 5 \end{bmatrix}$$

The characteristic equation of the matrix is given by

$$\begin{vmatrix} 5-\lambda & 0 & 1 \\ 0 & -2-\lambda & 0 \\ 1 & 0 & 5-\lambda \end{vmatrix} = 0$$

which gives $\lambda_1 = -2, \lambda_2 = 4$ and $\lambda_3 = 6$.

Determination of eigenvectors corresponding to $\lambda_1 = -2$. Let the eigenvector be

$$X_1 = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

Then we have:

$$A \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = -2 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix},$$

which gives the equations

$$7x_1 + x_3 = 0$$

$$\text{and } x_1 + 7x_3 = 0$$

The solution is $x_1 = x_3 = 0$ with x_2 arbitrary. In particular, we take $x_2 = 1$ and an eigenvector is

$$X_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

Determination of eigenvectors corresponding to $\lambda_2 = 4$. If

$$X_2 = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

is an eigenvector, the equations are

$$x_1 + x_3 = 0$$

$$\text{and } -6x_2 = 0$$

from which we obtain

$$x_1 = -x_3 \text{ and } x_2 = 0.$$

We choose, in particular, $x_1 = 1/\sqrt{2}$ and $x_3 = -1/\sqrt{2}$ so that $x_1^2 + x_2^2 + x_3^2 = 1$. The eigenvector chosen in this way is said to be normalized. We therefore have $X_2 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{bmatrix}$.

Determination of eigenvectors corresponding to $\lambda_3 = 6$. If

$$X_3 = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

is the required eigenvector, then the equations are

$$-x_1 + x_3 = 0$$

$$-8x_2 = 0$$

$$x_1 - x_3 = 0$$

which give $x_1 = x_3$ and $x_2 = 0$.

Choosing $x_1 = x_3 = 1/\sqrt{2}$, the normalized eigenvector is given by

$$X_3 = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{bmatrix}$$

Example Determine the largest eigen value and the corresponding eigenvector of the matrix

$$A = \begin{bmatrix} 1 & 6 & 1 \\ 1 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

Let the initial eigenvector be

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = X^{(0)}.$$

Then we have

$$AX^{(0)} = \begin{bmatrix} 1 & 6 & 1 \\ 1 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

Let $X^{(1)} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$. Then we have $AX^{(0)} = X^{(1)}$ and we have an approximate eigen value is 1 and an approximate eigenvector is $X^{(1)}$. Hence we have

$$AX^{(1)} = \begin{bmatrix} 1 & 6 & 1 \\ 1 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 7 \\ 3 \\ 0 \end{bmatrix} = 3 \begin{bmatrix} 2.3 \\ 1 \\ 0 \end{bmatrix}$$

from which we see that

$$X^{(2)} = \begin{bmatrix} 2.3 \\ 1 \\ 0 \end{bmatrix}$$

and that an approximate eigen value is 3.

Repeating the above procedure, we successively obtain

$$4 \begin{bmatrix} 2.1 \\ 1.1 \\ 0 \end{bmatrix}; \quad 4 \begin{bmatrix} 2.2 \\ 1.1 \\ 0 \end{bmatrix}; \quad 4.4 \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}; \quad 4 \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}; \quad 4 \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}.$$

It follows that the largest eigen value is 4 and the corresponding eigenvector is

$$\begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}.$$

Eigenvalues of a Symmetric Tridiagonal Matrix

Since symmetric matrices can be reduced to symmetric tridiagonal matrices, the determination of eigen values of a symmetric tridiagonal matrix is of particular interest. Consider the **tridiagonal matrix**

$$A_1 = \begin{bmatrix} a_{11} & a_{12} & 0 \\ a_{12} & a_{22} & a_{23} \\ 0 & a_{23} & a_{33} \end{bmatrix}.$$

To obtain the eigenvalues of A_1 , we form the determinant equation

$$|A_1 - \lambda I| = \begin{vmatrix} a_{11} - \lambda & a_{12} & 0 \\ a_{12} & a_{22} - \lambda & a_{23} \\ 0 & a_{23} & a_{33} - \lambda \end{vmatrix} = 0.$$

Suppose that the above equation is written in the form

$$w_3(\lambda) = 0 \quad \dots (1)$$

Expanding the determinants in terms of the third row, we obtain

$$w_3(\lambda) = (a_{33} - \lambda) \begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{12} & a_{22} - \lambda \end{vmatrix} - a_{23} \begin{vmatrix} a_{11} - \lambda & 0 \\ a_{12} & a_{23} \end{vmatrix}$$

$$= (a_{33} - \lambda)w_2(\lambda) - a_{23}(a_{11} - \lambda)a_{23},$$

$$\text{where } w_2(\lambda) = \begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{12} & a_{22} - \lambda \end{vmatrix}$$

$$= (a_{33} - \lambda)w_2(\lambda) - a_{23}^2 w_1(\lambda), \text{ where } w_1(\lambda) = (a_{11} - \lambda)$$

Hence (1) implies,

$$(a_{33} - \lambda)w_2(\lambda) - a_{23}^2 w_1(\lambda) = 0.$$

We thus obtain the recursion formula

$$w_0(\lambda) = 1$$

$$w_1(\lambda) = a_{11} - \lambda$$

$$= (a_{11} - \lambda)w_0(\lambda)$$

$$w_2(\lambda) = \begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{12} & a_{22} - \lambda \end{vmatrix}$$

$$= (a_{11} - \lambda)(a_{22} - \lambda) - a_{12}^2$$

$$= w_1(\lambda)(a_{22} - \lambda) - a_{12}^2 w_0(\lambda)$$

$$w_3(\lambda) = w_2(\lambda)(a_{33} - \lambda) - a_{23}^2 w_1(\lambda).$$

In general, if

$$w_k(\lambda) = \begin{vmatrix} a_{11} - \lambda & a_{12} & 0 & \dots & 0 \\ a_{12} & a_{22} - \lambda & a_{23} & \dots & 0 \\ 0 & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & a_{k-1,k} & a_{kk} - \lambda \end{vmatrix}, \quad (2 \leq k \leq n),$$

then the recursion formula is

$$w_k(\lambda) = (a_{kk} - \lambda)w_{k-1}(\lambda) - a_{k-1,k}^2 w_{k-2}(\lambda), \quad (2 \leq k \leq n)$$

The equation $w_k(\lambda) = 0$ is the characteristic equation and can be solved using the methods discussed in Chapter 2. When the eigen values are known its eigen vectors can be calculated.

Exercises

1. Find the eigen values and the corresponding eigen vectors of the following matrices:

(a) $\begin{bmatrix} -3 & 0 \\ 5 & -1 \end{bmatrix}$

(b) $\begin{bmatrix} 1 & -2 \\ -2 & 4 \end{bmatrix}$

$$(c) \begin{bmatrix} 2 & 1 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 2 \end{bmatrix}$$

$$(d) \begin{bmatrix} 3 & 10 & 5 \\ -2 & -3 & -4 \\ 3 & 5 & 7 \end{bmatrix}$$

$$(e) \begin{bmatrix} 3 & 0 & 0 \\ 5 & 4 & 0 \\ 3 & 6 & 1 \end{bmatrix}$$

$$(f) \begin{bmatrix} 5 & 1 & -1 \\ 1 & 3 & -1 \\ 1 & -1 & 3 \end{bmatrix}$$

$$(g) \begin{bmatrix} 5 & -6 & -6 \\ -1 & 4 & 2 \\ 3 & -6 & -4 \end{bmatrix}$$

$$(h) \begin{bmatrix} 2 & 2 & 0 \\ 2 & 1 & 1 \\ -7 & 2 & -3 \end{bmatrix}$$

$$(i) \begin{bmatrix} 2 & 2 & 1 \\ 1 & 3 & 1 \\ 1 & 2 & 2 \end{bmatrix}$$

$$(j) \begin{bmatrix} 3 & 1 & -1 \\ 1 & 3 & 1 \\ -1 & 1 & 3 \end{bmatrix}$$

$$(k) \begin{bmatrix} 2 & 1 & -1 \\ 0 & 3 & -2 \\ 2 & 4 & -3 \end{bmatrix}$$

$$(l) \begin{bmatrix} 2 & -1 & 1 \\ -1 & 2 & -1 \\ 1 & -1 & 2 \end{bmatrix}$$

2. Find the eigen values and eigen vectors of $\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$ Find the characteristic roots of

$$A = \begin{bmatrix} 1 & 0 & 2 \\ 0 & 2 & 1 \\ 2 & 0 & 1 \end{bmatrix}.$$

3. Find also the corresponding characteristic vectors.

4. Find the eigen values and the eigen vector corresponding to the largest eigen value of

the matrix $A = \begin{bmatrix} 8 & -6 & 2 \\ -6 & -1 & -4 \\ 2 & -4 & 3 \end{bmatrix}.$

5. Obtain the eigen values and the corresponding eigen vector of matrix

$$A = \begin{bmatrix} 6 & -2 & 2 \\ -2 & 3 & -1 \\ 2 & -1 & 3 \end{bmatrix}.$$

6. Use the iterative method to find the largest eigen value and the corresponding eigen vector of the matrix

$$A = \begin{bmatrix} 5 & 2 & 1 & -2 \\ 2 & 6 & 3 & -4 \\ 1 & 3 & 19 & 2 \\ -2 & -4 & 2 & 1 \end{bmatrix}.$$

14

TAYLOR SERIES METHOD

METHODS FOR NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS

There are differential equations that cannot be solved using the standard methods even though they possess solutions. In such situations, we apply numerical methods for obtaining approximate solutions, where the accuracy is sufficient. These methods yield the solution in one of the following forms:

- (i) **Single-step method:** A series for y in terms of powers of x , from which the value of y at a particular value of x can be obtained by direct substitution.
- (ii) **Multi-step method:** In multi step methods, the solution at any point x is obtained using the solution at a number of previous points.

Taylor's, Picard's, Euler's and Modified Euler's methods are coming under single-step method of solving an ordinary differential equation.

The need for finding the solution of the initial value problems occur frequently in Engineering and Physics. There are some first order differential equations that cannot be solved using the standard methods. In such situations we apply numerical methods. These methods yield the solution in one of the two forms:

- (iii) A series for y in terms of powers of x , from which the value of y can be obtained by direct substitution.
- (iv) A set of tabulated values of x and y .

The methods of Taylor and Picard belong to class (i), whereas those of Euler, Runge-Kutta, etc., belong to the class (ii). In this chapter we consider Taylor series method.

Taylor Series

We recall the following (Ref. Fourth Semester Core Text):

The Taylor series generated by f at $x = a$ is

$$\sum_{k=0}^{\infty} \frac{f^{(k)}(a)}{k!} (x-a)^k = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!} f''(a) + \dots$$

$$+ \frac{(x-a)^{n-1}}{(n-1)!} f^{(n-1)}(a) + \frac{(x-a)^n}{n!} f^{(n)}(a) + \dots$$

In most of the cases, the Taylor's series converges to $f(x)$ at every x and we often write the Taylor's series at $x = a$ as

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!} f''(a) + \dots \quad \dots (1)$$

Instead of $f(x)$ and a , we prefer $y(x)$ and x_0 , and in that case (1) becomes

$$y(x) = y(x_0) + (x-x_0)y'(x_0) + \frac{(x-x_0)^2}{2!} y''(x_0) + \dots \quad \dots (2)$$

Solution of First Order IVP by Taylor Series Method

Now consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0. \quad \dots (3)$$

If $y(x)$ is the exact solution of (3), then using (2) with $y(x_0) = y_0$, $y'(x_0) = y'_0$, $y''(x_0) = y''_0$, and so on, we obtain the Taylor's series for $y(x)$ around $x = x_0$ as

$$y(x) = y_0 + (x-x_0)y'_0 + \frac{(x-x_0)^2}{2!} y''_0 + \dots \quad \dots (4)$$

If the values of y'_0, y''_0, \dots are known, then (4) gives a power series for y . From (3) we have $y' = f$, which on differentiation with respect to x (using chain rule) gives

$$y'' = f' = \frac{df}{dx} = \frac{\partial f}{\partial x} + \left(\frac{\partial f}{\partial y} \right) y' \quad \dots (5)$$

Similarly, higher derivatives of y can be expressed in terms of f .

Example Using Taylor series, solve $y' = x - y^2$, $y(0) = 1$. Also find $y(0.1)$ correct to four decimal places.

