

Chapter 1

Solutions of Algebraic and Transcendental Equations

1.1 Introduction

In engineering and sciences, a frequently occurring problem is that of determining the solutions of equations of the form

$$\boxed{f(x) = 0} \tag{1.1}$$

where $f(x)$ can be a linear, quadratic, cubic or quartic expression, in which case algebraic methods of solution are available. However, when $f(x)$ is a polynomial of higher degrees, or a transcendental function, algebraic methods of solution are not available, hence we have to look for approximate methods of solution. In this section, we shall consider approximation methods such as the bisection method, fixed-point iterative method, method of false position and the Newton-Raphson method.

1.2 The Bisection Method

Recall from MTH103 the intermediate value theorem thus:

Theorem 1 *If $f(x)$ is a continuous function on $[a, b]$, and if $f(a)$ and $f(b)$ are of opposite signs, then there exists $\xi \in (a, b)$ such that $f(\xi)=0$.*

In particular, suppose that $f(a) < 0$ and $f(b) > 0$, then there is a root lying between a and b . The approximate value of this root is given by

$$x_0 = \frac{a + b}{2}.$$

If $f(x_0) = 0$, we conclude that x_0 is the root of the equation (1.1). Otherwise, the root lies between a and x_0 or between x_0 and b according as $f(x_0)$ is negative or positive. Continuing, we bisect the interval and repeat the process until a root is known to the desired accuracy. This process is shown in the diagram below:

Example 1

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

Solution

Note that $f(1) < 0$ and $f(2) > 0$, thus a root lies between 1 and 2 and we thus take

$$x_0 = \frac{1 + 2}{2} = \frac{3}{2}.$$

Hence

$$f(x_0) = f\left(\frac{3}{2}\right) = \frac{27}{8} - \frac{3}{2} - 1 = \frac{7}{8} > 0.$$

Thus the root lies between 1 and $\frac{3}{2}$. We then obtain $x_1 = \frac{1+1.5}{2} = 1.25$, and $f(x_1) = -\frac{19}{64} < 0$. We therefore conclude that the root lies between 1.25 and 1.5.

Continuing, one obtains

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

The procedure is repeated and we obtain the successive approximations

$$x_3 = 1.3125, x_4 = 1.34375, x_5 = 1.328125, \dots$$

Stop the iteration as soon as the required accuracy is attained.

1.3 Fixed Point Iteration Method

We transform the equation (1.1) algebraically into the form

$$\boxed{x = \phi(x)} \tag{1.2}$$

The solution of (1.2) is called a fixed point of ϕ , hence the name of the method.

From (1.1), we may get several forms of (1.2). For example, the equation

$$x^3 + x^2 - 1 = 0$$

can be expressed as

(i) $x = \frac{1}{\sqrt{1+x}}$

(ii) $x = \sqrt{1-x^2}$

(iii) $x = \sqrt[3]{1-x^2}$ and so on.

Suppose x_0 is an approximate value of the desired root ξ . Substituting it for x in (1.3), we obtain the first and successive approximations as

$$x_1 = \phi(x_0)$$

$$x_2 = \phi(x_1)$$

$$x_3 = \phi(x_2)$$

⋮

$$x_n = \phi(x_{n-1})$$

and in general,

$$x_{n+1} = \phi(x_n).$$

However, the sequence of successive approximations $x_0, x_1, x_2, \dots, x_n$ do not always converge to some value ξ . For example, take the equation

$$x = 10^x + 1.$$

If we take $x_0 = 0, x_1 = 2, x_2 = 10^2 + 1 = 101, x_3 = 10^{101} + 1, \dots$. This sequence obviously diverges as n increases. When does the iteration converge?

Theorem 2 (*Convergence of Fixed Point Iteration Method*)

Let $x = s$ be a solution of $x = g(x)$ and suppose that g has a continuous derivative in some interval I containing s . Then if $|g'(x)| \leq K \leq 1$ in I , the iteration process defined by $x = g(x)$ converges for any s in I .

Example 2

Use the fixed point iteration method to find the solution of the equation

$$x^3 + x - 1 = 0.$$

Solution:

The equation may be written in the form $x = \frac{1}{1+x^2}$, while the iteration can be expressed as

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

A rough sketch indicates that there is a solution near $x = 1$, and taking $x_0 = 1$, we obtain the iterations

$$x_1 = 0.5, x_2 = 0.800, x_3 = 0.610, x_4 = 0.729, x_5 = 0.653, x_6 = 0.701, \dots$$

The solution to 6 places of decimals is 0.682328.

Exercise

Use the fixed point iteration method to determine the solution of the equation $x^2 - x = 0$. Compare your solution with the exact solution.

1.4 Newton-Raphson Method

This is another iteration method for solving equation (1.1), where f is assumed to have a continuous first derivative f' . Suppose $x = x_0 + h$ is the correct root of (1.1), then expanding $f(x_0 + h)$ in Taylor series leads to

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \dots = 0.$$

Neglecting the second and higher order derivatives, one obtains

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

Therefore,

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

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

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

⋮

We then have the iteration scheme

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}} \quad (1.3)$$

If $f'(x_n) = 0$, then use a different starting value. The Newton-Raphson method is used to improve the results obtained by previous methods.

Example 3

Determine the solution of the equation $x^3 + x - 1 = 0$ using the Newton-Raphson method.

Solution:

$$f(x) = x^3 + x - 1, f'(x) = 3x^2 + 1,$$
$$\therefore x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^3 + x_n - 1}{3x_n^2 + 1}.$$

taking $x_0 = 1$, one obtains

$$x_1 = x_0 - \frac{x_0^3 + x_0 - 1}{3x_0^2 + 1} = 0.75,$$
$$x_2 = x_1 - \frac{x_1^3 + x_1 - 1}{3x_1^2 + 1} = 0.68604651,$$

and iterate to convergence to the required degree of accuracy.

Example 4

Find the root of the equation $x \sin x + \cos x = 0$ using the Newton-Raphson method.

Solution:

$$f(x) = x \sin x + \cos x, f'(x) = x \cos x,$$

The iteration formula then becomes

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

Take $x_0 = \pi$ and then obtain

$$x_1 = 2.823$$

$$x_2 = 2.7986$$

$$x_3 = 2.7984$$

$$x_4 = 2.7984,$$

Note the convergence of the solution above to 4 places of decimals.

1.4.1 Convergence of Newton-Raphson Method

Consider $\phi(x) = x - \frac{f(x)}{f'(x)}$, thus $\phi'(x) = \frac{f(x)f''(x)}{(f'(x))^2}$. We assume $f(x)$, $f'(x)$ and $f''(x)$ are continuous and bounded on any interval containing the root $x = \xi$ of equation (1.1). If ξ is a simple root, then $f'(\xi) \neq 0$, and since $f'(x)$ is continuous, $|f'(x)| \geq \epsilon$, for some $\epsilon > 0$ in a suitable neighbourhood of ξ . Within this neighbourhood, we can select an interval such that $|f(x)f''(x)| < \epsilon^2$ and this is possible since $f(\xi) = 0$ and since $f(x)$ is continuously twice differentiable. Thus, in this interval we have $|\phi'(x)| < 1$.

Hence by theorem 1, Newton-Raphson method converges, provided the initial approximation is sufficiently close to ξ . Newton-Raphson method still converges, but slowly when ξ is a multiple root. To determine the rate of convergence of the method, we note that $f(\xi) = 0$ so that Taylor's expansion gives

$$f(x_n) + (\xi - x_n)f'(x_n) + \frac{1}{2}(\xi - x_n)^2 f''(x_n) + \dots = 0$$

from which we get

$$(\xi - x_n) + \frac{\frac{1}{2}(\xi - x_n)^2 f''(x_n)}{f'(x_n)} = -\frac{f(x_n)}{f'(x_n)}.$$

Using Newton-Raphson iteration formula, we obtain

$$x_{n+1} - \xi = \frac{\frac{1}{2}(\xi - x_n)^2 f''(x_n)}{f'(x_n)}$$

and setting $\epsilon_n = x_n - \xi$, we have

$$\boxed{\epsilon_{n+1} = \frac{\frac{1}{2}\epsilon_n^2 f''(\xi)}{f'(\xi)}} \quad (1.4)$$

Hence Newton-Raphson method has a second order or quadratic convergence.

Assignment

Obtain a root of each of the equations

1. $2x = 3 + \cos x$

2. $e^x - \tan^{-1} x - \frac{3}{2} = 0$

3. $x^2 + \cos x - xe^{-x} = 0$

correct to 3 places of decimals using

(a) the bisection method

(b) fixed point iteration method

(c) Newton-Raphson method.

Compare the three results in tabular form.

1.5 Numerical Evaluation of Multiple Roots of Algebraic Equations

We say that the function $f(x)$ has a root α of multiplicity $p > 1$ if

$$\boxed{f(x) = (x - \alpha)^p h(x)} \quad (1.5)$$

with $h(\alpha) \neq 0$ and $h(x)$ continuous at $x = \alpha$. We restrict p to be a positive integer, although the result could be valid for non-integral values for some cases.