Here $x_0 = 0$; $y_0 = y(0) = 1$. Hence (4) takes the form

$$y(x) = y_0 + \frac{x}{1!} y'_0 + \frac{x^2}{2!} y''_0 + \frac{x^3}{3!} y'''_0 + \frac{x^4}{4!} y^{(4)}_0 + \frac{x^5}{5!} y^{(5)}_0 + \dots \quad \dots (6)$$

We have

$$y' = x - y^2, \quad y'_0 = y'(x = x_0, y = y_0) = x_0 - y_0^2 = 0 - 1^2 = -1.$$

$$y'' = 1 - 2yy', \quad y''_0 = y''(x = x_0, y = y_0) = 1 - 2y_0y'_0 = 1 - 2(1)(-1) = 3.$$

$$y''' = -2yy' - 2(y')^2, \quad y'''_0 = y'''(x = x_0, y = y_0) = -2y_0y'_0 - 2(y'_0)^2 = -8.$$

$$y^{(4)} = -2yy'' - 6y'y'',$$

$$y^{(4)}_0 = y^{(4)}(x = x_0, y = y_0) = -2y_0y''_0 - 6y'_0y''_0 = 34.$$

$$y^{(5)} = -2yy^{(4)} - 8y'y''' - 6(y')^2,$$

$$y^{(5)}_0 = y^{(5)}(x = x_0, y = y_0) = -2y_0y^{(4)}_0 - 8y'_0y'''_0 - 6(y'_0)^2 = -186.$$

Substituting these values in (6), we obtain

$$y(x) = 1 - x + \frac{3}{2}x^2 - \frac{4}{3}x^3 + \frac{17}{12}x^4 - \frac{31}{20}x^5 + \dots \quad \dots(7)$$

To obtain $y(0.1)$ correct to four decimal places, we consider the terms upto x^4 and putting $x=0.1$, we obtain

$$y(0.1) = 0.9138.$$

Remark to the Example (*Truncation and range of x*) Suppose that we wish to find the range of values of x for which the above series, truncated after the term containing x^4 , can be used to compute the values of y correct to four decimal places. We need only to write

$$\frac{31}{20}x^5 \leq 0.00005,$$

so that $x \leq 0.126$.

Example Solve using Taylor series method $\frac{dy}{dx} = x + y$ numerically starting with $x=1$, $y=0$.

Also find y at $x=1.1$.

Here $x_0 = 1$; $y_0 = y(1) = 0$. Hence (4) takes the form

$$y(x) = y_0 + (x-1)y'_0 + \frac{(x-1)^2}{2!}y''_0 + \frac{(x-1)^3}{3!}y'''_0 + \frac{(x-1)^4}{4!}y^{(4)}_0 + \dots \quad \dots(7)$$

Here

$$y' = x + y ; \quad y'_0 = y'(x = x_0, y = y_0) = x_0 + y_0 = 1 + 0 = 1 \quad y'' = \frac{d}{dx}(x + y) = 1 + y' ;$$

$$y''_0 = y''(x = x_0, y = y_0) = 1 + y'_0 = 1 + 1 = 2$$

$$y''' = y'' ; \quad y'''_0 = y''(x = x_0, y = y_0) = y''_0 = 2.$$

$$y^{(4)} = y''' ; \quad y^{(4)}_0 = y'''(x = x_0, y = y_0) = y'''_0 = 2.$$

Substituting these values in (7), we obtain

$$y(x) = (x-1) + (x-1)^2 + \frac{(x-1)^3}{3} + \frac{(x-1)^4}{12} + \dots$$

Now to find $y(1.1)$, we put $x=1.1$ in the above series (considering terms upto 4th power of x) we get

$$y(1.1) = 0.1 + (0.1)^2 + \frac{(0.1)^3}{3} + \frac{(0.1)^4}{12} = 0.11.$$

Exact solution of the above initial value problem is

$$y = -x - 1 + 2e^{x-1}$$

and hence the exact value of y at $x=1.1$ is

$$y(1.1) = 0.11034.$$

Example Using Taylor series, solve

$$5xy' + y^2 - 2 = 0, \quad y(4) = 1.$$

Also, find $y(4.1)$.

Here $x_0 = 4$; $y_0 = y(4) = 1$. Hence (4) takes the form

$$y(x) = y_0 + (x-4)y'_0 + \frac{(x-4)^2}{2!}y''_0 + \frac{(x-4)^3}{3!}y'''_0 + \frac{(x-4)^4}{4!}y^{(4)}_0 + \dots \quad \dots(8)$$

Here y'_0, y''_0, \dots are evaluated as follows:

Consider the differential equation

$$5xy' + y^2 - 2 = 0 \quad \dots(9)$$

Differentiating (9) with respect to x , we get

$$5xy'' + 5y' + 2yy' = 0. \quad \dots(10)$$

Differentiating successively with respect to x , we obtain

$$5xy''' + 10y'' + 2yy'' + 2(y')^2 = 0 \quad \dots(11)$$

$$5xy'''' + 15y''' + 2yy''' + 6y'y'' = 0 \quad \dots(12)$$

$$5xy''''' + 20y'''' + 2yy'''' + 8y'y''' + 6(y'')^2 = 0 \dots(13)$$

Using $x_0 = 4$; $y_0 = 1$, (9) gives $5x_0y'_0 + y_0^2 - 2 = 0$ or $5 \cdot 4 \cdot y'_0 + 1^2 - 2 = 0$ which gives $y'_0 = 0.05$.
 (10) gives

$$5x_0y''_0 + 5y'_0 + 2y_0y'_0 = 0 \quad \text{or} \quad 5 \times 4y''_0 + 5 \times 0.05 + 2 \times 1 \times 0.05 = 0$$

and gives $y''_0 = -0.0175$.

Similarly, $y'''_0 = 0.01025$, $y^{(4)}_0 = -0.00845$, $y^{(5)}_0 = 0.008998125$,

Hence (8) gives

$$y(x) = 1 + (x-4)(0.05) + \frac{(x-4)^2}{2!}(-0.0175) + \frac{(x-4)^3}{3!}(0.01025) \\ + \frac{(x-4)^4}{4!}(-0.00845) + \frac{(x-4)^5}{5!}(0.008998125)$$

Putting $x = 4.1$, we get

$$y(4.1) = 1 + (0.1)(0.05) + \frac{(0.1)^2}{2!}(-0.0175) + \frac{(0.1)^3}{3!}(0.01025) \\ + \frac{(0.1)^4}{4!}(-0.00845) + \frac{(0.1)^5}{5!}(0.008998125) \\ = 1.0049$$

Solution of Second Order IVP by Taylor Series Method

Consider the second order initial value problem

$$y'' = f(x, y, y'), \quad y(x_0) = y_0, \quad y'(x_0) = l_0. \quad \dots(14)$$

Setting $y' = p$, we get $y'' = p'$, and the differential equation in (14) becomes

$$p' = f(x, y, p) \quad \dots(15)$$

with the initial conditions

$$y(x_0) = y_0 \quad \dots(16)$$

and

$$p(x_0) = p_0 = l_0. \quad \dots(17)$$

Now Taylor series is given by

$$y(x) = y_0 + (x-x_0)y'_0 + \frac{(x-x_0)^2}{2!}y''_0 + \dots \quad \dots(18)$$

where y'_0, y''_0, \dots are determined using (16) and (17) and successive differentiation. The method is illustrated in the following example.

Example Using Taylor series method, prove that the solution of

$$\frac{d^2y}{dx^2} + xy = 0$$

with the initial conditions $y(0) = d$ and $y'(0) = 0$ is given by

$$y(x) = d \left[1 - \frac{1}{3!}x^3 + \frac{4}{6!}x^6 - \frac{28}{9!}x^9 + \dots \right] \quad \dots(19)$$

Set $y' = p$.

Then, $y'' = p'$,

and the given differential equation becomes

$$p' + xy = 0. \quad \dots(20)$$

Now we have to determine the coefficients of the Taylor series:

$$y(x) = y_0 + (x - x_0)y'_0 + \frac{(x - x_0)^2}{2!}y''_0 + \dots \quad \dots (21)$$

Here $x_0 = 0$, $y_0 = y(x_0) = y(0) = d$, $y'_0 = y'(x_0) = y'(0) = 0$.

From (20), $p' = -xy$,

so

$$\begin{aligned} y'' &= p' = -xy, & y''_0 &= -x_0 y_0 = 0; \\ y''' &= p'' = -y - xy', & y'''_0 &= -y_0 - x_0 y'_0 = -d; \\ y^{(4)} &= -2y' - xy'', & y^{(4)}_0 &= -2y'_0 - x_0 y''_0 = 0; \\ y^{(5)} &= -3y'' - xy''', & y^{(5)}_0 &= -3y''_0 - x_0 y'''_0 = 0; \\ y^{(6)} &= -4y''' - xy^{(4)}, & y^{(6)}_0 &= -4y'''_0 - x_0 y^{(4)}_0 = -4d; \\ y^{(7)} &= -5y^{(4)} - xy^{(5)}, & y^{(7)}_0 &= -5y^{(4)}_0 - x_0 y^{(5)}_0 = 0; \\ y^{(8)} &= -6y^{(5)} - xy^{(6)}, & y^{(8)}_0 &= -6y^{(5)}_0 - x_0 y^{(6)}_0 = 0; \\ y^{(9)} &= -7y^{(6)} - xy^{(7)}, & y^{(9)}_0 &= -7y^{(6)}_0 - x_0 y^{(7)}_0 = -7 \times 4d = -28d. \end{aligned}$$

Putting these values in (21), we obtain (19).

Example 9 Evaluate $y(0.1)$, using Taylor series method, given

$$y'' - x(y')^2 + y^2 = 0, \quad y(0) = 1, \quad y'(0) = 0$$

Solution

Set $y' = p$.

Then, $y'' = p'$,

and the given differential equation becomes

$$p' - xp^2 + y^2 = 0. \quad \dots(22)$$

Now we have to determine the coefficients of the Taylor series:

$$y(x) = y_0 + (x - x_0)y'_0 + \frac{(x - x_0)^2}{2!}y''_0 + \dots \quad \dots (23)$$

Here $x_0 = 0$, $y_0 = y(x_0) = y(0) = 1$, $p_0 = y'_0 = y'(x_0) = y'(0) = 0$.

From (22), $p' = xp^2 - y^2$,

so

$$\begin{aligned} y'' &= p' = xp^2 - y^2, & y''_0 &= x_0 p_0^2 - y_0^2 = 0 - 1 = -1; \\ y''' &= p'' = p^2 + 2xpp' - 2yy', & y'''_0 &= p_0^2 + 2x_0 p_0 p'_0 - 2y_0 y'_0 = 0; \end{aligned}$$

$$y''' = p'' = p^2 + 2xpp' - 2yy', \quad y_0''' = p_0^2 + 2x_0p_0p_0' - 2y_0y_0' = 0;$$

Putting these values in (23), we obtain

$$y(x) = 1 - \frac{x^2}{2!} + \dots \quad \dots (24)$$

Putting $x = 0.1$ in (24), neglecting higher powers of x , we obtain

$$y(0.1) \approx 1 - \frac{(0.1)^2}{2!} = 1 - 0.005 = 0.995.$$

Exercises

In Exercises 1–12, solve the given initial value problem using Taylor series method. Also find the value of y for the given x .

1. $\frac{dy}{dx} - 1 = xy$, $y(0) = 1$. Also find $y(0.1)$.
2. $\frac{dy}{dx} = x^2 + y^2 - 2$, $y = 1$ at $x = 0$. Also find $y(0.1)$.
3. $\frac{dy}{dx} = y^2 + 1$, $y(0) = 0$. Also find $y(0.1)$ and $y(0.2)$.
4. $\frac{dy}{dx} = x - y^2$, $y(0) = 1$. Obtain numerical values for $x = 0.2(0.2)0.6$.
5. $y' = x + y^2$, $y(0) = 0$. Obtain numerical values for
 $x = 0.0(0.2)0.4$.
6. $y' = x^2 + y^2$, $y(1) = 0$. Find $y(1.3)$.
7. Solve $y' = x + y$, $y(1) = 0$. Obtain numerical values for $x = 1.0(0.1)1.2$.
8. Solve $\frac{dy}{dx} = \frac{1}{x^2 + y}$, $y(4) = 4$. Also find $y(4.1)$ and $y(4.2)$.
9. Solve $\frac{dy}{dx} = 1 - 2xy$, $y(0) = 0$. Also find $y(0.2)$ and $y(0.4)$.
10. Solve $\frac{dy}{dx} = xy^{1/3}$, $y(1) = 1$. Also find $y(1.1)$ and $y(1.2)$.
11. Solve $\frac{dy}{dx} = x^2 - y$, $y(0) = 1$. Also find y at $x = 0.1(0.1)0.4$.