1.5.1 Newton-Raphson Method and Multiple Roots

Most of the rootfinding methods considered so far perform poorly when the root being sought is multiple. We now investigate this for Newton-Raphson method as a fixed point method with $f(x)$ satisfying (1.5). Thus

$$x_{n+1} = g(x_n), g(x) = x - \frac{f(x)}{f'(x)}, x \neq \alpha.$$

The expression for $g(x)$ on using (1.5) is obtained as

$$f'(x) = (x - \alpha)^p h'(x) + p(x - \alpha)^{p-1} h(x)$$

$$\therefore g(x) = x - \frac{(x - \alpha)^p h(x)}{(x - \alpha)^{p-1} [(x - \alpha)h'(x)]} = x - \frac{(x - \alpha)h(x)}{ph(x) + (x - \alpha)h'(x)}.$$

One then obtains

$$g'(x) = 1 - \frac{h(x)}{ph(x) + (x - \alpha)h'(x)} - (x - \alpha) \frac{d}{dx} \left[\frac{h(x)}{ph(x) + (x - \alpha)h'(x)} \right]$$

and $g'(\alpha) = 1 - \frac{1}{p} \neq 0$ for $p > 1$. You can then find p for any given α . This shows that Newton-Raphson Method is a linear method with rate of convergence $\frac{p-1}{p}$.

Example 5

Determine the multiplicity of the root of the equation

$$x^4 - 5.4x^3 + 10.56x^2 - 8.954x + 2.7951 = 0$$

lying in the interval $1 \leq x \leq 2$.

Solution:

$$f(x) = x^4 - 5.4x^3 + 10.56x^2 - 8.954x + 2.7951,$$

$$f'(x) = 4x^3 - 16.2x^2 + 21.12x - 8.954$$

$$\therefore x_1 = 1.032352941, x_2 = 1.054435334, x_3 = 1.069406530,$$

$$x_4 = 1.079501623, x_5 = 1.086286231, \dots$$

Thus

$$g(x) = x - \frac{f(x)}{f'(x)}.$$

Now taking $x \approx 1.086$ as the approximate root, we obtain

$$g'(1.086) = 0.6698244,$$

thus we solve the equation $\frac{p-1}{p} = 0.6698244$ which yields $p = 3.02869144$.

Hence $p \approx 3$. Therefore the root has multiplicity 3.

1.6 Solutions of Systems of Nonlinear Equations

We consider in this section the numerical solution of simultaneous equations by two methods:

(a) Fixed Point Iteration method and

(b) Newton-Raphson Method

We shall consider the case of two equations in two unknowns only.

1.6.1 Fixed Point Iteration Method

Consider the nonlinear system of equations

$$f(x, y) = 0 \tag{1.6}$$

$$g(x, y) = 0$$

Re-write the system in the form

$$x = F(x, y) \tag{1.7}$$

$$y = G(x, y)$$

where F and G satisfy the conditions of convergence

$$\left| \frac{\partial F}{\partial x} \right| + \left| \frac{\partial G}{\partial x} \right| < 1$$

and

$$\left| \frac{\partial F}{\partial y} \right| + \left| \frac{\partial G}{\partial y} \right| < 1$$

in the neighbourhood of the root. Suppose (x_0, y_0) is the initial approximation to the root. Then the sequence of successive approximations becomes

$$x_1 = F(x_0, y_0), y_1 = G(x_1, y_0),$$

$$x_2 = F(x_1, y_1), y_1 = G(x_2, y_1),$$

$$x_3 = F(x_2, y_2), y_3 = G(x_3, y_2),$$

⋮

$$x_{n+1} = F(x_n, y_n), y_{n+1} = G(x_{n+1}, y_n).$$

Iterate to convergence.

Example 6

Find the root of the system of equations

$$x^2 + y^2 - 1 = 0 \tag{1.8}$$

$$\frac{x^2}{2} + 4y^2 - 1 = 0 \tag{1.9}$$

correct to 3 places of decimals using the initial value $(x_0, y_0) = (1, 1)$. Transforming the equations lead to the iteration scheme

$$x_{n+1} = \sqrt{1 - y_n^2}, y_{n+1} = \sqrt{\frac{1}{4} - \frac{x_{n+1}^2}{8}}.$$

Thus we obtain the iterations

$$x_1 = 0, y_1 = 0.5$$

$$x_2 = 0.866025404, y_2 = 0.3952847075$$

$$x_3 = 0.9185586535, y_3 = 0.3801726581$$

$$x_4 = 0.9249155367, y_4 = 0.3782412011$$

$$x_5 = 0.9257070778, y_5 = 0.3779990751$$

$$x_6 = 0.9258059728, y_6 = 0.3779687984$$

We have then achieved 3 places of decimals accuracy.

That is $x \approx 0.926, y \approx 0.378$.

1.6.2 Newton-Raphson Method

Suppose the initial approximation to the root of the system is (x_0, y_0) , and if $(x_0 + h, y_0 + k)$ is the exact root of the system, then we must have that

$$f(x_0 + h, y_0 + k) = 0, g(x_0 + h, y_0 + k) = 0.$$

If f and g are sufficiently differentiable, we can expand them in Taylor's series as

$$\begin{aligned} f_0 + h \frac{\partial f}{\partial x_0} + k \frac{\partial f}{\partial y_0} + \dots &= 0 \\ g_0 + h \frac{\partial g}{\partial x_0} + k \frac{\partial g}{\partial y_0} + \dots &= 0 \end{aligned} \quad (1.10)$$

where

$$f_0 = f(x_0, y_0), g_0 = g(x_0, y_0), \frac{\partial f}{\partial x_0} = \left[\frac{\partial f}{\partial x} \right]_{x=x_0}, \frac{\partial f}{\partial y_0} = \left[\frac{\partial f}{\partial y} \right]_{y=y_0}.$$

Neglecting the second and higher order terms, we obtain the system of linear equations

$$\begin{aligned} h \frac{\partial f}{\partial x_0} + k \frac{\partial f}{\partial y_0} &= -f_0 \\ h \frac{\partial g}{\partial x_0} + k \frac{\partial g}{\partial y_0} &= -g_0 \end{aligned} \quad (1.11)$$

The system (1.9) can be solved for h and k to obtain the new solution as

$$x_1 = x_0 + h, y_1 = y_0 + k.$$

The process is repeated until the required accuracy is attained.

Example 6

Find the real roots of the equations

$$x^2 - y^2 = 4$$

$$x^2 + y^2 = 16$$

Solution:

This system has the solutions $x = \sqrt{10} = 3.162$ and $y = \sqrt{6} = 2.449$. To apply the Newton-Raphson method, we replace the hyperbola by its asymptote $y = x$. This produces the initial values $x_0 = y_0 = 2\sqrt{2} = 2.828$. However, in general, this is obtained from a rough graph.

Taking $f = x^2 - y^2 - 4, g = x^2 + y^2 - 16$

$$\Rightarrow \frac{\partial f}{\partial x} = 2x, \frac{\partial f}{\partial y} = -2y, \frac{\partial g}{\partial x} = 2x, \frac{\partial g}{\partial y} = 2y,$$

$$\text{and } f_0 = x_0^2 - y_0^2 - 4 = -4, g_0 = x_0^2 + y_0^2 - 16 = 0.$$

$\therefore \frac{\partial f}{\partial x_0} = 2x_0 = 4\sqrt{2}, \frac{\partial f}{\partial y_0} = -2y_0 = -4\sqrt{2}, \frac{\partial g}{\partial x_0} = 2x_0 = 4\sqrt{2}, \frac{\partial g}{\partial y_0} = 2y_0 = 4\sqrt{2}$. Thus one obtains the equations

$$h - k = 0.707$$

$$h + k = 0$$

which have the solutions $h = 0.354, k = -0.354$. The second approximation is then given by

$$x_1 = x_0 + h = 3.182, y_1 = y_0 + k = 2.474.$$

Using (x_1, y_1) and repeating the process, we obtain $h = -0.0204, k = -0.0242$ and thus $x_2 = x_1 + h = 3.162, y_2 = y_1 + k = 2.450$.