12. Solve $\frac{dy}{dx} - 2y = 3e^x$, $y(0) = 0$. Also find $y(0.1)$ and $y(0.2)$.

In Exercises 13–15, solve the given second order initial value problem using Taylor series method. Also find the value of y for the given x .

13. $\frac{d^2y}{dx^2} = y + x \frac{dy}{dx}$, $y(0) = 1$, $y'(0) = 0$. Also find $y(0.1)$.
14. $\frac{d^2y}{dx^2} + xy = 0$, $y(0) = 1$, $y'(0) = 0.5$. Also find $y(0.1)$ and $y(0.2)$.
15. $\frac{d^2y}{dx^2} = x^2 - xy$, $y(0) = 1$, $y'(0) = 0$. Also find $y(0.1)$ and $y(0.2)$.

15

PICARDS ITERATION METHOD

Consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0. \quad \dots(1^*)$$

Also, assume (1*) have a unique solution on some interval containing x_0 . By separating variables, the differential equation in (1) becomes

$$dy = f(x, y)dx. \quad \dots(1^{**})$$

Integrating (1**) from x_0 to x with respect to x , (at the same time y changes from y_0 to y) we get

$$\int_{y_0}^y dy = \int_{x_0}^x f(x, y)dx$$

or
$$y(x) - y_0 = \int_{x_0}^x f(x, y)dx$$

or
$$y(x) = y_0 + \int_{x_0}^x f(x, y)dx \quad \dots(2)$$

It can be verified, by substituting $x = x_0$ and $y = y_0$ in (2), that (2) satisfies the initial condition in (1).

To find the approximations to the solution $y(x)$ of (2) we proceed as follows:

We substitute the first approximation $y = y_0$ on the right side of (2), and obtain the better approximation

$$y^{(1)}(x) = y_0 + \int_{x_0}^x f(x, y_0)dx \quad \dots(3)$$

In the next step we substitute the function $y^{(1)}(x)$ on the right side of (2) and obtain

$$y^{(2)}(x) = y_0 + \int_{x_0}^x f(x, y^{(1)}(x))dx, \quad \dots(4)$$

The n^{th} step of this iteration gives an approximating function

$$y^{(n)}(x) = y_0 + \int_{x_0}^x f(x, y^{(n-1)}(x))dx \quad \dots(5)$$

In this way we obtain a sequence of approximations

$$y^{(1)}(x), y^{(2)}(x), \dots, y^{(n)}(x), \dots$$

Working Rule

Consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0.$$

Then Picard's iterative formula is

$$y^{(n)} = y_0 + \int_{x_0}^x f(x, y^{(n-1)}) dx \quad (n = 1, 2, 3, \dots) \quad \dots(6)$$

with $y^{(0)} = y_0$.

Example Find approximate solutions by Picard's iteration method to the initial value problem $y' = 1 + y^2$ with the initial condition $y(0) = 0$. Hence find the approximate value of y at $x = 0.1$ and $x = 0.2$.

Picard's iteration's n^{th} step is given by (6).

In this problem

$$f(x, y) = 1 + y^2; \quad x_0 = 0, \quad y^{(0)} = y_0 = y(x_0) = y(0) = 0,$$

and hence

$$f(x, y^{(n-1)}) = 1 + (y^{(n-1)})^2.$$

Substituting these values in (6),

$$y^{(n)} = 0 + \int_0^x [1 + (y^{(n-1)})^2] dx \quad (n = 1, 2, 3, \dots)$$

i.e.,
$$y^{(n)} = x + \int_0^x (y^{(n-1)})^2 dx \quad (n = 1, 2, 3, \dots)$$

$$y^{(1)} = x + \int_0^x (y^{(0)})^2 dx$$

Putting $y^{(0)} = 0$,

$$y^{(1)} = x + \int_0^x 0^2 dx = x.$$

$$y^{(2)} = x + \int_0^x (y^{(1)})^2 dx$$

Putting $y^{(1)} = x$,

$$y^{(2)} = x + \int_0^x x^2 dx = x + \frac{1}{3}x^3.$$

$$y^{(3)} = x + \int_0^x \left(y^{(2)}\right)^2 dx$$

Putting $y^{(2)} = x + \frac{1}{3}x^3$,

$$\begin{aligned} y^{(3)} &= x + \int_0^x \left(x + \frac{1}{3}x^3\right)^2 dx \\ &= x + \frac{1}{3}x^3 + \frac{2}{15}x^5 + \frac{1}{63}x^7. \end{aligned}$$

We can continue the process. But we take the above as an approximate solution to the given initial value problem. That is,

$$y = y(x) = x + \frac{1}{3}x^3 + \frac{2}{15}x^5 + \frac{1}{63}x^7. \quad \dots(7)$$

Substituting $x = 0.1$, and $x = 0.2$, in (7), we obtain

$$y(0.1) = 0.100334$$

and $y(0.2) = 0.202709$.

The above are not exact values for y at the given x points, but the approximate values.

Example Given $\frac{dy}{dx} = x + y$ with the initial condition $y(0) = 1$. Find approximately the value of y for $x = 0.2$ and $x = 1$.

Here $f(x, y) = x + y$; $x_0 = 0$, $y^{(0)} = y_0 = y(x_0) = y(0) = 1$, and hence using (6)

$$y^{(n)} = 1 + \int_0^x (x + y^{(n-1)}) dx$$

i.e.,
$$y^{(n)} = 1 + \frac{x^2}{2} + \int_0^x y^{(n-1)} dx$$

$$y^{(1)} = 1 + \frac{x^2}{2} + \int_0^x y^{(0)} dx$$

Putting $y^{(0)} = 1$, we obtain

$$y^{(1)} = 1 + \frac{x^2}{2} + \int_0^x dx = 1 + x + \frac{x^2}{2}.$$

$$y^{(2)} = 1 + \frac{x^2}{2} + \int_0^x y^{(1)} dx$$

Putting $y^{(1)} = 1 + x + \frac{x^2}{2}$, we obtain

$$y^{(2)} = 1 + \frac{x^2}{2} + \int_0^x \left(1 + x + \frac{x^2}{2} \right) dx$$

$$= 1 + x + x^2 + \frac{x^3}{6}$$

$$y^{(3)} = 1 + \frac{x^2}{2} + \int_0^x y^{(2)} dx$$

Putting $y^{(2)} = 1 + x + x^2 + \frac{x^3}{6}$, we obtain

$$y^{(3)} = 1 + \frac{x^2}{2} + \int_0^x \left(1 + x + x^2 + \frac{x^3}{6} \right) dx$$

$$= 1 + x + x^2 + \frac{x^3}{3} + \frac{x^4}{24}$$

We accept

$$y = 1 + x + x^2 + \frac{x^3}{3} + \frac{x^4}{24}$$

as an approximate solution.

When $x = 0.2$, we have

$$y(0.2) = 1 + 0.2 + (0.2)^2 + \frac{(0.2)^3}{3} + \frac{(0.2)^4}{24} = 1.2427.$$

When $x = 1.0$, we have

$$y(1.0) = 1 + 1 + 1 + \frac{1}{3} + \frac{1}{24} = 3.3751.$$

Example Solve by Picard's method

$$y' - xy = 1, \text{ given } y = 0, \text{ when } x = 2.$$

Also find $y(2.05)$ correct to four places of decimal.

Here $y' = 1 + xy.$

Hence $f(x, y) = 1 + xy; \quad x_0 = 2, \quad y^{(0)} = y_0 = y(x_0) = y(2) = 0,$

and hence

$$f(x, y^{(n-1)}) = 1 + xy^{(n-1)}.$$

Substituting these values in (5), we obtain

$$y^{(n)} = 0 + \int_2^x (1 + xy^{(n-1)}) dx \quad (n = 1, 2, 3, \dots)$$

i.e.,
$$y^{(n)} = x - 2 + \int_2^x xy^{(n-1)} dx \quad (n = 1, 2, 3, \dots)$$

$$y^{(1)} = x - 2 + \int_2^x xy^{(0)} dx$$

Putting $y^{(0)} = 0$, we obtain

$$y^{(1)} = x - 2 + \int_2^x x \cdot 0 dx$$

i.e.,
$$y^{(1)} = x - 2.$$

$$y^{(2)} = x - 2 + \int_2^x xy^{(1)} dx$$

Putting $y^{(1)} = x - 2$, we obtain

$$y^{(2)} = x - 2 + \int_2^x x(x - 2) dx$$

$$= -\frac{2}{3} + x - x^2 + \frac{x^3}{3}.$$

$$y^{(3)} = x - 2 + \int_2^x xy^{(2)} dx$$

Putting $y^{(2)} = -\frac{2}{3} + x - x^2 + \frac{x^3}{3}$, we obtain

$$y^{(3)} = x - 2 + \int_2^x x \left(-\frac{2}{3} + x - x^2 + \frac{x^3}{3} \right) dx$$

$$= -\frac{22}{15} + x - \frac{x^2}{3} + \frac{x^3}{3} - \frac{x^4}{4} + \frac{x^5}{15}.$$

We consider

$$y = -\frac{22}{15} + x - \frac{x^2}{3} + \frac{x^3}{3} - \frac{x^4}{4} + \frac{x^5}{15}$$

as an approximate solution. Substituting $x = 2.05$, we get

$$y(2.05) \approx 0.0526.$$

Example Solve the $\frac{dy}{dx} = \frac{y-x}{y+x}$, $y(0) = 1$ using Picard's method. Find the value of y at $x = 0.1$ approximately.

Here $f(x, y) = \frac{y-x}{y+x}$; $x_0 = 0$, $y^{(0)} = y_0 = y(x_0) = y(0) = 1$, and hence by (6),

$$y^{(n)} = 1 + \int_0^x \frac{y^{(n-1)} - x}{y^{(n-1)} + x} dx$$

$$y^{(1)} = 1 + \int_0^x \frac{y^{(0)} - x}{y^{(0)} + x} dx$$

Putting $y^{(0)} = 1$, we obtain

$$y^{(1)} = 1 + \int_0^x \frac{1-x}{1+x} dx$$

By actual division,

$$\frac{1-x}{1+x} = -1 + \frac{2}{1+x}$$

and hence the above can be written as

$$\begin{aligned} y^{(1)} &= 1 + \int_0^x \left(-1 + \frac{2}{1+x} \right) dx \\ &= 1 - x + 2\ln(1+x). \end{aligned}$$

We take $y = 1 - x + 2\ln(1+x)$ as an approximate solution and hence the value of y at $x = 0.1$ (with $\ln 1.1 =$ natural logarithm of $1.1 = 0.0953$) is given by

$$y(0.1) \approx 1 - 0.1 + 2\ln(1+0.1) = 0.9 + 2\ln 1.1 = 1.0906.$$

Example Given the differential equation

$$\frac{dy}{dx} = \frac{x^2}{y^2 + 1}$$

with the initial condition $y = 0$ when $x = 0$, use Picard's method to obtain y for $x = 0.25, 0.5$ and 1.0 correct to three decimal places.

Here $f(x, y) = \frac{x^2}{y^2 + 1}$; $x_0 = 0$, $y^{(0)} = y_0 = y(x_0) = y(0) = 0$, and hence by (6),

$$y^{(n)} = \int_0^x \frac{x^2}{\left(y^{(n-1)}\right)^2 + 1} dx$$

$$y^{(1)} = \int_0^x \frac{x^2}{\left(y^{(0)}\right)^2 + 1} dx$$

Putting $y^{(0)} = 0$, we obtain

$$y^{(1)} = \int_0^x x^2 dx = \frac{1}{3} x^3$$

$$y^{(2)} = \int_0^x \frac{x^2}{\left(y^{(1)}\right)^2 + 1} dx$$

Putting $y^{(1)} = \frac{1}{3} x^3$, we obtain

$$\begin{aligned} y^{(2)} &= \int_0^x \frac{x^2}{(1/9)x^6 + 1} dx = \int_0^x \frac{d(\frac{1}{3}x^3)}{(\frac{1}{3}x^3)^2 + 1} dx \\ &= \tan^{-1}\left(\frac{1}{3}x^3\right) = \frac{1}{3}x^3 - \frac{1}{81}x^9 + \dots \end{aligned}$$

so that $y^{(1)}$ and $y^{(2)}$ agree to the first term, viz., $(1/3)x^3$. To find the range of values of x so that the series with the term $(1/3)x^3$ alone will give the result correct to three decimal places, we put

$$\frac{1}{81}x^9 \leq 0.0005$$

which yields

$$x \leq 0.7$$

Hence

$$y(0.25) = \frac{1}{3}(0.25)^3 = 0.005$$

$$y(0.5) = \frac{1}{3}(0.5)^3 = 0.042$$

When $x=1.0$ ($x \leq 0.7$ is not true) so we have to consider the second term $-\frac{1}{81}x^9$ also into consideration and get

$$y(1.0) = \frac{1}{3} - \frac{1}{81} = 0.321.$$

Exercises

In Exercises 1-7, solve the initial value problem by Picard's iteration method (Do three steps).