For a system of equations, the procedure is modified accordingly. Thus to obtain the solution to the system

$$f(x, y) = x^2 + y^2 - 1 = 0$$

$$g(x, y) = \frac{x^2}{2} + 4y^2 - 1 = 0$$

subject to the initial approximation $[x_0, y_0] = [1, 1]$, we replace $f'(x)$ in the Newton-Raphson iteration scheme with the Jacobian $J(\mathbf{x})$ of the system. Thus the iteration scheme becomes

$$\boxed{\mathbf{x}_{n+1} = \mathbf{x}_n - \frac{f(\mathbf{x}_n)}{J(\mathbf{x}_n)} = \mathbf{x}_n - f(\mathbf{x}_n)J^{-1}(\mathbf{x}_n)} \quad (1.12)$$

where $\mathbf{X}_n = (x_n, y_n)$ and $J(\mathbf{x}_n) = \begin{pmatrix} \frac{\partial f}{\partial x_n} & \frac{\partial f}{\partial y_n} \\ \frac{\partial g}{\partial x_n} & \frac{\partial g}{\partial y_n} \end{pmatrix}$ and $J^{-1}(\mathbf{x}_n)$ is the inverse of

$J(\mathbf{x}_n)$. Thus the iteration scheme becomes

$$\boxed{(x_{n+1}, y_{n+1}) = (x_n, y_n) - \frac{(f(x_n, y_n), g(x_n, y_n))}{\begin{pmatrix} \frac{\partial f}{\partial x_n} & \frac{\partial f}{\partial y_n} \\ \frac{\partial g}{\partial x_n} & \frac{\partial g}{\partial y_n} \end{pmatrix}}} \quad (1.13)$$

Hence, for the above system, we obtain

$$(x_{n+1}, y_{n+1}) = (x_n, y_n) - \frac{\left(x^2 + y^2 - 1, \frac{x^2}{2} + 4y^2 - 1\right)}{\begin{pmatrix} 2x_n & 2y_n \\ x_n & 8y_n \end{pmatrix}}$$

Taking $x_0 = (1, 1)$ leads to the following sequence of approximations:

$$(x_1, y_1) = (1, 1) - \frac{(1, 3.5)}{\begin{pmatrix} 2 & 2 \\ 1 & 8 \end{pmatrix}} = (1, 1) - (1, 3.5) \begin{pmatrix} 0.57142857 & -0.14285714 \\ -0.07142857 & 0.14285714 \end{pmatrix} \\ = (0.67857143, 0.64285714).$$

$$\begin{aligned} (x_1 \ y_1) &= (0.67857143 \ 0.64285714) \\ (x_2 \ y_2) &= (0.88305212 \ 0.41999860) \\ (x_3 \ y_3) &= (0.92764766 \ 0.38043036) \\ (x_4 \ y_4) &= (0.92613160 \ 0.37779498) \\ (x_5 \ y_5) &= (0.92581236 \ 0.37794889) \end{aligned} \quad (1.14)$$

Hence we have achieved convergence to three places of decimals, that is

$$x \approx 0.926, y \approx 0.378.$$

Class Exercise:

Use the fixed point iteration method to obtain the solution of example 6 above.

General Exercises

1. Obtain a root for each of the following equations using the bisection method

$$(a) \ x^3 + x^2 + x + 7 = 0 \quad (b) \ x^3 - x^2 - 1 = 0$$

2. Use the fixed point iteration method to find a root of each of the following equations correct to 4 s.f.

(a) $\cos x = 3x - 1$ (b) $x = \frac{1}{(1+x)^2}$

3. Use Newton-Raphson method to solve the equation

(a) $x^4 - x^3 - 2x - 34 = 0$ (b) $\tan x = 4x$.

Chapter 2

Interpolation

Given a function $f(x)$ defined on the interval $x_0 < x < x_n$, and assuming that $f(x)$ is single-valued and continuous and that it is known explicitly, then the values of $f(x)$ corresponding to certain given values of x , say $x_0, x_1, x_2, \dots, x_n$, can easily be computed and tabulated. However, the major problem of numerical analysis is the converse, that is, given the set of tabular values

$(x_0, y_0), (x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ satisfying the relation $y = f(x)$ where the explicit nature of $f(x)$ is unknown, it is required to find a simpler function $\phi(x)$ such that $f(x)$ and $\phi(x)$ agree at the set of tabulated points. Such a process is known as *interpolation*. If $\phi(x)$ is a polynomial, then the process is called *polynomial interpolation* and $\phi(x)$ is called the *interpolating polynomial*.

2.1 Finite Differences

Assuming we have a table of values $(x_i, y_i), i = 0, 1, 2, \dots, n$ of any function $y = f(x)$, the values of x being equally spaced, i.e. $x_i = x_0 + ih, i = 0, 1, 2, \dots, n$. Suppose that we are required to recover the values of $f(x)$ for some intermediate values of x or to obtain the derivative of $f(x)$ for some x in the range $x_0 < x < x_n$.

The methods for the solution of these problems are based on the concept of the differences of a function which we now proceed to define.

2.1.1 Forward Differences

If $y_0, y_1, y_2, \dots, y_n$ denote a set of values of y , then

$$y_1 - y_0, y_2 - y_1, y_3 - y_2, \dots, y_n - y_{n-1}$$

are called the *differences* of y . Denoting the differences by $\Delta y_0, \Delta y_1, \Delta y_2, \dots, \Delta y_{n-1}$ respectively, we have

$$\Delta y_0 = y_1 - y_0, \Delta y_1 = y_2 - y_1, \Delta y_2 = y_3 - y_2, \dots, \Delta y_{n-1} = y_n - y_{n-1}.$$

where Δ is called the *forward difference operator* and $\Delta y_0, \Delta y_1, \Delta y_2, \dots$ are called *first forward differences*. The differences of the first forward differences are called *second forward differences* and are denoted by $\Delta^2 y_0, \Delta^2 y_1, \Delta^2 y_2, \dots$. Similarly, one can define the third and higher differences. Thus,

$$\begin{aligned} \Delta^2 y_0 &= \Delta(y_1 - y_0) = \Delta y_1 - \Delta y_0 = y_2 - 2y_1 + y_0 \\ \Delta^3 y_0 &= \Delta^2 y_1 - \Delta^2 y_0 = \Delta y_2 - \Delta y_1 - (\Delta y_1 - \Delta y_0) \\ &= y_3 - y_2 - (y_1 - y_0) - [y_2 - y_1 - (y_1 - y_0)] \\ &= y_3 - 3y_2 + 3y_1 - y_0. \end{aligned}$$

Similarly,

$$\Delta^4 y_0 = \Delta^3 y_1 - \Delta^3 y_0 = y_4 - 4y_3 + 6y_2 - 4y_1 + y_0.$$

Note that the coefficients in the above expansions are binomial coefficients.

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
x_0	y_0	Δy_0					
x_1	y_1	Δy_1	$\Delta^2 y_0$	$\Delta^3 y_0$			
x_2	y_2	Δy_2	$\Delta^2 y_1$	$\Delta^3 y_1$	$\Delta^4 y_0$		
x_3	y_3	Δy_3	$\Delta^2 y_2$	$\Delta^3 y_2$	$\Delta^4 y_1$	$\Delta^5 y_0$	
x_4	y_4	Δy_4	$\Delta^2 y_3$	$\Delta^3 y_3$	$\Delta^4 y_2$	$\Delta^5 y_1$	$\Delta^6 y_0$
x_5	y_5	Δy_5	$\Delta^2 y_4$	$\Delta^3 y_4$	$\Delta^4 y_3$		
x_6	y_6	Δy_6	$\Delta^2 y_5$				

Table 2.1: The table of forward differences.

2.1.2 Backward differences

The differences $y_1 - y_0, y_2 - y_1, y_3 - y_2, \dots, y_n - y_{n-1}$ are called *first backward differences* if they are denoted by $\nabla y_1, \nabla y_2, \nabla y_3, \dots, \nabla y_n$ respectively so that $\nabla y_1 = y_1 - y_0, \nabla y_2 = y_2 - y_1, \dots, \nabla y_n = y_n - y_{n-1}$, where ∇ is called the *backward difference operator*. In a similar way, one can define backward differences of higher orders. Thus we have

$$\nabla^2 y_2 = \nabla y_2 - \nabla y_1 = y_2 - 2y_1 + y_0,$$

$$\nabla^3 y_3 = \nabla^2 y_3 - \nabla^2 y_2 = y_3 - 3y_2 + 3y_1 - y_0,$$

and so forth.

2.1.3 Central Differences

The central difference operator is defined by the relations

$$\delta y_{\frac{1}{2}} = y_1 - y_0, \delta y_{\frac{3}{2}} = y_2 - y_1, \dots, \delta y_{n-\frac{1}{2}} = y_n - y_{n-1}.$$

Higher order central differences can be obtained in a similar manner. Using the values from the two tables above, the central difference table can be formed thus

x	y	∇	∇^2	∇^3	∇^4	∇^5	∇^6
x_0	y_0						
x_1	y_1	∇y_1					
x_2	y_2	∇y_2	$\nabla^2 y_2$				
x_3	y_3	∇y_3	$\nabla^2 y_3$	$\nabla^3 y_3$			
x_4	y_4	∇y_4	$\nabla^2 y_4$	$\nabla^3 y_4$	$\nabla^4 y_4$		
x_5	y_5	∇y_5	$\nabla^2 y_5$	$\nabla^3 y_5$	$\nabla^4 y_5$	$\nabla^5 y_5$	
x_6	y_6	∇y_6	$\nabla^2 y_6$	$\nabla^3 y_6$	$\nabla^4 y_6$	$\nabla^5 y_6$	$\nabla^6 y_6$

Table 2.2: The table of backward differences.

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

Table 2.3: The table of central differences.

Note from the three tables that

$$\Delta y_0 = \nabla y_1 = \delta y_{\frac{1}{2}},$$

$$\Delta^3 y_2 = \nabla^3 y_5 = \delta^3 y_{\frac{7}{2}},$$

and so on.

2.1.4 symbolic Relations

We can establish difference formulae by using the shift operator E in addition to the operators Δ , ∇ and δ defined above. The shift operator E is defined by

$$Ey_i = y_{i+1}$$

$$E^2y_i = E(Ey_i) = E(y_{i+1}) = y_{i+2}$$

and in general

$$\boxed{E^n(y_i) = y_{i+n}} \quad (2.1)$$

Now, a relationship between Δ and E can be derived as follows:

$\Delta y_0 = y_1 - y_0 = Ey_0 - y_0 = (E - 1)y_0$. Hence $\Delta = E - 1$ or $E = 1 + \Delta$. This implies that the effect of E on y_0 is the same as that of the operator $(1 + \Delta)$ on y_0 .

The higher order forward differences in terms of the given function values are

$$\Delta^2 y_0 = (E - 1)^2 y_0 = (E^2 - 2E + 1)y_0 = E^2 y_0 - 2E y_0 + E^0 y_0 = y_2 - 2y_1 + y_0,$$

$$\Delta^3 y_0 = (E - 1)^3 y_0 = (E^3 - 3E^2 + 3E - 1)y_0 = y_3 - 3y_2 + 3y_1 - y_0.$$

The following relations can also be established from the definitions

$$\nabla y_0 = y_0 - E^{-1}y_0 = (1 - E^{-1})y_0$$

$$\Rightarrow \nabla \equiv 1 - E^{-1}.$$

Also,

$$\delta y_0 = E^{\frac{1}{2}}y_0 - E^{-\frac{1}{2}}y_0 = (E^{\frac{1}{2}} - E^{-\frac{1}{2}})y_0$$

$$\therefore \delta \equiv E^{\frac{1}{2}} - E^{-\frac{1}{2}},$$

Hence

$$\Delta \equiv \nabla E \equiv \delta E^{\frac{1}{2}}.$$

2.1.5 Detecting Errors by Use of Difference Tables

Errors in tabulated values can easily be detected using difference tables. For example, if we introduce an error e in a tabulated values of zeroes, we can notice how the error propagates fanwise at higher differences and also gets magnified. The following characteristics of error propagation can be deduced from the table that follows:

- (i) Error increases with the order of the differences
- (ii) The errors in any one column are the binomial coefficients with alternating signs
- (iii) The algebraic sum of the errors in any difference column is zero
- (iv) The maximum error occurs opposite the function value containing the error.

Suppose an error e is introduced into the table of values of a given function, then these indicators can be used to detect errors in difference tables as can be seen from table (2.4) below.

2.2 Differences of a Polynomial

Suppose $y(x)$ is a polynomial of degree n so that

$$\boxed{y(x) = a_0x^n + a_1x^{n-1} + a_2x^{n-2} + \dots + a_n} \quad (2.2)$$

We then obtain the difference of $y(x)$ as

$$\begin{aligned} \Delta y(x) &= y(x+h) - y(x) \\ &= a_0 [(x+h)^n - x^n] + a_1 [(x+h)^{n-1} - x^{n-1}] + \dots \\ &= a_0 n h x^{n-1} + a_1' x^{n-2} + \dots + a_n' \end{aligned} \quad (2.3)$$

y	Δ	Δ^2	Δ^3	Δ^4	Δ^5
0					
0	0	0	0		
0	0	0	0	0	e
0	0	0	e	e	$-5e$
0	e	e	$-3e$	$-4e$	$10e$
e	$-e$	$-2e$	$3e$	$6e$	$-10e$
0	0	e	$-e$	$-4e$	$5e$
0	0	0	0	e	$-e$
0	0	0	0	0	
0	0	0			
0	0				

Table 2.4: Error spread in a difference table

which shows that the difference of a polynomial of degree n is a polynomial of degree $n - 1$. Similarly, the second difference will be a polynomial of degree $n - 2$ and $\Delta^n y(x)$ will then be a constant.

For example, consider the polynomial $y(x) = ax^2 + bx + c$.

The first and second forward differences become

$$\begin{aligned}
 \Delta y(x) &= y(x+h) - y(x) \\
 &= a(x+h)^2 + b(x+h) + c - ax^2 - bx - c \\
 &= (2ax + ah + b)h \\
 \Delta^2 y(x) &= \Delta y(x+h) - \Delta y(x) \\
 &= 2ah^2
 \end{aligned}$$

2.2.1 Newton's Interpolation Formulae

Given the set of $n + 1$ values, $(x_0, y_0), (x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$, of x and y , it is required to find $y_n(x)$, a polynomial of degree n such that y and $y_n(x)$ agree at the tabulated points. Suppose the values of x are equidistant, and let $x_i = x_0 + ih, i = 0, 1, 2, \dots, n$. Since $y_n(x)$ is a polynomial of degree n , it may be written as

$$\boxed{y_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \dots + a_n(x - x_0)(x - x_1) \dots (x - x_{n-1})} \quad (2.4)$$

Now, we impose the condition that y and $y_n(x)$ should agree at the set of tabulated points, i.e $y(x_i) = y_i(x_i)$, we obtain

$$y_0 = a_0, y_1 = a_1(x_1 - x_0) + y_0 \Rightarrow a_1 = \frac{y_1 - y_0}{x_1 - x_0} = \frac{\Delta y_0}{h}.$$

$$\begin{aligned} y_2 &= a_0 + a_1(x_2 - x_0) + a_2(x_2 - x_0)(x_2 - x_1) \\ &= y_0 + \frac{y_1 - y_0}{x_1 - x_0}(x_2 - x_0) + a_2h(x_2 - x_0) \\ &\quad \therefore \frac{y_2 - y_0}{x_2 - x_0} = \frac{\Delta y_0}{h} + a_2h \\ \Rightarrow a_2 &= \frac{1}{h} \left[\frac{y_2 - y_0}{2h} - \frac{y_1 - y_0}{h} \right] \\ &= \frac{y_2 - 2y_1 + y_0}{2h^2} = \frac{\Delta^2 y_0}{2h^2}. \end{aligned}$$

Similarly,

$$a_3 = \frac{\Delta^3 y_0}{3!h^3}, a_4 = \frac{\Delta^4 y_0}{4!h^4}, \dots, a_n = \frac{\Delta^n y_0}{n!h^n}.$$

Setting $x = x_0 + ph$ and substituting for $a_0, a_1, a_2, \dots, a_n$ in (2.4) above gives

$$\begin{aligned} y_n(x) &= y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 \\ &\quad + \dots + \frac{p(p-1)(p-2) \dots (p-n+1)}{n!}\Delta^n y_0 \end{aligned} \quad (2.5)$$

This is called *Newton's forward interpolation formula* and it is useful for interpolation near the beginning of a set of tabular values.

The error committed in replacing the function $y(x)$ by the polynomial $y_n(x)$ can be obtained as

$$\boxed{y(x) - y_n(x) = \frac{(x - x_0)(x - x_1) \cdots (x - x_n)}{(n + 1)!} y^{(n+1)}(\xi)} \quad (2.6)$$

for $x_0 < \xi < x_n$. However, (2.6) is not useful in practice, since we have no information concerning $y^{(n)}(x)$. In any case, if $y^{(n)}(x)$ does not vary rapidly in the interval, a useful estimate of the derivative can be obtained thus:

We obtain the Taylor's series expansion of $y(x + h)$ as

$$y(x + h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \cdots$$

and neglecting the term containing h^2 and higher powers of h , produces

$$y'(x) = \frac{1}{h} [y(x + h) - y(x)] = \frac{1}{h} \Delta y(x).$$

Thus $y^{(n+1)}(x) = \frac{1}{h^{n+1}} \Delta^{n+1} y(x)$. Equation (2.6) can then be written as

$$\boxed{y(x) - y_n(x) = \frac{p(p - 1)(p - 2) \cdots (p - n)}{(n + 1)!} \Delta^{n+1} y(\xi)} \quad (2.7)$$

a form suitable for computation.

If we assume (2.4) in the form

$$y_n(x) = a_0 + a_1(x - x_n) + a_2(x - x_n)(x - x_{n-1}) + \cdots + a_n(x - x_n)(x - x_{n-1}) \cdots (x - x_1)$$

and then impose the condition that $y(x)$ and $y_n(x)$ should agree at the tabulated points $x_n, x_{n-1}, x_{n-2}, \cdots, x_2, x_1, x_0$, we obtain in a similar manner as above

$$\boxed{y_n(x) = y_n + p \nabla y_n + \frac{p(p + 1)}{2!} \nabla^2 y_n + \cdots + \frac{p(p + 1) \cdots (p + n - 1)}{n!} \nabla^n y_n} \quad (2.8)$$

where $p = \frac{x-x_n}{h}$. This is called *Newton's backward difference interpolating formula* and it uses tabular values to the left of y_n . This formula is useful for interpolation near the end of tabulated values. The error is estimated as

$$y(x) - y_n(x) = \frac{p(p+1)(p+2)\cdots(p+n)}{(n+1)!} h^{n+1} y^{(n+1)}(\xi) \quad (2.9)$$

where $x_0 < \xi < x_n$ and $x = x_n + ph$.