1. $y' = y$, $y(0) = 1$.
2. $y' = x + y$, $y(0) = -1$.
3. $y' = xy + 2x - x^3$, $y(0) = 0$.
4. $y' = y - y^2$, $y(0) = \frac{1}{2}$.
5. $y' = y^2$, $y(0) = 1$.
6. $y' = 2\sqrt{y}$, $y(1) = 0$.

7. $y' = \frac{3y}{x}$, $y(1) = 1$.

In Exercises 8-16, solve the initial value problem by Picard's iteration method (Do four steps). Also find the value of y at the given points of x .

8. $y' = 2x - y$, $y(1) = 3$. Also find $y(1.1)$.

9. $y' = x - y$, $y(0) = 1$. Also find $y(0.2)$.

10. $y' = x^2 y$, $y(1) = 2$. Also find $y(1.2)$.

11. $y' = 3x + y^2$, $y(0) = 1$. Also find $y(0.1)$.

12. $y' = 2x + 3y$, $y(0) = 1$. Also find $y(0.25)$.

13. $2\frac{dy}{dx} = x + y$, $y(0) = 2$. Also find $y(0.1)$.

14. $\frac{dy}{dx} + \frac{y}{x} = \frac{1}{x^2}$, $y(1) = 1$. Also find $y(1.1)$.

15. $\frac{dy}{dx} - 1 = xy$, $y(0) = 1$. Also find $y(0.1)$.

16. $\frac{dy}{dx} = x(1 + x^3 y)$, $y(0) = 3$. Also find $y(0.1)$ and $y(0.2)$.

17. Obtain the approximate solution of

$$\frac{dy}{dx} = x + x^4 y, \quad y(0) = 3$$

by Picard's iteration method. Tabulate the values of y , for $x = 0.1(0.1)0.5, 3D$.

16

EULER METHODS

Consider the initial value problem of first order

$$y' = f(x, y), \quad y(x_0) = y_0. \quad \dots(1)$$

Starting with given x_0 and the value of h is chosen so small, we suppose x_0, x_1, x_2, \dots be equally spaced x values (called *mesh points*) with interval h .

i.e., $x_1 = x_0 + h, \quad x_2 = x_1 + h, \dots$

Also denote $y_0 = y(x_0), \quad y_1 = y(x_1), \quad y_2 = y(x_2), \dots$

By separating variables, the differential equation in (1) becomes

$$dy = f(x, y)dx. \quad \dots(1A)$$

Integrating (1A) from x_0 to x_1 with respect to x , (at the same time y changes from y_0 to y_1) we get

$$\int_{y_0}^{y_1} dy = \int_{x_0}^{x_1} f(x, y)dx$$

or
$$y_1 - y_0 = \int_{x_0}^{x_1} f(x, y)dx$$

or
$$y_1 = y_0 + \int_{x_0}^{x_1} f(x, y)dx \quad \dots(2)$$

Assuming that $f(x, y) \approx f(x_0, y_0)$ in $x_0 \leq x \leq x_1$, (2) gives

$$y_1 \approx y_0 + f(x_0, y_0)(x_1 - x_0)$$

or
$$y_1 \approx y_0 + hf(x_0, y_0).$$

Similarly, for the range $x_1 \leq x \leq x_2$, we have

$$y_2 = y_1 + \int_{x_1}^{x_2} f(x, y)dx \quad \dots(3)$$

Assuming that $f(x, y) \approx f(x_1, y_1)$ in $x_1 \leq x \leq x_2$, (3) gives

$$y_2 \approx y_1 + hf(x_1, y_1).$$

Proceeding in this way, we obtain the general formula

$$y_{n+1} = y_n + hf(x_n, y_n) \quad (n = 0, 1, \dots) \quad \dots(4)$$

The above is called the **Euler method** or **Euler-Cauchy method**.

Working Rule (Euler method)

Given the initial value problem (1). Suppose x_0, x_1, x_2, \dots be equally spaced x values with interval h . i.e., $x_1 = x_0 + h, x_2 = x_1 + h, \dots$ Also denote $y_0 = y(x_0), y_1 = y(x_1), y_2 = y(x_2), \dots$

Then the iterative formula of **Euler method** is:

$$y_{n+1} = y_n + hf(x_n, y_n) \quad (n = 0, 1, \dots) \quad \dots(5)$$

Example Use Euler's method with $h = 0.1$ to solve the initial value problem

$$\frac{dy}{dx} = x^2 + y^2 \text{ with } y(0) = 0 \text{ in the range } 0 \leq x \leq 0.5.$$

Here $f(x, y) = x^2 + y^2, x_0 = 0, y_0 = 0, h = 0.1$.

Hence

$$x_1 = x_0 + h = 0.2, \quad x_2 = x_1 + h = 0.3, \quad x_3 = x_2 + h = 0.4, \quad x_4 = x_3 + h = 0.5, \quad x_5 = x_4 + h = 0.6.$$

We determine y_1, y_2, y_3, y_4, y_5 using the Euler formula (5). Substituting the given value in

$$y_{n+1} = y_n + hf(x_n, y_n)$$

we obtain

$$y_{n+1} = y_n + 0.1(x_n^2 + y_n^2) \quad (n = 0, 1, \dots)$$

$$y_1 = y_0 + 0.1(x_0^2 + y_0^2) = 0 + 0.1(0 + 0) = 0.$$

$$y_2 = y_1 + 0.1(x_1^2 + y_1^2) = 0 + 0.1[(0.1)^2 + 0^2] = 0.001.$$

$$y_3 = y_2 + 0.1(x_2^2 + y_2^2) = 0.001 + 0.1[(0.2)^2 + (0.001)^2] = 0.005.$$

$$y_4 = y_3 + 0.1(x_3^2 + y_3^2) = 0.005 + 0.1[(0.3)^2 + (0.005)^2] = 0.014.$$

$$y_5 = y_4 + 0.1(x_4^2 + y_4^2) = 0.014 + 0.1[(0.4)^2 + (0.014)^2] = 0.0300196.$$

Hence

$$y(0) = 0 \qquad y(0.1) = 0 \qquad y(0.2) = 0.001$$

$$y(0.3) = 0.005 \qquad y(0.4) = 0.014 \qquad y(0.5) = 0.0300196.$$

Example Using Euler method solve the equation $y' = 2xy + 1$ with $y(0) = 0, h = 0.02$ for $x = 0.1$.

Here $f(x, y) = 2xy + 1, x_0 = 0, y_0 = 0, h = 0.02$. Hence

$$x_1 = x_0 + h = 0.02, \quad x_2 = x_1 + h = 0.04, \quad x_3 = x_2 + h = 0.06, \quad x_4 = x_3 + h = 0.08, \quad x_5 = x_4 + h = 0.1.$$

We determine y_1, y_2, y_3, y_4, y_5 using the Euler formula (5). Substituting the given value in

$$y_{n+1} = y_n + hf(x_n, y_n)$$

we obtain

$$y_{n+1} = y_n + 0.02(2x_n y_n + 1) \quad (n = 0, 1, \dots)$$

$$y_1 = y_0 + 0.02(2x_0 y_0 + 1) = 0 + 0.02(0 + 1) = 0.02.$$

$$y_2 = y_1 + 0.02(2x_1 y_1 + 1) = 0.02 + 0.02(2 \times 0.02 \times 0.02 + 1) = 0.04,$$

approximate to 2 places of decimals

$$y_3 = y_2 + 0.02(2x_2 y_2 + 1) = 0.04 + 0.02(2 \times 0.04 \times 0.04 + 1) = 0.06$$

$$y_4 = y_3 + 0.02(2x_3 y_3 + 1) = 0.06 + 0.02(2 \times 0.06 \times 0.06 + 1) = 0.08$$

$$y_5 = y_4 + 0.02(2x_4 y_4 + 1) = 0.08 + 0.02(2 \times 0.08 \times 0.08 + 1) = 0.1$$

Hence

$$y(0) = 0 \qquad y(0.02) = 0.02 \qquad y(0.04) = 0.04$$

$$y(0.06) = 0.06 \qquad y(0.08) = 0.08 \qquad y(0.1) = 0.1.$$

That is the approximate value of $y(0.1)$ is 0.1.

Example Given the initial value problem $y' = x + y, y(0) = 0$. Find the value of y approximately for $x = 1$ by Euler method in five steps. Compare the result with the exact value.

Here $f(x, y) = x + y, x_0 = 0, y_0 = y(x_0) = y(0) = 0$. As we have to calculate the value of y in

five steps, we have to take $h = \frac{x_n - x_0}{n} = \frac{1 - 0}{5} = 0.2$. Hence

$$x_1 = x_0 + h = 0.2, \quad x_2 = x_1 + h = 0.4, \quad x_3 = x_2 + h = 0.6, \quad x_4 = x_3 + h = 0.8, \quad x_5 = x_4 + h = 1.0.$$

We determine y_1, y_2, y_3, y_4, y_5 using the Euler formula (5). Substituting the given value in (5), we obtain

$$y_{n+1} = y_n + 0.2(x_n + y_n) \quad (n = 0, 1, \dots)$$

The steps are given in the following Table.

Also the exact solution to the linear differential equation $y' = x + y$ with the initial condition $y(0) = 0$ can be found out to be

$$y = e^x - x - 1. \quad \dots(6)$$

The exact values of y can be evaluated from (6) by substituting the corresponding x values, in particular,

$$y_1 = y(x_1) = e^{x_1} - x_1 - 1 = e^{0.2} - 0.2 - 1 = 0.000, \text{ approximately.}$$

The other exact values are also shown in the following table.

n	x_n	approximate value of y_n	$0.2(x_n + y_n)$	Exact values	Absolute value of Error
0	0.0	0.000	0.000	0.000	0.000
1	0.2	0.000	0.040	0.021	0.021
2	0.4	0.040	0.088	0.092	0.052
3	0.6	0.128	0.146	0.222	0.094
4	0.8	0.274	0.215	0.426	0.152
5	1.0	0.489		0.718	0.229

The approximate value of $y(1.0)$ by Euler's method is 0.489, while exact value is 0.718.

Exercises

In Exercises 1-11, solve the initial value problem using Euler's method for value of y at the given point of x with given (h is given in brackets)

1. $\frac{dy}{dx} = 1 - y$, $y(0) = 0$ at the point $x = 0.2$ ($h = 0.1$).
2. $\frac{dy}{dx} = \frac{y - x}{1 + x}$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.02$).
3. $yy' = x$, $y(0) = 1.5$ at the point $x = 0.2$ ($h = 0.1$).
4. $\frac{dy}{dx} = 3x + \frac{1}{2}y$, $y(0) = 1$ at the point $x = 0.2$ ($h = 0.05$).
5. $y' = x + y + xy$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.02$).

6. $\frac{dy}{dx} = 1 + y^2$, $y(0) = 0$ at the point $x = 0.4$ ($h = 0.2$).
7. $\frac{dy}{dx} = xy$, $y(0) = 1$ at the point $x = 0.4$ ($h = 0.2$).
8. $\frac{dy}{dx} = 1 + \ln(x + y)$, $y(0) = 1$ at the point $x = 0.2$ ($h = 0.1$).
9. $y' = x^2 + y$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.05$).
10. $y' = 2xy$, $y(0) = 1$ at the point $x = 0.5$ ($h = 0.1$).
11. $y' = -y$, $y(0) = 1$ at the point $x = 0.04$ ($h = 0.01$).

In Exercises 12-15, apply Euler's method. Do 10 steps. Also solve the problem exactly. Compute the errors to see that the method is too inaccurate for practical purposes.

12. $y' + 0.1y = 0$, $y(0) = 2$, $h = 0.1$
13. $y' = \frac{1}{2}f\sqrt{1 - y^2}$, $y(0) = 0$, $h = 0.1$
14. $y' + 5x^4y^2 = 0$, $y(0) = 1$, $h = 0.2$
15. $y' = (y + x)^2$, $y(0) = 1$, $h = 0.1$
16. Solve using Euler's method $y'(x + y) = y - x$ with $y(0) = 2$ for the range 0.00(0.02)0.06.
17. Solve using Euler's method $y' = y - \frac{2x}{y}$ with $y = 1$ at $x = 0$ for $h = 0.5$ on the interval $[0, 1]$.
18. Using Euler's method find $y(0.2)$ of the initial value problem $y' = x + 2y$, $y(0) = 1$, taking $h = 0.1$.
19. Using Euler's method find the value of y at the point $x = 2$ in steps of 0.2 of the initial value problem $\frac{dy}{dx} = 2 + \sqrt{xy}$, $y(1) = 1$.

Modified Euler Method

Modified Euler method is given by the iteration formula

$$y_1^{(n+1)} = y_0 + \frac{h}{2} [f(x_0, y_0) + f(x_1, y_1^{(n)})], \quad n = 0, 1, 2, \dots$$

where $y_1^{(n)}$ is the n th approximation to y_1 . The iteration formula can be started by choosing $y_1^{(0)}$ from Euler's formula

$$y_1^{(0)} = y_0 + hf(x_0, y_0).$$

Example Using modified Euler's method, determine the value of y when $x = 0.1$ given that

$$y' = x^2 + y; \quad y(0) = 1. \quad (\text{Take } h = 0.05)$$

Here $f(x, y) = x^2 + y; \quad x_0 = 0, \quad y_0 = 1.$

$$y_1^{(0)} = y_0 + hf(x_0, y_0) = 1 + 0.05(1) = 1.05$$

$$\begin{aligned} y_1^{(1)} &= y_0 + \frac{h}{2} [f(x_0, y_0) + f(x_1, y_1^{(0)})] \\ &= 1 + \frac{0.05}{2} [f(0, 1) + f(0.05, 1.05)] \\ &= 1 + 0.025[1 + (0.05)^2 + 1.05] \\ &= 1.0513 \end{aligned}$$

$$\begin{aligned} y_1^{(2)} &= y_0 + \frac{h}{2} [f(x_0, y_0) + f(x_1, y_1^{(1)})] \\ &= 1 + \frac{0.05}{2} [f(0, 1) + f(0.05, 1.0513)] \\ &= 1 + 0.025[1 + (0.05)^2 + 1.0513] \\ &= 1.0513 \end{aligned}$$

Hence we take $y_1 = 1.0513$, which is correct to four decimal places.

Formula takes the form

$$y_2^{(n+1)} = y_1 + \frac{h}{2} [f(x_1, y_1) + f(x_2, y_2^{(n)})] \quad n = 0, 1, 2, \dots$$

where we first evaluate $y_2^{(0)}$ using the Euler formula

$$\begin{aligned} y_2^{(0)} &= y_1 + hf(x_1, y_1). \\ &= 1.0513 + 0.05[(0.05)^2 + 1.0513] = 1.1040 \end{aligned}$$

$$\begin{aligned} y_2^{(1)} &= y_1 + \frac{h}{2} [f(x_1, y_1) + f(x_2, y_2^{(0)})] \\ &= 1 + \frac{0.05}{2} \left\{ [(0.05)^2 + 1.0513] + [(0.1)^2 + 1.1040] \right\} \\ &= 1.1055 \end{aligned}$$

$$\begin{aligned}
 y_2^{(2)} &= y_1 + \frac{h}{2} [f(x_1, y_1) + f(x_2, y_2^{(1)})] \\
 &= 1 + \frac{0.05}{2} \{ [(0.05)^2 + 1.0513] + [(0.1)^2 + 1.1055] \} \\
 &= 1.1055
 \end{aligned}$$

Hence we take $y_2 = 1.1055$.

Hence the value of y when $x = 0.1$ is 1.1055 correct to four decimal places.

Example Using modified Euler's method, determine the value of y when $x = 0.2$ given that

$$\frac{dy}{dx} = x + \sqrt{y}; \quad y(0) = 1. \quad (\text{Take } h = 0.2)$$

Here $f(x, y) = x + \sqrt{y}$; $x_0 = 0$, $y_0 = 1$.

$$y_1^{(0)} = y_0 + hf(x_0, y_0) = 1 + 0.2(0 + 1) = 1.2$$

$$\begin{aligned}
 y_1^{(1)} &= y_0 + \frac{h}{2} [f(x_0, y_0) + f(x_1, y_1^{(0)})] \\
 &= 1 + \frac{0.2}{2} [1 + (0.2 + \sqrt{1.2})] = 1.2295.
 \end{aligned}$$

$$\begin{aligned}
 y_1^{(2)} &= y_0 + \frac{h}{2} [f(x_0, y_0) + f(x_1, y_1^{(1)})] \\
 &= 1 + \frac{0.2}{2} [1 + (0.2 + \sqrt{1.2295})] = 1.2309.
 \end{aligned}$$

$$\begin{aligned}
 y_1^{(3)} &= y_0 + \frac{h}{2} [f(x_0, y_0) + f(x_1, y_1^{(2)})] \\
 &= 1 + \frac{0.2}{2} [1 + (0.2 + \sqrt{1.2309})] = 1.2309.
 \end{aligned}$$

Hence we take $y(0.2) = y_1 = 1.2309$.

Exercises

In Exercises 1-11, solve the initial value problem using modified Euler's method for value of y at the given point of x with given (h is given in brackets)

1. $\frac{dy}{dx} = 1 - y$, $y(0) = 0$ at the point $x = 0.2$ ($h = 0.1$).
2. $\frac{dy}{dx} = \frac{y - x}{1 + x}$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.02$).

3. $yy' = x$, $y(0) = 1.5$ at the point $x = 0.2$ ($h = 0.1$).
4. $\frac{dy}{dx} = 3x + \frac{1}{2}y$, $y(0) = 1$ at the point $x = 0.2$ ($h = 0.05$).
5. $y' = x + y + xy$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.02$).
6. $\frac{dy}{dx} = 1 + y^2$, $y(0) = 0$ at the point $x = 0.4$ ($h = 0.2$).
7. $\frac{dy}{dx} = xy$, $y(0) = 1$ at the point $x = 0.4$ ($h = 0.2$).
8. $\frac{dy}{dx} = 1 + \ln(x + y)$, $y(0) = 1$ at the point $x = 0.2$ ($h = 0.1$).
9. $y' = x^2 + y$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.05$).
10. $y' = 2xy$, $y(0) = 1$ at the point $x = 0.5$ ($h = 0.1$).
11. $y' = -y$, $y(0) = 1$ at the point $x = 0.04$ ($h = 0.01$).

RUNGE KUTTA METHODS

The Taylor series method has desirable features, particularly in its ability to keep the errors small, but that it also has the strong disadvantage of requiring the evaluation of higher derivatives of the function $f(x,y)$. In the Taylor series method, each of these higher order derivatives is evaluated at the point x_i at the beginning of the step, in order to evaluate $y(x_i)$ at the end of the step. We observed that the Euler method could be improved by computing the function $f(x,y)$ at a predicted point at the far end of the step in x . The Runge-Kutta approach is to aim for the desirable features of the Taylor series method, but with the replacement of the requirement for the evaluation of higher order derivatives with the requirement to evaluate $f(x,y)$ at some points within the step x_i to x_{i+1} . Since it is not initially known at which points in the interval these evaluations should be done, it is possible to choose these points in such a way that the result is consistent with the Taylor series solution to some particular, which we shall call the order of the Runge-Kutta method. The Runge-Kutta method of order $N = 4$ is most popular. It is a good choice for common purposes because it is quite accurate, stable, and easy to program. Most authorities proclaim that it is not necessary to go to a higher-order method because the increased accuracy is offset by additional computational effort. If more accuracy is required, then either a smaller step size or an adaptive method should be used.

We use the fact that Runge-Kutta method of r^{th} order agree with Taylor's series solution up to the terms of h^r .

Second Order Runge-Kutta Method

Computationally, most efficient methods in terms of accuracy were developed by two German mathematicians, Carl Runge and Wilhelm Kutta. These methods are well known as Runge-Kutta methods (R-K methods). In this and the coming section we consider second and fourth order R-K methods.

There are several second order Runge-Kutta formulas and we consider one among them.

Working Method (Second Order Runge-Kutta Method)

Given the initial value problem (1). Suppose x_0, x_1, x_2, \dots be equally spaced x values with interval h . i.e.,

$$x_1 = x_0 + h, \quad x_2 = x_1 + h, \dots$$

Also denote $y_0 = y(x_0), y_1 = y(x_1), y_2 = y(x_2), \dots$

For $n = 0, 1, \dots$ until termination do:

$$x_{n+1} = x_n + h$$

$$k_n = hf(x_n, y_n) \quad \dots(8)$$

$$l_n = hf(x_{n+1}, y_n + k_n) \quad \dots(9)$$

$$y_{n+1} = y_n + \frac{1}{2}(k_n + l_n) \quad \dots(10)$$

Remark Modified Euler method is a special case of second order Runge-Kutta method given by (10).

Example Use second order Runge-Kutta method with $h = 0.1$ to find $y(0.2)$, given

$$\frac{dy}{dx} = x^2 + y^2 \text{ with } y(0) = 0.$$

Here $f(x, y) = x^2 + y^2, x_0 = 0, y_0 = 0, h = 0.1$. Hence

$$x_1 = x_0 + h = 0.1, \quad x_2 = x_1 + h = 0.2.$$

To determine y_1, y_2 we use second order Runge-Kutta method and using (8) – (10),

$$k_n = hf(x_n, y_n) = 0.1(x_n^2 + y_n^2)$$

$$l_n = hf(x_{n+1}, y_n + k_n) = 0.1[x_{n+1}^2 + (y_n + k_n)^2]$$

and
$$y_{n+1} = y_n + \frac{1}{2}(k_n + l_n)$$

$$k_0 = 0.2(x_0^2 + y_0^2) = 0.1(0^2 + 0^2) = 0.$$

$$l_0 = 0.2(x_1^2 + (y_0 + k_0)^2) = 0.1[(0.1)^2 + (0 + 0)^2] = 0.001$$

and
$$y_1 = y_0 + \frac{1}{2}(k_0 + l_0) = 0 + \frac{1}{2}(0 + 0.001) = 0.0005.$$

$$k_1 = 0.2(x_1^2 + y_1^2) = 0.1[(0.1)^2 + (0.0005)^2] = 0.001, \text{ correct to three places of decimals.}$$

$$l_1 = 0.2(x_2^2 + (y_1 + k_1)^2) = 0.1[(0.2)^2 + (0.0015)^2] = 0.004$$

and
$$y_2 = y_1 + \frac{1}{2}(k_1 + l_1) = 0.0005 + \frac{1}{2}(0.001 + 0.004) = 0.003.$$

Hence $y(0.1) = 0.0005$, $y(0.2) = 0.003$.

Example Given the initial value problem $y' = x + y$, $y(0) = 0$. Find the value of y approximately for $x = 1$ by second order Runge-Kutta method in five steps. Compare the result with the exact value.

Here $f(x, y) = x + y$, $x_0 = 0$, $y_0 = 0$. As we have to calculate the value of y when $x = 1$ in five steps, we have to take $h = \frac{x_n - x_0}{n} = \frac{1 - 0}{5} = 0.2$. Hence

$$x_1 = x_0 + h = 0.2, \quad x_2 = x_1 + h = 0.4, \quad x_3 = x_2 + h = 0.6, \quad x_4 = x_3 + h = 0.8, \quad x_5 = x_4 + h = 1.0.$$

We determine y_1, y_2, y_3, y_4, y_5 we use second order Runge-Kutta formula:

$$k_n = hf(x_n, y_n) = 0.2(x_n + y_n)$$

$$l_n = hf(x_{n+1}, y_n + k_1) = 0.2(x_{n+1} + (y_n + k_n))$$

$$= 0.2[x_n + 0.2 + y_n + 0.2(x_n + y_n)], \text{ as } x_{n+1} = x_n + h = x_n + a_2 \text{ and } y_{n+1} = y_n + \frac{1}{2}(k_n + l_n)$$

$$= y_n + \frac{1}{2}\{0.2(x_n + y_n) + 0.2[x_n + 0.2 + y_n + 0.2(x_n + y_n)]\}$$

$$= y_n + 0.22(x_n + y_n) + 0.02$$

The successive steps and calculations are plotted in the following table.

n	x_n	approximate value of y_n	$x_n + y_n$	$0.22(x_n + y_n) + 0.02$	y_{n+1}
0	0.0	0.0000	0.0000	0.0200	0.0200
1	0.2	0.0200	0.2200	0.0684	0.0884
2	0.4	0.0884	0.4884	0.1274	0.2158
3	0.6	0.2158	0.8158	0.1995	0.4153
4	0.8	0.4153	1.2153	0.2874	0.7027
5	1.0	0.7027			

Hence $y(1) = 0.7027$. In an earlier example we have noted that the exact value is 0.718.