Example 7

Find the cubic polynomial which takes the following values:

x	0	1	2	3
y	1	0	1	10

Hence or otherwise obtain $y(4)$.

Solution:

We form the forward difference table thus:

x	y	Δ	Δ^2	Δ^3
0	1	-1		
1	0	1	2	
2	1	9	8	6
3	10			

Here, $h = 1$ (from the forward difference table). Using $x = x_0 + ph$ and choosing $x_0 = 0$, one obtains $x = 0 + p = p$. Thus substituting for p in (2.5), one obtains

$$y(x) = 1 + x(-1) + \frac{x(x-1)}{2!}(2) + \frac{x(x-1)(x-2)}{3!}(6) = x^3 - 2x^2 + 1,$$

which is the polynomial from which we obtained the tabulated values above. $y(4)$ can be obtained by substituting $x = 4$ in the polynomial obtained above. Note that this process of obtaining the value of y for some value of x outside the given range is called *extrapolation* and this demonstrates the fact that if a tabulated function is a polynomial, then interpolation and extrapolation would yield exact values.

Example 8

The table below gives the values of $\tan x$ for $0.10 \leq x \leq 0.30$.

x	0.10	0.15	0.20	0.25	0.30
$y = \tan x$	0.1003	0.1511	0.2027	0.2553	0.3093

Find: (a) $\tan(0.12)$ (b) $\tan(0.26)$ (c) $\tan(0.40)$ (d) $\tan(0.50)$.

Solution:

The table of forward differences is

x	y	Δ	Δ^2	Δ^3	Δ^4
0.10	0.1003				
0.15	0.1511	0.0508	0.0008		
0.20	0.2027	0.0516	0.0010	0.0002	
0.25	0.2553	0.0526	0.0014	0.0004	0.0002
0.30	0.3093	0.0540			

(i) Taking $x = x_0 + ph$, where $x_0 = 0.10$, $h = 0.05$, thus to find the value of $\tan(0.12)$, we have that $0.12 = 0.10 + 0.05p \Rightarrow p = 0.4$, and using (2.5) yields

$$\begin{aligned} \tan(0.12) &= 0.1003 + 0.4(0.0508) + \frac{0.4(0.4-1)}{2}(0.0008) \\ &+ \frac{0.4(0.4-1)(0.4-2)}{6}(0.0002) + \frac{0.4(0.4-1)(0.4-2)(0.4-3)}{24}(0.0002) = 0.1205. \end{aligned}$$

(i) To obtain $\tan(0.26)$, we have $0.26 = 0.30 + p(0.05) \Rightarrow p = -0.8$. We now use Newton's backward interpolation formula (2.8), since we are estimating a value at

the end of the data. Hence one obtains

$$\begin{aligned} \tan(0.26) &= 0.3093 - 0.8(0.0540) - \frac{0.8(-0.8+1)}{2}(0.0014) \\ &- \frac{0.8(-0.8+1)(-0.8+2)}{6}(0.0004) - \frac{0.8(-0.8+1)(-0.8+2)(-0.8+3)}{24}(0.0002) \\ &= 0.2662. \end{aligned}$$

Using formula (2.5) and proceeding as in (i), one gets

$$(iii) \tan(0.40) = 0.4241 \text{ and}$$

$$(iv) \tan(0.50) = 0.5543.$$

Note that the actual values of $\tan(0.12)$, $\tan(0.26)$, $\tan(0.40)$, $\tan(0.50)$ are respectively 0.1206, 0.2660, 0.4228 and 0.5463. Thus if the tabulated function is not a polynomial, then extrapolation very far from the table limits would be dangerous, although interpolation can be carried out very accurately.

2.3 Interpolation with unevenly spaced points

In the previous section, we derived interpolation formulae and discussed their practical use in some detail. However, they possess a major disadvantage of requiring the values of the independent variable to be equally spaced (i.e uniform grids). It is therefore desirable to have interpolation formulae with unequally spaced values of the argument (non-uniform grids). We discuss in this section Lagrange's interpolation formula which uses only the function values.

2.3.1 Lagrange's interpolation formula

Let $y(x)$ be continuous and differentiable $(n+1)$ times in the interval (a, b) . Given the $n+1$ points $(x_0, y_0), (x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$, where the values of x need not necessarily be equally spaced, we wish to find a polynomial of degree n , say

$\phi_n(x)$ such that

$$\boxed{\phi_i(x_i) = y(x_i) = y_i, i = 0, 1, 2, \dots, n} \quad (2.10)$$

Let

$$\boxed{\phi_n(x) = a_0 + a_1x + a_2x^2 + \dots + a_nx^n} \quad (2.11)$$

be the desired polynomial. Substituting the condition (2.10) into (2.11), we obtain the system of equations

$$\begin{aligned} y_0 &= a_0 + a_1x_0 + a_2x_0^2 + \dots + a_nx_0^n \\ y_1 &= a_0 + a_1x_1 + a_2x_1^2 + \dots + a_nx_1^n \\ y_2 &= a_0 + a_1x_2 + a_2x_2^2 + \dots + a_nx_2^n \\ &\vdots \quad \quad \quad \vdots \quad \quad \quad \dots \quad \quad \quad \vdots \\ y_n &= a_0 + a_1x_n + a_2x_n^2 + \dots + a_nx_n^n \end{aligned} \quad (2.12)$$

The system (2.12) will have a solution if the determinant

$$\begin{vmatrix} 1 & x_0 & x_0^2 & \dots & x_0^n \\ 1 & x_1 & x_1^2 & \dots & x_1^n \\ 1 & x_2 & x_2^2 & \dots & x_2^n \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^n \end{vmatrix} \neq 0 \quad (2.13)$$

The value of this determinant called *Vandermonde's determinant* is

$$(x_0 - x_1)(x_0 - x_2) \dots (x_0 - x_n)(x_1 - x_2) \dots (x_1 - x_n) \dots (x_{n-1} - x_n).$$

Eliminating $a_0, a_1, a_2, \dots, a_n$ from equations (2.11) and (2.12), we obtain

$$\begin{vmatrix} \phi_n(x) & 1 & x & x^2 & \cdots & x^n \\ y_0 & 1 & x_0 & x_0^2 & \cdots & x_0^n \\ y_1 & 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ y_n & 1 & x_n & x_n^2 & \cdots & x_n^n \end{vmatrix} = 0 \quad (2.14)$$

which shows that $\phi_n(x)$ is a linear combination of $y_0, y_1, y_2, \dots, y_n$. Hence we write

$$\phi_n(x) = \sum_{i=0}^n L_i(x)y_i \quad (2.15)$$

where $L_i(x)$ are polynomials in x of degree n . Since $\phi_j(x_j) = y_j$ for $j = 0, 1, 2, \dots, n$, equation (2.15) gives

$$\delta_{ij} = \begin{cases} L_i(x_j) = 0, & \text{if } i \neq j \\ L_i(x_j) = 1, & \text{if } i = j \end{cases}$$

where δ_{ij} is the Kronecker delta. Hence $L_i(x)$ may be written as

$$\boxed{L_i(x) = \frac{(x - x_0)(x - x_1) \cdots (x - x_{i-1})(x - x_{i+1}) \cdots (x - x_n)}{(x_i - x_0)(x_i - x_1) \cdots (x_i - x_{i-1})(x_i - x_{i+1}) \cdots (x_i - x_n)}} \quad (2.16)$$

which satisfies the condition above. The function

$$\begin{aligned} \pi(x) &= (x - x_0)(x - x_1) \cdots (x - x_{i-1})(x - x_{i+1}) \cdots (x - x_n) \\ &= \prod_{i=0}^n (x - x_i) \end{aligned} \quad (2.17)$$

may be used to express the Lagrange multiplier function in the more compact form

$$L_i(x) = \frac{\pi(x)}{(x - x_i)\pi'(x_i)}.$$

Hence (2.15) yields

$$\boxed{\phi_n(x) = \sum_{i=0}^n \frac{\pi(x)}{(x - x_i)\pi'(x_i)} y_i} \quad (2.18)$$

which is known as *Lagrange's interpolation formula*. The $L_i(x)$ are called *Lagrange's interpolation coefficients*. Interchanging x and y in (2.18) yields the formula

$$\boxed{\phi_n(y) = \sum_{i=0}^n \frac{\pi(y)}{(y - y_i)\pi'(y_i)} x_i}, \quad (2.19)$$

which is useful for inverse interpolation. It is important to note that the Lagrange's interpolation polynomial is unique. From (2.18), we note that

$$\boxed{\phi_1(x) = L_0(x)y_0 + L_1(x)y_1} \quad (2.20)$$

where

$$\begin{aligned} L_0(x) &= \frac{\pi(x)}{(x - x_0)\pi'(x)} = \frac{(x - x_0)(x - x_1)}{(x - x_0)(x_0 - x_1)} = \frac{x - x_1}{x_0 - x_1} \\ L_1(x) &= \frac{\pi(x)}{(x - x_1)(x_0 - x_1)} = \frac{(x - x_0)(x - x_1)}{(x - x_1)(x_0 - x_1)} = \frac{x - x_0}{x_1 - x_0} \\ \therefore \phi(x) &= \frac{x - x_1}{x_0 - x_1}y_0 + \frac{x - x_0}{x_1 - x_0}y_1. \end{aligned}$$