Exercises

In Exercises 1-10, solve the initial value problem using second order Runge-Kutta method for value of y at the given point of x with given h .

1. $\frac{dy}{dx} = 1 - y$, $y(0) = 0$ at the point $x = 0.2$ (Take $h = 0.1$).
2. $\frac{dy}{dx} = \frac{y - x}{1 + x}$, $y(0) = 1$ at the point $x = 0.1$ (Take $h = 0.02$).
3. $yy' = x$, $y(0) = 1.5$ at the point $x = 0.2$ (Take $h = 0.1$).
4. $\frac{dy}{dx} = x - y$, $y(0) = 1$ at the point $x = 0.2$ (Take $h = 0.1$).
5. $y' = x + y + xy$, $y(0) = 1$ at the point $x = 0.1$ (Take $h = 0.02$).
6. $\frac{dy}{dx} = 1 + y^2$, $y(0) = 0$ at the point $x = 0.4$ (Take $h = 0.2$).
7. $\frac{dy}{dx} = xy$, $y(0) = 1$ at the point $x = 0.4$ (Take $h = 0.2$).
8. $\frac{dy}{dx} = 1 + \ln(x + y)$, $y(0) = 1$ at the point $x = 0.2$ (Take $h = 0.1$).
9. $y' = x^2 + y$, $y(0) = 1$ at the point $x = 0.1$ (Take $h = 0.05$).
10. $y' = 2xy$, $y(0) = 1$ at the point $x = 0.5$ (Take $h = 0.1$).

In Exercises 11-13, apply second order Runge-Kutta method. Do 10 steps.

11. $y' = y$, $y(0) = 1$, $h = 0.1$
12. $y' = y - y^2$, $y(0) = 0.5$, $h = 0.1$
13. $y' = 2(1 + y^2)$, $y(0) = 0$, $h = 0.05$
14. $y' + 2xy^2 = 0$, $y(0) = 1$, $h = 0.2$
15. Solve using second order Runge-Kutta method $y'(x + y) = y - x$ with $y(0) = 2$ for the range $0.00(0.02)0.06$.
16. Solve using second order Runge-Kutta method $y' = y - \frac{2x}{y}$ with $y = 1$ at $x = 0$ for $h = 0.5$ on the interval $[0, 1]$.

17. Using second order Runge-Kutta method find $y(0.2)$ of the initial value problem $y' = x + 2y$, $y(0) = 1$, taking $h = 0.1$.
18. Using second order Runge-Kutta method find the value of y at the point $x = 2$ in steps of 0.2 of the initial value problem $\frac{dy}{dx} = 2 + \sqrt{xy}$, $y(1) = 1$.

Fourth Order Runge-Kutta method

The **Runge-Kutta method**¹ of fourth order (also known as *classical Runge-Kutta method*) gives greater accuracy and is most widely used for finding the approximate solution of first order ordinary differential equations. The method is well suited for computers. The method is shown in the following algorithm.

Algorithm (The Runge-Kutta method)

Given the initial value problem (1). Suppose x_0, x_1, x_2, \dots be equally spaced x values with interval h . i.e.,

$$x_1 = x_0 + h, \quad x_2 = x_1 + h, \dots$$

Also denote $y_0 = y(x_0), y_1 = y(x_1), y_2 = y(x_2), \dots$

For $n = 0, 1, \dots$, until termination do:

$$x_{n+1} = x_n + h$$

$$A_n = hf(x_n, y_n) \quad \dots(11)$$

$$B_n = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}A_n) \quad \dots(12)$$

$$C_n = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}B_n) \quad \dots(13)$$

$$D_n = hf(x_n + h, y_n + C_n) \quad \dots(14)$$

$$y_{n+1} = y_n + \frac{1}{6}(A_n + 2B_n + 2C_n + D_n) \quad \dots(15)$$

Example Use Runge-Kutta method with $h = 0.1$ to find $y(0.2)$ given $\frac{dy}{dx} = x^2 + y^2$ with $y(0) = 0$.

Here $f(x, y) = x^2 + y^2$, $x_0 = 0$, $y_0 = 0$, $h = 0.1$. Hence

$$x_1 = x_0 + h = 0.1, \quad x_2 = x_1 + h = 0.2.$$

To determine y_1, y_2 we use improved Euler formula. Using Eqs. (12) (15),

$$x_{n+1} = x_n + h = x_n + 0.1$$

$$A_n = hf(x_n, y_n) = 0.1(x_n^2 + y_n^2)$$

$$B_n = hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}A_n\right) = 0.1\left[(x_n + 0.05)^2 + \left(y_n + \frac{1}{2}A_n\right)^2\right]$$

$$C_n = hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}B_n\right) = 0.1\left[(x_n + 0.05)^2 + \left(y_n + \frac{1}{2}B_n\right)^2\right]$$

$$D_n = hf(x_n + h, y_n + C_n) = 0.1\left[x_{n+1}^2 + (y_n + C_n)^2\right]$$

$$y_{n+1} = y_n + \frac{1}{6}(A_n + 2B_n + 2C_n + D_n)$$

$$x_1 = x_0 + 0.1 = 0 + 0.1 = 0.1$$

$$A_0 = 0.1(x_0^2 + y_0^2) = 0.1(0^2 + 0^2) = 0$$

$$\begin{aligned} B_0 &= 0.1\left[(x_0 + 0.05)^2 + \left(y_0 + \frac{1}{2}A_0\right)^2\right] \\ &= 0.1\left[(0.05)^2 + 0^2\right] = 0.00025. \end{aligned}$$

$$\begin{aligned} C_0 &= 0.1\left[(x_0 + 0.05)^2 + \left(y_0 + \frac{1}{2}B_0\right)^2\right] \\ &= 0.1\left[(0.05)^2 + (0.000125)^2\right] = 0.00025. \end{aligned}$$

$$\begin{aligned} D_0 &= 0.1\left[x_1^2 + (y_0 + C_0)^2\right] \\ &= 0.1\left[(0.1)^2 + (0.00025)^2\right] = 0.001. \end{aligned}$$

$$\begin{aligned} y_1 &= y_0 + \frac{1}{6}(A_0 + 2B_0 + 2C_0 + D_0) \\ &= 0 + \frac{1}{6}(0 + 2 \times 0.00025 + 2 \times 0.00025 + 0.001) = 0.00033. \end{aligned}$$

$$x_2 = x_1 + 0.1 = 0.1 + 0.1 = 0.2$$

$$A_1 = 0.1(x_1^2 + y_1^2) = 0.1\left[(0.1)^2 + (0.00033)^2\right] = 0.001$$

$$\begin{aligned} B_1 &= 0.1\left[(x_1 + 0.05)^2 + \left(y_1 + \frac{1}{2}A_1\right)^2\right] \\ &= 0.1\left[(0.15)^2 + (0.00083)^2\right] = 0.00225. \end{aligned}$$

$$\begin{aligned} C_1 &= 0.1\left[(x_1 + 0.05)^2 + \left(y_1 + \frac{1}{2}B_1\right)^2\right] \\ &= 0.1\left[(0.15)^2 + (0.001455)^2\right] = 0.00025. \end{aligned}$$

$$\begin{aligned} D_1 &= 0.1 \left[x_2^2 + (y_1 + C_1)^2 \right] \\ &= 0.1 \left[(0.2)^2 + (0.0058)^2 \right] = 0.004. \end{aligned}$$

$$\begin{aligned} y_2 &= y_1 + \frac{1}{6}(A_1 + 2B_1 + 2C_1 + D_1) \\ &= 0.00033 + \frac{1}{6}(0.014) = 0.002663. \end{aligned}$$

Example Use Runge-Kutta method with $h=0.2$ to find the value of y at $x=0.2$, $x=0.4$, and $x=0.6$, given $\frac{dy}{dx} = 1 + y^2$, $y(0) = 0$.

Here $f(x, y) = 1 + y^2$, $x_0 = 0$, $y_0 = 0$, $h = 0.2$. Hence

$$x_1 = x_0 + h = 0.2, \quad x_2 = x_1 + h = 0.4.$$

To determine y_1 , y_2 we use improved Euler formula:

$$\begin{aligned} x_{n+1} &= x_n + h = x_n + 0.2 \\ A_n &= hf(x_n, y_n) = 0.2(1 + y_n^2) \\ B_n &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}A_n\right) = 0.2 \left[1 + \left(y_n + \frac{1}{2}A_n\right)^2 \right] \\ C_n &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}B_n\right) = 0.2 \left[1 + \left(y_n + \frac{1}{2}B_n\right)^2 \right] \\ D_n &= hf(x_n + h, y_n + C_n) = 0.2 \left[1 + (y_n + C_n)^2 \right] \\ y_{n+1} &= y_n + \frac{1}{6}(A_n + 2B_n + 2C_n + D_n) \\ x_1 &= x_0 + 0.2 = 0 + 0.2 = 0.2 \\ A_0 &= 0.2(1 + y_0^2) = 0.2(1 + 0^2) = 0.2 \\ B_0 &= 0.2 \left[1 + \left(y_0 + \frac{1}{2}A_0\right)^2 \right] = 0.2 \left[1 + (0.1)^2 \right] = 0.202. \\ C_0 &= 0.2 \left[1 + \left(y_0 + \frac{1}{2}B_0\right)^2 \right] = 0.2 \left[1 + (0.101)^2 \right] = 0.20204. \\ D_0 &= 0.2 \left[1 + (y_0 + C_0)^2 \right] \\ &= 0.2 \left[1 + (0.20204)^2 \right] = 0.20816. \end{aligned}$$

$$y_1 = y_0 + \frac{1}{6}(A_0 + 2B_0 + 2C_0 + D_0)$$

$$= 0 + \frac{1}{6}(0.2 + 2 \times 0.202 + 2 \times 0.20204 + 0.20816) = 0.2027.$$

i.e., $y(0.2) = 0.2027$.

$$x_2 = x_1 + 0.1 = 0.2 + 0.2 = 0.4$$

$$A_1 = 0.2(1 + y_1^2) = 0.2[1 + (0.2027)^2] = 0.2082$$

$$B_1 = 0.2\left[1 + \left(y_1 + \frac{1}{2}A_1\right)^2\right] = 0.2[1 + (0.3068)^2] = 0.2188.$$

$$C_1 = 0.2\left[1 + \left(y_1 + \frac{1}{2}B_1\right)^2\right] = 0.2[1 + (0.3121)^2] = 0.2195. \quad D_1 = 0.2[1 + (y_1 + C_1)^2]$$

$$= 0.2[1 + (0.4222)^2] = 0.2356.$$

$$y_2 = y_1 + \frac{1}{6}(A_1 + 2B_1 + 2C_1 + D_1)$$

$$= 0.00033 + \frac{1}{6}(0.2082 + 2 \times 0.2195 + 2 \times 0.2195 + 0.2356)$$

$$= 0.4228.$$

i.e., $y(0.4) = 0.4228$, correct to four decimal places.

$$x_3 = x_2 + 0.1 = 0.4 + 0.2 = 0.6$$

$$A_2 = 0.2(1 + y_2^2); \quad B_2 = 0.2\left[1 + \left(y_2 + \frac{1}{2}A_2\right)^2\right];$$

$$C_2 = 0.2\left[1 + \left(y_2 + \frac{1}{2}B_2\right)^2\right]; \quad D_2 = 0.2[1 + (y_2 + C_2)^2].$$

Substituting the values, and using

$$y_3 = y_2 + \frac{1}{6}(A_2 + 2B_2 + 2C_2 + D_2)$$

we obtain $y(0.6) = y_3 = 0.6841$, correct to four decimal places.

Example Given the initial value problem $y' = x + y$, $y(0) = 0$. Find the value of y approximately for $x = 1$ by Runge-Kutta method in five steps. Compare the result with the exact value.