This is a linear interpolation formula. For a quadratic interpolation, we have

$$\boxed{\phi_2(y) = L_0(x)y_0 + L_1(x)y_1 + L_2(x)y_2} \quad (2.21)$$

where

$$\begin{aligned} L_0(x) &= \frac{(x - x_0)(x - x_1)(x - x_2)}{(x - x_0)(x_0 - x_1)(x_0 - x_2)} = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}, \\ L_1(x) &= \frac{(x - x_0)(x - x_1)(x - x_2)}{(x - x_1)(x_1 - x_0)(x_1 - x_2)} = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \end{aligned}$$

and

$$\begin{aligned} L_2(x) &= \frac{(x - x_0)(x - x_1)(x - x_2)}{(x - x_2)(x_2 - x_0)(x_2 - x_1)} = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}. \\ \therefore \phi_2(x) &= \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}y_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}y_1 + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}y_2. \end{aligned}$$

Example 9

Obtain a linear Lagrange's polynomial for the tabulated values for $y = \ln x$.

Hence find the value of $y(9.2)$ correct to 4 places of decimals, and determine the error in the estimate.

x	9.0	9.5
$y = \ln x$	2.1972	2.2513

Solution:

Here, $x_0 = 9.0, x_1 = 9.5, y_0 = 2.1972, y_1 = 2.2513$.

$$\begin{aligned} \therefore \phi_1(x) &= L_0(x)y_0 + L_1(x)y_1 = \frac{x - x_1}{x_0 - x_1}y_0 + \frac{x - x_0}{x_1 - x_0}y_1 \\ &= \frac{x - 9.5}{9.0 - 9.5} \ln(9.0) + \frac{x - 9.0}{9.5 - 9.0} \ln(9.5) = \frac{x - 9.5}{-0.5}(2.1972) + \frac{x - 9.0}{0.5}(2.2513) \\ \therefore \phi_1(9.2) &= \frac{9.2 - 9.5}{-0.5}(2.1972) + \frac{9.2 - 9.0}{0.5}(2.2513) = 2.2188. \\ \therefore \text{error} &= 2.2192 - 2.2188 = 0.0004. \end{aligned}$$

Thus linear interpolation is not sufficient to get 4 d.p. accuracy, it would suffice for 3 d.p. accuracy.

Example 10

Obtain the value of $\ln(9.2)$ using the quadratic interpolation polynomial using the data below:

x	9.0	9.5	11.0
$y = \ln x$	2.1972	2.2513	2.3979

Solution:

$$\begin{aligned} L_0(x) &= \frac{(x - 9.5)(x - 11.0)}{(9.0 - 9.5)(9.0 - 11.0)} = x^2 - 20.5x - 104.5, L_0(9.2) = 0.5400 \\ L_1(x) &= \frac{(x - 9.0)(x - 11.0)}{(9.5 - 9.0)(9.5 - 11.0)} = -\frac{4}{3}(x^2 - 20x + 99), L_1(9.2) = 0.4800 \\ L_2(x) &= \frac{(x - 9.0)(x - 9.5)}{(11.0 - 9.0)(11.0 - 9.5)} = \frac{1}{3}(x^2 - 18.5x + 85.5), L_2(9.2) = -0.0200. \end{aligned}$$

$$\therefore \phi_2(9.2) = \ln(9.2) = 0.5400(2.1972) + 0.4800(2.2513) - 0.0200(2.3979) = 2.2192$$

which is exact to 4 d.p.

Example 11

Fit a cubic Lagrange's interpolation polynomial to the data below:

x	0	1	2	3
y	1	0	1	10

Solution:

$$L_0(x) = \frac{(x - x_1)(x - x_2)(x - x_3)}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)}y_0 = -\frac{1}{6}(x - 1)(x - 2)(x - 3)$$

$$L_1(x) = \frac{(x - x_0)(x - x_2)(x - x_3)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)}y_1 = 0$$

$$L_2(x) = \frac{(x - x_0)(x - x_1)(x - x_3)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)}y_2 = \frac{1}{2}x(x - 1)(x - 3)$$

$$L_3(x) = \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)}y_3 = \frac{5}{3}x(x - 1)(x - 2).$$

$$\therefore \phi_3(x) = L_0(x)y_0 + L_1(x)y_1 + L_2(x)y_2 + L_3(x)y_3$$

$$= -\frac{1}{6}(x - 1)(x - 2)(x - 3) + 0 - \frac{1}{2}x(x - 1)(x - 3) + \frac{5}{3}x(x - 1)(x - 2) = (x - 1)(x^2 - x - 1)$$

$$\therefore \phi_3(x) = x^3 - 2x + 1.$$

This is the same polynomial we have earlier obtained using Newton's forward interpolation.

2.4 Least Squares Method for Curve Fitting

The least squares method is one of the most systematic procedures for fitting a unique curve through given data points and is widely used in practical computations.

Let the set of data points be $(x_i, y_i), i = 0, 1, 2, \dots, m$, and let the curve given by $y = f(x)$ be fitted to this data. At $x = x_i$, the experimental (or observed) value of the ordinate is y_i and the corresponding value on the fitting curve is $f(x_i)$. If e_i is the error of approximation at $x = x_i$, then we have

$$\boxed{e_i = y_i - f(x_i)} \quad (2.22)$$

Now, if we let

$$\begin{aligned} S &= [y_1 - f(x_1)]^2 + [y_2 - f(x_2)]^2 + \dots + [y_m - f(x_m)]^2 \\ &= e_1^2 + e_2^2 + \dots + e_m^2, \end{aligned} \quad (2.23)$$

then the method of least squares consists of minimising S , that is the sum of the squares of the errors.

2.4.1 Fitting a straight line

Let $y = a_0 + a_1x$ be the straight line to be fitted to the given data. Then, corresponding to equation (2.23), we have

$$\boxed{S = [y_1 - (a_0 + a_1x_1)]^2 + [y_2 - (a_0 + a_1x_2)]^2 + \dots + [y_m - (a_0 + a_1x_m)]^2} \quad (2.24)$$

For S to be minimum, we have

$$\frac{\partial S}{\partial a_0} = -2[y_1 - (a_0 + a_1x_1)] - 2[y_2 - (a_0 + a_1x_2)] - \dots - 2[y_m - (a_0 + a_1x_m)] = 0$$

and

$$\frac{\partial S}{\partial a_1} = -2x_1[y_1 - (a_0 + a_1x_1)] - 2x_2[y_2 - (a_0 + a_1x_2)] - \dots - 2x_m[y_m - (a_0 + a_1x_m)] = 0$$

Simplifying the above equations yield

$$ma_0 + a_1(x_1 + x_2 + \dots + x_m) = y_0 + y_1 + y_2 + \dots + y_m$$

and

$$a_0(x_1 + x_2 + \cdots + x_m) + a_1(x_1^2 + x_2^2 + \cdots + x_m^2) = x_1y_1 + x_2y_2 + \cdots + x_my_m.$$

We then have the equations

$$\begin{aligned} ma_0 + a_1 \sum_{i=1}^m x_i &= \sum_{i=1}^m y_i \\ a_0 \sum_{i=1}^m x_i + a_1 \sum_{i=1}^m x_i^2 &= \sum_{i=1}^m x_i y_i \end{aligned} \quad (2.25)$$

where

$$a_0 = \frac{(\sum y_i)(\sum x_i^2) - (\sum x_i)(\sum x_i y_i)}{m \sum x_i^2 - (\sum x_i)^2}$$

and

$$a_1 = \frac{m \sum x_i y_i - (\sum x_i)(\sum y_i)}{m \sum x_i^2 - (\sum x_i)^2}.$$

Since the x_i and y_i are known quantities, the equations (2.25) are called the *normal equations*, and can be solved for the unknowns a_0 and a_1 . We also note that $\frac{\partial^2 S}{\partial a_0^2}$ and $\frac{\partial^2 S}{\partial a_1^2}$ are both positive at the points a_0 and a_1 . Thus these values provide a minimum of S .

Now, dividing the first of equations (2.25) by m yields

$$\boxed{a_0 + a_1 \bar{x} = \bar{y}} \quad (2.26)$$

where (\bar{x}, \bar{y}) is the centroid of the given data points. Hence the fitted straight line passes through the centroid of the data points.

Example 12

The table below gives the temperatures T (in $^{\circ}C$) and lengths l (in mm) of heated rod. If $l = a + bT$, find the best values for a and b that approximate the data of the table below.

T	20	30	40	50	60	70
l	800.3	800.4	800.6	800.7	800.9	801.0

Solution:

T	l	T^2	lT
20	800.3	400	16006
30	800.4	900	24012
40	800.6	1600	32024
50	800.7	2500	40035
60	800.9	3600	48054
70	801.0	4900	56070
270	4803.9	13900	216201

Using the normal equations, one obtains

$$6a + 270b = 4803.9$$

$$270a + 13900b = 216201$$

which lead to $a = 800$ and $b = 0.0146$.

$$\therefore l = 800 + 0.0146b.$$

2.4.2 Nonlinear curve fitting

A nonlinear function $y = \alpha x^c$ can be fitted to the given set of data points. Taking the logarithms of both sides yields

$$\boxed{Y = a_0 + a_1 X} \quad (2.27)$$

where $Y = \log y$, $a_0 = \log \alpha$, $a_1 = c$ and $X = \log x$. Thus the procedure outlined above can be followed to obtain the values of a_0 and a_1 , hence α and c can be calculated.

Now consider the parabola

$$\boxed{y = a_0 + a_1 x + a_2 x^2} \quad (2.28)$$

The least squares parabola approximating the set of points $(x_i, y_i), i = 0, 1, 2, \dots, n$ has the equation (2.28). The constants a_0, a_1 and a_2 can be determined by solving simultaneously the equations.

$$\begin{aligned} \sum y &= na_0 + a_1 \sum x + a_2 \sum x^2 \\ \sum xy &= a_0 \sum x + a_1 \sum x^2 + a_2 \sum x^3 \\ \sum x^2y &= a_0 \sum x^2 + a_1 \sum x^3 + a_2 \sum x^4 \end{aligned} \quad (2.29)$$

The equations (2.29) are called the *normal equations* for the least squares parabola (2.28). This parabola is said to be the regression curve of y on x , since an estimate of y is obtained for any given value of x . Similarly, we can have a regression equation of x on y .

Example 13

Fit a curve of the form $Y = \alpha e^{\beta x}$ to the data below

x	1	2	3	4
Y	7	11	17	27

Solution:

Taking the natural logarithms of both sides leads to

$$\ln y = \ln \alpha + \beta x.$$

This is of the form $y = a + bx$, where $y = \ln Y, a = \ln \alpha$ and $b = \beta$. Thus we fit a least squares line to the data

x	1	2	3	3
y	1.95	2.40	2.83	3.30

and one obtains $\alpha = 4.48$ and $\beta = 0.45$. Thus the curve becomes

$$Y = 4.48e^{0.45x}.$$

Exercise

Obtain a quadratic curve which fits the data in the table below, using the least squares method.

x	1.2	1.8	3.1	4.9	5.7	7.1	8.6	9.8
y	4.5	5.9	7.0	7.8	7.2	6.8	4.5	2.7

Chapter 3

Numerical Differentiation and Integration

3.1 Introduction

In chapter 2, we considered the problem of interpolation, that is, given a set of tabulated values $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ of x and y , can we find a polynomial $y_n(x)$ of the lowest degree such that $y(x)$ and $y_n(x)$ agree at the set of tabulated points? In this chapter, we are concerned with numerical differentiation and integration. This involves deriving formulae for derivatives and integrals from given set of tabulated values of x and y in the interval $[x_0, x_n]$.

3.2 Numerical Differentiation

A straightforward method for deriving numerical differentiation formulae is to differentiate the interpolation formulae obtained in the previous chapter. Differentiating the Newton's forward interpolating formula

$$y_n(x) = y_0 + \binom{p}{1} \Delta y_0 + \binom{p}{2} \Delta^2 y_0 + \binom{p}{3} \Delta^3 y_0 + \dots + \binom{p}{n} \Delta^n y_0 \quad (3.1)$$

where $\binom{p}{r} = \frac{p!}{(p-r)!r!}$, leads to the following results:

$$y'_n(x) = \frac{1}{h} \left[\Delta y_0 + \left(p - \frac{1}{2}\right) \Delta^2 y_0 + \frac{3p^2 - 6p + 2}{6} \Delta^3 y_0 + \frac{2p^3 - 9p^2 + 11p - 3}{12} \Delta^4 y_0 + \dots \right] \quad (3.2)$$

$$y''_n(x) = \frac{1}{h^2} \left[\Delta^2 y_0 + (p - 1) \Delta^3 y_0 + \frac{6p^2 - 18p + 11}{12} \Delta^4 y_0 + \dots \right] \quad (3.3)$$

$$y'''_n(x) = \frac{1}{h^3} \left[\Delta^3 y_0 + \frac{2p - 3}{2} \Delta^4 y_0 + \dots \right] \quad (3.4)$$

$$y_n^{(iv)}(x) = \frac{1}{h^4} [\Delta^4 y_0 + \dots] \quad (3.5)$$

For tabulated value x_0 , $p = 0$ and hence equations (3.2) - (3.4) simplify to

$$y'_n(x) = \frac{1}{h} \left[\Delta y_0 - \frac{1}{2} \Delta^2 y_0 + \frac{1}{3} \Delta^3 y_0 - \frac{1}{4} \Delta^4 y_0 + \dots \right] \quad (3.6)$$

$$y''_n(x) = \frac{1}{h^2} \left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 + \dots \right] \quad (3.7)$$

$$y'''_n(x) = \frac{1}{h^3} \left[\Delta^3 y_0 - \frac{3}{2} \Delta^4 y_0 + \dots \right] \quad (3.8)$$

Using only the first terms of the formulae above, one obtains the forward finite difference approximations to the following derivatives:

$$y'(x) = \frac{1}{h} \Delta y_0 = \frac{y(x+h) - y(x)}{h}$$

$$y''(x) = \frac{1}{h^2} \Delta^2 y_0 = \frac{y(x+2h) - 2y(x+h) + y(x)}{h^2}$$

$$y'''(x) = \frac{1}{h^3} \Delta^3 y_0 = \frac{y(x+3h) - 3y(x+2h) + 3y(x+h) - y(x)}{h^3}$$

and so on.

In a similar vein, we obtain other formulae using Newton's backward differ-

ence interpolating formula (2.8) as

$$\begin{aligned}
 y'_n(x) &= \frac{1}{h} \left[\nabla y_n + \left(p + \frac{1}{2} \right) \nabla^2 y_n + \frac{3p^2 + 6p + 2}{6} \nabla^3 y_n + \frac{2p^3 + 9p^2 + 11p + 3}{12} \nabla^4 y_n + \dots \right] \\
 y''_n(x) &= \frac{1}{h^2} \left[\nabla^2 y_n + (p + 1) \nabla^3 y_n + \frac{6p^2 + 18p + 11}{12} \nabla^4 y_n + \dots \right] \\
 y'''_n(x) &= \frac{1}{h^3} \left[\nabla^3 y_n + \frac{2p + 3}{2} \nabla^4 y_n + \dots \right] \\
 y_n^{(iv)}(x) &= \frac{1}{h^4} [\nabla^4 y_n + \dots]
 \end{aligned}
 \tag{3.9}$$

For tabulated value $x = x_n, p = 0$ and the formulae listed in (3.9) simplify to

$$y'_n(x) = \frac{1}{h} \left[\nabla y_n + \frac{1}{2} \nabla^2 y_0 + \frac{1}{3} \nabla^3 y_n + \frac{1}{4} \nabla^4 y_n + \dots \right] \tag{3.10}$$

$$y''_n(x) = \frac{1}{h^2} \left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12} \nabla^4 y_n + \dots \right] \tag{3.11}$$

$$y'''_n(x) = \frac{1}{h^3} \left[\nabla^3 y_n + \frac{3}{2} \nabla^4 y_n + \dots \right] \tag{3.12}$$

Similar finite difference approximations to the derivatives can be obtained from the first terms of the above formulae as in the case of forward differences.

Example 14

From the table of values below, obtain the value of (i) $y'(x)$ and (ii) $y''(x)$ at the point $x = 1.2$.

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

Solution:

We construct the difference table for the tabulated values as follows

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	0.1333				
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	
2.2	9.0250	1.6359	0.2964	0.0535	0.0096	0.0014	0.0001

From the difference table, we obtain

$$(i) y'(1.2) = \frac{1}{0.2} \left[0.7351 - \frac{1}{2}(0.1627) + \frac{1}{3}(0.0361) - \frac{1}{4}(0.008) + \frac{1}{5}(0.0014) \right] \\ \approx 3.3203$$

$$(ii) y''(1.2) = \frac{1}{(0.2)^2} \left[0.1627 - 0.0361 + \frac{11}{12}(0.008) - \frac{10}{12}(0.0014) \right] \approx 3.3192.$$

3.3 Numerical Integration

Numerical integration refers to the evaluation of the integral

$$I = \int_a^b y(x) dx \quad (3.13)$$

where $y(x)$ is a function given analytically by a formula or empirically by a table of values. Geometrically, the integral is the area under the graph of $y(x)$ between a and b . To determine this area, we divide the interval $[a, b]$ into n subintervals such that

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b$$

where $x_n = x_0 + nh$. Thus the integral becomes

$$I = \int_{x_0}^{x_n} y(x) dx.$$

Approximating $y(x)$ by Newton's forward difference interpolating formula leads to the integral

$$I = \int_{x_0}^{x_n} \left(y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \dots \right) dx \quad (3.14)$$

Since $x = x_0 + ph$, $dx = hdp$ and so the integral (3.14) becomes

$$I = h \int_0^n \left(y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \dots \right) dp \quad (3.15)$$

which on simplification yields

$$\int_{x_0}^{x_n} y(x)dx = nh \left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \dots \right] \quad (3.16)$$

Equation (3.16) is a general formula from which one can obtain different integration formulae by putting $n = 1, 2, 3, \dots$.