Here $f(x, y) = x + y$, $x_0 = 0$, $y_0 = 0$. As we have to calculate the value of y when $x = 1$ in five steps, we have to take $h = \frac{x_n - x_0}{n} = \frac{1 - 0}{5} = 0.2$. Hence

$$x_1 = x_0 + h = 0.2, \quad x_2 = x_1 + h = 0.4, \quad x_3 = x_2 + h = 0.6, \quad x_4 = x_3 + h = 0.8, \quad x_5 = x_4 + h = 1.0.$$

We determine y_1, y_2, y_3, y_4, y_5 we use Runge-Kutta formula:

$$x_{n+1} = x_n + h = x_n + 0.2$$

$$A_n = hf(x_n, y_n) = 0.2(x_n + y_n)$$

$$B_n = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}A_n) = 0.2[x_n + 0.1 + y_n + 0.1(x_n + y_n)]$$

$$= 0.22(x_n + y_n) + 0.02$$

$$C_n = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}B_n)$$

$$= 0.2[x_n + 0.1 + y_n + 0.11(x_n + y_n) + 0.01]$$

$$= 0.222(x_n + y_n) + 0.022$$

$$D_n = hf(x_n + h, y_n + C_n)$$

$$= 0.2[x_n + 0.2 + y_n + 0.222(x_n + y_n) + 0.022]$$

$$= 0.2444(x_n + y_n) + 0.0444$$

$$y_{n+1} = y_n + \frac{1}{6}(A_n + 2B_n + 2C_n + D_n)$$

i.e., $y_{n+1} = y_n + 0.2214(x_n + y_n) + 0.0214.$

The successive steps and calculations are plotted in the following table.

n	x_n	approximate value of y_n	$x_n + y_n$	$0.2214(x_n + y_n)$	$0.2214(x_n + y_n) + 0.0214$
0	0.0	0.0000	0.0000	0.0000	0.021 400
1	0.2	0.021 400	0.221 400	0.049 018	0.070 418
2	0.4	0.091 818	0.491 818	0.108 889	0.130 289
3	0.6	0.222 107	0.822 107	0.182 014	0.203 414
4	0.8	0.425 521	1.225 521	0.271 330	0.292 730
5	1.0	0.718 251			

Table:

Comparison of the accuracy of three methods discussed in earlier sections in the case of the initial value problem $y' = x + y$, $y(0) = 0$.

x_n	Exact value	Approximate values to y obtained by			Absolute value of Error		
		Euler method	R-K Second Order	R-K Fourth Order	Euler method	R-K Second Order	R-K Fourth Order
0.2	0.021403	0.000	0.0200	0.021400	0.021	0.0014	0.000003
0.4	0.091825	0.040	0.0884	0.091818	0.052	0.0034	0.000007
0.6	0.222119	0.128	0.2158	0.222107	0.094	0.0063	0.000011
0.8	0.425541	0.274	0.4153	0.425521	0.152	0.0102	0.000020
1.0	0.718282	0.489	0.7027	0.718251	0.229	0.0156	0.000031

Exercises

In Exercises 1-10, solve the initial value problem using fourth order Runge-Kutta method for value of y at the given point of x (with h given in brackets)

1. $\frac{dy}{dx} = y$, $y(0) = 1$ at the point $x = 1$ ($h = 0.5$)
2. $\frac{dy}{dx} = 1 - y$, $y(0) = 0$ at the point $x = 0.2$ ($h = 0.1$).
3. $\frac{dy}{dx} = y - x$, $y(0) = 2$ at the point $x = 0.2$ ($h = 0.1$).
4. $yy' = x$, $y(0) = 1.5$ at the point $x = 0.2$ ($h = 0.1$).
5. $\frac{dy}{dx} = x - y$, $y(1) = 0.4$ at the point $x = 1.6$ ($h = 0.6$).
6. $y' = x + y + xy$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.02$).
7. $\frac{dy}{dx} = \frac{y - x}{1 + x}$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.02$).
8. $\frac{dy}{dx} = xy$, $y(1) = 2$ at the point $x = 1.6$ ($h = 0.2$).

9. $\frac{dy}{dx} = 1 + \ln(x + y)$, $y(0) = 1$ at the point $x = 0.2$ ($h = 0.1$).
10. $y' = x^2 + y$, $y(0) = 1$ at the point $x = 0.1$ ($h = 0.05$).
11. $y' = 2xy$, $y(0) = 1$ at the point $x = 0.5$ ($h = 0.1$).
12. $y' = 3x + \frac{1}{2}$, $y(0) = 1$ at the point $x = 0.2$ ($h = 0.05$).
13. Solve using Runge-Kutta method $y'(x + y) = y - x$ with $y(0) = 2$ for the range $0.00(0.02)0.06$.
14. Using Runge-Kutta method find $y(0.2)$ of the initial value problem $y' = x^2 + 2y$, $y(0) = 0$, taking $h = 0.2$.
15. Using Runge-Kutta method find the value of y at the point $x = 2$ in steps of 0.2 of the initial value problem $\frac{dy}{dx} = 2 + \sqrt{xy}$, $y(1) = 1$.
16. Using Runge-Kutta method find $y(1.3)$, given $y' = x^2y$ and $y(1) = 2$. Take $h = 0.3$.
17. Solve using Runge-Kutta method $y' = y - \frac{2x}{y}$ with $y = 1$ at $x = 0$ for $h = 0.5$ on the interval $[0, 1]$.
18. Solve $y' = 2x^{-1}\sqrt{y - \ln x} + x^{-1}$, $y(1) = 0$ for $1 \leq x \leq 1.8$
 - (a) by Euler method with $h = 0.1$.
 - (b) by improved Euler method with $h = 0.2$.
 - (c) by Runge-Kutta method with $h = 0.4$.
 - (d) Compare the above results with the exact value. Determine the errors. Comment.

18

PREDICTOR CORRECTOR METHODS

Introduction

Euler method and fourth order Runge-Kutta methods are called single-step methods, where we have seen that the computation of y_{n+1} requires the knowledge of y_n only. But modified Euler method is a multi-step method since for the computation of y_{n+1} the knowledge of y_n is not enough. It is a *predictor-corrector method*, in which a *predictor* formula is used to predict the value y_{n+1} of y at x_{n+1} and then a *corrector* formula is used to improve the value of y_{n+1} .

For example, consider the initial value problem

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0.$$

Using simple Euler's and modified Euler's method, we can write down a simple predictor-corrector pair (P-C) as

$$P: \quad y_{n+1}^{(0)} = y_n + hf(x_n, y_n).$$

$$C: \quad y_{n+1}^{(1)} = y_n + \frac{h}{2} [f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(0)})].$$

Here, $y_{n+1}^{(1)}$ is the first corrected value of y_{n+1} . The corrector formula may be used iteratively as defined below:

$$y_{n+1}^{(r)} = y_n + \frac{h}{2} [f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(r-1)})] \quad (r=1, 2, \dots)$$

The iteration terminate when two successive iterates agree to the desired accuracy. We have considered modified Euler method in the previous chapter.

In this chapter we consider two methods: Adams-Moulton and Milne's Methods. They require function values at $x_n, x_{n-1}, x_{n-2}, \dots$ for the computation of the function value at x_{n+1} .

Adams-Moulton Method

Consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0. \quad \dots(1)$$

Starting with given x_0 and given the step size h , we have
 $x_1 = x_0 + h$, $x_{-1} = x_0 - h$, $x_{-2} = x_0 - 2h$, and $x_{-3} = x_0 - 3h$. We denote
 $f_0 = f(x_0, y_0)$, $f_1 = f(x_1, y_1)$, $f_{-1} = f(x_{-1}, y_{-1})$, $f_{-2} = f(x_{-2}, y_{-2})$, and $f_{-3} = f(x_{-3}, y_{-3})$.

In Adams-Moulton Method, we predict by

$$y_1^p = y_0 + \frac{h}{24}(55f_0 - 59f_{-1} + 37f_{-2} - 9f_{-3}) \quad \dots(1)$$

and correct by

$$y_1^c = y_0 + \frac{h}{24}(9f_1^p + 19f_0 - 5f_{-1} + f_{-2}), \quad \dots(2)$$

where $f_1^p = f(x_1, y_1^p)$.

The general forms for formulae (1) and (2) are given by

$$y_{n+1}^p = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}) \quad \dots(1)$$

with correction

$$y_{n+1}^c = y_n + \frac{h}{24}(9f_{n+1}^p + 19f_n - 5f_{n-1} + f_{n-2}), \quad \dots(2)$$

where $f_{n+1}^p = f(x_{n+1}, y_{n+1}^p)$.

The formulae given above are example of *explicit predictor –corrector* formulae as they are expressed in ordinate form.

Example Given $\frac{dy}{dx} = 1 + y^2$; $y(0) = 0$. Compute $y(0.8)$ using Adams-Moulton Method.

Here $x_1 = 0.8$, $h = 0.2$. Hence $x_0 = x_1 - h = 0.8 - 0.2 = 0.6$,

$x_{-1} = x_0 - h = 0.4$, $x_{-2} = x_0 - 2h = 0.2$, and $x_{-3} = x_0 - 3h = 0$.

The starter values are $y(0.6)$, $y(0.4)$ and $y(0.2)$. Using fourth-order Runge-Kutta method (Ref. Example 7 in the previous chapter), the values are found to be:

$$y(0.6) = 0.6841, \quad y(0.4) = 0.4228, \quad y(0.2) = 0.2027.$$

Hence $y_0 = y(x_0) = y(0.6) = 0.6841$, $y_{-1} = y(x_{-1}) = y(0.4) = 0.4228$,

$$y_{-2} = 0.2027 \quad \text{and} \quad y_{-3} = y(x_{-3}) = y(0) = 0.$$

Also, $f_0 = f(x_0, y_0) = 1 + y_0^2 = 1 + (0.6841)^2$;

$$f_{-1} = f(x_{-1}, y_{-1}) = 1 + y_{-1}^2 = 1 + (0.4228)^2;$$

and so on. We tabulate them below:

x	y	$f(x) = 1 + y^2$
$x_{-3} = 0.0$	$y_{-3} = 0.000$	$f_{-3} = 1.0000$
$x_{-2} = 0.2$	$y_{-2} = 0.2027$	$f_{-2} = 1.0411$
$x_{-1} = 0.4$	$y_{-1} = 0.4228$	$f_{-1} = 1.1787$
$x_0 = 0.6$	$y_0 = 0.6841$	$f_0 = 1.4681$

Substituting these values in (1), we obtain the predicted value of y_1 at $x_1 = 0.8$ as

$$\begin{aligned} y_1^P &= 0.6841 + \frac{0.2}{24} \{ 55[1 + (0.6841)^2] - 59[1 + (0.4228)^2] \\ &\quad + 37[1 + (0.4228)^2] - 9 \} \\ &= 1.0233, \text{ on simplification.} \end{aligned}$$

Corrected value of y_1 at $x_1 = 0.8$ is obtained using (2) as below:

$$\begin{aligned} y_1^C &= 0.6841 + \frac{0.2}{24} \{ 9[1 + (0.0233)^2] + 19[1 + (0.6841)^2] \\ &\quad - 5[1 + (0.4228)^2] + [1 + (0.2027)^2] \} \\ &= 1.0296, \text{ on simplification.} \end{aligned}$$

Exercises

- Using Adams-Moulton predictor-corrector method, find the value of y at $x = 4.4$ from the differential equation

$$5x \frac{dy}{dx} + y^2 = 2,$$

given that

x	4.0	4.1	4.2	4.3
y	1.0000	1.0049	1.0097	1.0143

- Using Adams-Moulton predictor-corrector method, find the value of y at $x = 0.8$, and $x = 1.0$ of the initial value problem

$$\frac{dy}{dx} = y - x^2, \quad y(0) = 1$$

(Take $h = 0.2$.)

3. Using Adams-Moulton predictor-corrector method, find the value of y at $x = 1.4$ of the initial value problem

$$x^2 y' + xy = 1, \quad y(1) = 1.0$$

with starter values $y(1.1) = 0.996$, $y(1.2) = 0.986$, $y(1.3) = 0.972$.

4. Find the solution of the initial value problem

$$y' = y^2 \sin t, \quad y(0) = 1$$

using Adams-Moulton predictor-corrector method, in the interval $(0.2, 0.5)$ given that

$$y(0.05) = 1.00125, \quad y(0.1) = 1.00502, \quad y(0.15) = 1.01136.$$

Milne's Method

Consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0. \quad \dots(1)$$

Starting with given x_0 and given the step size h , we have
 $x_1 = x_0 + h$, $x_{-1} = x_0 - h$, $x_{-2} = x_0 - 2h$, and $x_{-3} = x_0 - 3h$. We denote
 $f_0 = f(x_0, y_0)$, $f_1 = f(x_1, y_1)$, $f_{-1} = f(x_{-1}, y_{-1})$, $f_{-2} = f(x_{-2}, y_{-2})$, and $f_{-3} = f(x_{-3}, y_{-3})$.

In Milne's Method, we predict by

$$y_1^P = y_{-3} + \frac{4h}{3}(2f_{-2} - f_{-1} + 2f_0) \quad \dots(1)$$

and correct by

$$y_1^C = y_{-1} + \frac{h}{3}(f_{-1} + 4f_0 + f_1^P), \quad \dots(2)$$

where $f_1^P = f(x_1, y_1^P)$.

The general forms for formulae (1) and (2) are given by

$$y_{n+1}^P = y_{n-3} + \frac{4h}{3}(2f_{n-2} - f_{n-1} + 2f_n) \quad \dots(3)$$

and correct by

$$y_{n+1}^C = y_{n-1} + \frac{h}{3}(f_{n-1} + 4f_n + f_{n+1}^P), \quad \dots(4)$$

where $f_{n+1}^P = f(x_{n+1}, y_{n+1}^P)$.

The formulae given above is also *explicit predictor -corrector* formulae as they are expressed in ordinate form.

Example Given $\frac{dy}{dx} = 1 + y^2$; $y(0) = 0$. Compute $y(0.8)$ and $y(1.0)$ using Milne's Method.

Solution

Determination of $y(0.8)$:

Here take $x_1 = 0.8$, $h = 0.2$. Hence

$$x_0 = x_1 - h = 0.8 - 0.2 = 0.6, \quad x_{-1} = 0.4, \quad x_{-2} = 0.2, \quad x_{-3} = 0.$$

The starter values are $y(0.6)$, $y(0.4)$ and $y(0.2)$. Using fourth-order Runge-Kutta method, the values are found to be:

$$y(0.6) = 0.6841, \quad y(0.4) = 0.4228, \quad y(0.2) = 0.2027.$$

Hence

$$y_0 = 0.6841, \quad y_{-1} = 0.4228, \quad y_{-2} = 0.2027 \quad \text{and}$$

$$y_{-3} = y(x_{-3}) = y(0) = 0.$$

Also, $f_0 = f(x_0, y_0) = 1 + y_0^2 = 1 + (0.6841)^2$;

$$f_{-1} = 1 + y_{-1}^2 = 1 + (0.4228)^2 ;$$

and so on. We tabulate them below:

x	y	$f(x) = 1 + y^2$
$x_{-3} = 0.0$	$y_{-3} = 0.000$	$f_{-3} = 1.0000$
$x_{-2} = 0.2$	$y_{-2} = 0.2027$	$f_{-2} = 1.0411$
$x_{-1} = 0.4$	$y_{-1} = 0.4228$	$f_{-1} = 1.1787$
$x_0 = 0.6$	$y_0 = 0.6841$	$f_0 = 1.4681$

Substituting these values in (1), we obtain the predicted value of y_1 at $x_1 = 0.8$ as

$$y_1^P = 0 + \frac{0.8}{3} [2(1.0411) - 1.1787 + 2(1.4681)] = 1.0239$$

Hence $f_1 = 1 + (y_1^P)^2 = 1 + (1.0239)^2 = 2.0480$

and hence the corrected value of y_1 at $x_1 = 0.8$ is obtained using (2) as below:

$$y_1^C = 0.4228 + \frac{0.2}{3} [1.1787 + 4(1.4681) + 2.0480] = 1.0294.$$

Hence $y(0.8) = 1.0294$, correct to four places of decimal.

Determination of $y(1.0)$:

Here take $x_1 = 1.0$, $h = 0.2$. Hence

$$x_0 = x_1 - h = 1.0 - 0.2 = 0.8, \quad x_{-1} = 0.6, \quad x_{-2} = 0.4, \quad x_{-3} = 0.2.$$

The starter values are $y(0.8)$, $y(0.6)$, and $y(0.4)$. We have the values

$$y(0.8) = 1.0294, \quad y(0.6) = 0.6841, \quad y(0.4) = 0.4228.$$

Hence

$$y_0 = 1.0294, \quad y_{-1} = 0.6841, \quad y_{-2} = 0.4228 \quad \text{and} \quad y_{-3} = 0.$$

Also, $f_0 = 1 + y_0^2 = 1 + (1.0294)^2$; $f_{-1} = 1 + y_{-1}^2 = 1 + (0.6841)^2$; and so on.

x	y	$f(x) = 1 + y^2$
$x_{-3} = 0.2$	$y_{-3} = 0.2027$	$f_{-3} = 1.0411$
$x_{-2} = 0.4$	$y_{-2} = 0.4228$	$f_{-2} = 1.1787$
$x_{-1} = 0.6$	$y_{-1} = 0.6841$	$f_{-1} = 1.4681$
$x_0 = 0.8$	$y_0 = 1.0294$	$f_0 = 2.0597$

Substituting these values in (1), we obtain the predicted value of y_1 at $x_1 = 1.0$ as

$$y_1^P = 1.5384$$

Hence $f_1 = 1 + (y_1^P)^2 = 3.3667$

Corrected value of y_1 at $x_1 = 0.8$ is obtained using (2) as below:

$$y_1^C = 1.5557.$$

Example Find, using Milne's predictor-corrector method, $y(2.0)$ if $y(x)$ is the solution of

$$\frac{dy}{dx} = \frac{x + y}{2}$$

assuming $y(0) = 2$, $y(0.5) = 2.636$, $y(1.0) = 3.595$ and $y(1.5) = 4.968$.

Here take $x_1 = 2.0$, $h = 0.5$. Hence

$$x_0 = x_1 - h = 2.0 - 0.5 = 1.5, \quad x_{-1} = 1, \quad x_{-2} = 0.5, \quad x_{-3} = 0.$$

Also, by the assumption,

$$y_0 = 4.968, \quad y_{-1} = 3.595, \quad y_{-2} = 2.636 \quad \text{and} \quad y_{-3} = 2.$$

As $f(x, y) = \frac{x+y}{2}$, we have

$$f_0 = f(x_0, y_0) = \frac{x_0 + y_0}{2} = \frac{1.5 + 4.968}{2} = 3.2340. ;$$

$$f_{-1} = f(x_{-1}, y_{-1}) = \frac{x_{-1} + y_{-1}}{2} = \frac{1.0 + 3.595}{2} = 2.2975. ;$$

$$f_{-2} = f(x_{-2}, y_{-2}) = \frac{x_{-2} + y_{-2}}{2} = \frac{0.5 + 2.636}{2} = 1.5680. ;$$

Now, using predictor formula we compute

$$\begin{aligned} y_1^P &= y_{-3} + \frac{4h}{3}(2f_{-2} - f_{-1} + 2f_0) \\ &= 2 + \frac{4(0.5)}{3}[2(1.5680) - 2.2975 + 2(3.2340)] = 6.8710. \end{aligned}$$

Using the predicted value, we shall compute the corrected value of y_1 from the corrector formula

$$y_1^C = y_{-1} + \frac{h}{3}(f_{-1} + 4f_0 + f_1^P), \quad (2)$$

where $f_1^P = f(x_1, y_1^P)$.

Now using the available predicted value y_1^P ,

$$f_1^P = f(x_1, y_1^P) = \frac{x_1 + y_1^P}{2} = \frac{2 + 6.871}{2} = 4.4355.$$

Thus the corrected value is given by

$$y_1^C = 3.595 + \frac{0.5}{3}[2.2975 + 4(3.234) + 4.4355] = 6.8731667.$$

Hence an approximate value of y at $x = 2$ is taken as $y(2) = y_1^C = 6.8731667$.

Example Tabulate the solution of

$$\frac{dy}{dx} = x + y; \quad y(0) = 1$$

in the interval $0 \leq x \leq 0.4$, with $h = 0.1$, using Milne's predictor-corrector method.

We take $x_1 = 0.4$. We cannot immediately use Milne's predictor-corrector method as it need the value of y at the previous four points $x_0 = x_1 - h = 0.4 - 0.1 = 0.3$, $x_{-1} = 0.2$, $x_{-2} = 0.1$, $x_{-3} = 0$. Clearly, $y_{-3} = y(x_{-3}) = y(0) = 1$. For the calculation of the rest three y values we use Runge-Kutta method of fourth order and then switch over to Milne's P-C method.

By Runge-Kutta method of fourth order it can be seen that (work is left as an exercise)

$$y_0 = y(x_0) = y(0.3) = 1.3997, \quad y_{-1} = y(x_{-1}) = y(0.2) = 1.2428, \quad y_{-2} = y(x_{-2}) = y(0.1) = 1.1103.$$

From the given differential equation $f(x, y) = x + y$, and we have

$$f_0 = f(x_0, y_0) = x_0 + y_0 = 0.3 + 1.3997 = 1.6997.$$

$$f_{-1} = f(x_{-1}, y_{-1}) = x_{-1} + y_{-1} = 0.2 + 1.2428 = 1.4428.$$

$$f_{-2} = f(x_{-2}, y_{-2}) = x_{-2} + y_{-2} = 0.1 + 1.1103 = 1.2103.$$

Now, using predictor formula we compute

$$\begin{aligned} y_1^p &= y_{-3} + \frac{4h}{3}(2f_{-2} - f_{-1} + 2f_0) \\ &= 1 + \frac{4(0.1)}{3}[2(1.2103) - 1.4428 + 2(1.6997)] = 1.58363 \end{aligned}$$

Before using the corrector formula

$$y_1^c = y_{-1} + \frac{h}{3}(f_{-1} + 4f_0 + f_1^p), \quad \dots(2)$$

we compute

$$f_1^p = f(x_1, y_1^p) = x_1 + y_1^p = 0.4 + 1.5836 = 1.9836.$$

Hence

$$y_1^c = 1.2428 + \frac{0.1}{3}[1.4428 + 4(1.6997) + 1.9836] = 1.5836.$$

The required solution is tabulated below:

x	0	0.1	0.2	0.3	0.4
y	1.0000	1.1103	1.2428	1.3997	1.5836

Example Find, using Milne's predictor-corrector method, $y(2.0)$ if $y(x)$ is the solution of $\frac{dy}{dx} = \frac{x+y}{2}$ assuming $y(0) = 2$, $y(0.5) = 2.636$, $y(1.0) = 3.595$ and $y(1.5) = 4.968$.

Here take $x_1 = 2.0$, $h = 0.5$. Hence

$$x_0 = x_1 - h = 2.0 - 0.5 = 1.5, \quad x_{-1} = 1, \quad x_{-2} = 0.5, \quad x_{-3} = 0.$$

Also, by the assumption,

$$y_0 = 4.968, \quad y_{-1} = 3.595, \quad y_{-2} = 2.636 \quad \text{and} \quad y_{-3} = 2.$$

As $f(x, y) = \frac{x+y}{2}$, we have

$$f_0 = f(x_0, y_0) = \frac{x_0 + y_0}{2} = \frac{1.5 + 4.968}{2} = 3.2340. ;$$

$$f_{-1} = f(x_{-1}, y_{-1}) = \frac{x_{-1} + y_{-1}}{2} = \frac{1.0 + 3.595}{2} = 2.2975. ;$$

$$f_{-2} = f(x_{-2}, y_{-2}) = \frac{x_{-2} + y_{-2}}{2} = \frac{0.5 + 2.636}{2} = 1.5680. ;$$

Now, using predictor formula we compute

$$\begin{aligned} y_1^P &= y_{-3} + \frac{4h}{3}(2f_{-2} - f_{-1} + 2f_0) \\ &= 2 + \frac{4(0.5)}{3}[2(1.5680) - 2.2975 + 2(3.2340)] = 6.8710. \end{aligned}$$

Using the predicted value, we shall compute the corrected value of y_1 from the corrector formula

$$y_1^C = y_{-1} + \frac{h}{3}(f_{-1} + 4f_0 + f_1^P),$$

where $f_1^P = f(x_1, y_1^P)$.

Now using the available predicted value y_1^P ,

$$f_1^P = f(x_1, y_1^P) = \frac{x_1 + y_1^P}{2} = \frac{2 + 6.871}{2} = 4.4355.$$

Thus the corrected value is given by

$$y_1^C = 3.595 + \frac{0.5}{3} [2.2975 + 4(3.234) + 4.4355] = 6.8731667.$$

Hence an approximate value of y at $x = 2$ is taken as $y(2) = y_1^C = 6.8731667$.

Exercises

1. Find $y(0.8)$ using Milne's P-C method, if $y(x)$ is the solution of the differential equation

$$\frac{dy}{dx} = -xy^2; \quad y(0) = 2$$

assuming $y(0.2) = 1.92308$, $y(0.4) = 1.72414$, $y(0.6) = 1.47059$.

2. Find the solution of

$$\frac{dy}{dx} = y(x + y), \quad y(0) = 1$$

using Milne's P-C method, at $x = 0.4$ given that

$y(0.1) = 1.11689$, $y(0.2) = 1.27739$ and $y(0.3) = 1.50412$.