We derive from this general formula a few important numerical integration formulae such as the trapezoidal and Simpson's rules.

3.3.1 The Trapezoidal Rule

Putting $n = 1$ into (3.16), all differences higher than the first become zero and one obtains

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

Similarly, we deduce for the remaining intervals $[x_1, x_2], \dots, [x_{n-1}, x_n]$ as

$$\int_{x_1}^{x_2} y(x)dx = \frac{h}{2}[y_1 + y_2]$$

⋮

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

Combining these integrals, we obtain the formula

$$\boxed{\int_{x_0}^{x_n} y(x) dx = \frac{h}{2} [y_0 + 2y_1 + 2y_2 + 2y_3 + \cdots + y_n]} \quad (3.17)$$

which is normally referred to as the *trapezoidal rule*. The geometrical interpretation of this rule is that the curve $y = f(x)$ is replaced by n straight lines joining the points (x_0, y_0) and (x_1, y_1) , (x_1, y_1) and (x_2, y_2) , \cdots , (x_{n-1}, y_{n-1}) and (x_n, y_n) . The area bounded by the curve $y = f(x)$, the ordinates $x = x_0$ and $x = x_n$ and the x -axis is then approximately equivalent to the sum of the areas of the n trapeziums obtained [see fig.], hence the name of the formula.

3.3.2 Error bounds and estimate for the Trapezoidal Rule

The error of the trapezoidal formula can be estimated as follows: Let $y = f(x)$ be continuous and many times differentiable in $[x_0, x_n]$. Thus expanding $f(x)$ in Taylor series about $x = x_0$, we get

$$\begin{aligned} \int_{x_0}^{x_n} f(x) dx &= \int_{x_0}^{x_n} \left[y_0 + (x - x_0)y'_0 + \frac{(x - x_0)^2}{2!}y''_0 + \cdots \right] dx \\ &= hy_0 + \frac{h^2}{2}y'_0 + \frac{h^3}{6}y''_0 + \cdots \end{aligned} \quad (3.18)$$

In a similar vein,

$$\begin{aligned} \frac{h}{2}[y_0 + y_1] &= \frac{h}{2} \left[y_0 + y_0 + hy'_0 + \frac{h^2}{2}y''_0 + \frac{h^3}{6}y'''_0 + \cdots \right] \\ &= hy_0 + \frac{h^2}{2}y'_0 + \frac{h^3}{4}y''_0 + \cdots \end{aligned} \quad (3.19)$$

From (3.18) and (3.19) we obtain

$$\boxed{\int_{x_0}^{x_n} f(x) dx - \frac{h}{2}[y_0 + y_1] \approx -\frac{h^3}{12}y''_0 + \cdots} \quad (3.20)$$

which is the error in the interval $[x_0, x_1]$. Continuing in a similar way, we obtain the errors in the remaining subintervals $[x_1, x_2]$, $[x_2, x_3]$, \cdots , $[x_{n-1}, x_n]$.

Summing all these, one obtains the error ϵ as

$$\epsilon \approx -\frac{h^3}{12}[y_0'' + y_1'' + y_2'' + \cdots + y_{n-1}''] \quad (3.21)$$

Taking $y''(\bar{x})$ as the largest value of the n quantities on the right hand side of (3.21), we get

$$\epsilon \approx -\frac{h^3}{12}ny''(\bar{x}) \approx -\frac{(b-a)}{12}h^2y''(\bar{x}) \quad (3.22)$$

where $nh = b - a$.

Error bounds can now be obtained by taking the largest value for $y''(\bar{x})$, say M_U and the smallest value M_L , in the interval of integration, hence

$$KM_L \leq \epsilon \leq KM_U,$$

where $K = -\frac{b-a}{12}h^2$.

3.3.3 Simpson's Rule

To obtain *Simpson's rule*, otherwise called *Simpson's $\frac{1}{3}$ -rule*, we need to divide the interval of integration $a \leq x \leq b$ into an **even** number of subintervals $n = 2m$.

Thus, Simpson's $\frac{1}{3}$ -rule can easily be obtained from (3.16) by substituting $n = 2$.

This leads to the relation

$$\int_{x_0}^{x_2} y(x)dx = 2h \left[y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0 \right] = \frac{h}{3}[y_0 + 4y_1 + y_2] \quad (3.23)$$

Similarly, for the remaining intervals $[x_2, x_4], [x_4, x_6] \cdots, [x_{n-2}, x_n]$, one obtains

$$\begin{aligned} \int_{x_2}^{x_4} y(x)dx &= \frac{h}{3}[y_2 + 4y_3 + y_4] \\ \int_{x_4}^{x_6} y(x)dx &= \frac{h}{3}[y_4 + 4y_5 + y_6] \\ &\vdots \\ \int_{x_{n-2}}^{x_n} y(x)dx &= \frac{h}{3}[y_{n-2} + 4y_{n-1} + y_n]. \end{aligned}$$

Summing the above integrals, we obtain the *composite Simpson's $\frac{1}{3}$ -rule* as

$$\int_{x_0}^{x_n} y(x)dx = \frac{h}{3} [y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \cdots + 2y_{n-2} + 4y_{n-1} + y_n]$$
(3.24)

Simpson's $\frac{1}{3}$ -rule has the error term

$$\epsilon \approx -\frac{(b-a)}{180}h^4 f^{(4)}(\bar{x})$$

and it is highly accurate for most problems.

3.3.4 Simpson's $\frac{3}{8}$ -Rule

The scheme is obtained from (3.16) by substituting $n = 3$, thus yielding

$$\begin{aligned} \int_{x_0}^{x_3} y(x)dx &= 3h \left[y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0 \right] \\ &= \frac{3h}{8} [y_0 + 3y_1 + 3y_2 + y_3] \end{aligned}$$
(3.25)

Computing the integrals for the remaining subintervals $[x_3, x_6], [x_6, x_9], \cdots, [x_{n-3}, x_n]$,

the composite Simpson's $\frac{3}{8}$ -rule as

$$\int_{x_0}^{x_n} y(x)dx = \frac{3h}{8} [y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \cdots + 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n]$$
(3.26)

Simpson's $\frac{3}{8}$ -rule has the error term

$$\epsilon \approx -\frac{3}{80}h^5 f^{(4)}(\bar{x})$$

and it is much less accurate than the Simpson's $\frac{1}{3}$ -rule, hence it is rarely used for computations.

Example 15

Evaluate $I = \int_0^1 \frac{dx}{1+x^2}$, correct to 4 places of decimals.

Using the Trapezoidal, Simpson's $\frac{1}{3}$ - and $\frac{3}{8}$ -rules for $h = 0.5, 0.25$ and 0.125 , we

have the following results:

(a) $h = 0.5$. The values are tabulated below

x	0	0.5	1.0
y	1.00000	0.80000	0.50000

(i) Trapezoidal rule yields

$$I = \frac{0.5}{2}(1.00000 + 2 \times 0.80000 + 0.50000) = 0.77500$$

(ii) Simpson's $\frac{1}{3}$ -rule yields

$$I = \frac{0.5}{3}(1.00000 + 4 \times 0.80000 + 0.50000) = 0.78333$$

(b) $h = 0.25$. The values are tabulated thus

x	0	0.25	0.50	0.75	1.00
y	1.00000	0.94118	0.80000	0.64000	0.50000

(i) Trapezoidal rule yields

$$I = \frac{0.25}{2}[1.00000 + 2(0.94118 + 0.80000 + 0.64000) + 0.50000] = 0.78280$$

(ii) Simpson's $\frac{1}{3}$ -rule gives

$$I = \frac{0.25}{3}[1.00000 + 4(0.94118 + 0.64000) + 2(0.80000) + 0.50000] = 0.78539$$

(c) $h = 0.125$. The tabulated data become

x	0	0.125	0.250	0.375	0.500	0.625	0.750	0.875	1.000
y	1.00000	0.98452	0.94118	0.87671	0.80000	0.71910	0.64000	0.56637	0.50000

(i) Using Trapezoidal rule, one obtains

$$I = \frac{0.125}{2}[1.500 + 2(0.98452 + 0.94118 + 0.87671 + 0.80000 + 0.71910 + 0.64000 + 0.56637)] = 0.78474$$

(ii) Simpson's $\frac{1}{3}$ -rule yields

$$I = \frac{0.125}{3}[1.50000 + 4(0.98452 + 0.87671 + 0.71910 + 0.56637) + 2(0.94118 + 0.80000 + 0.64000)] = 0.78538$$

Simpson's $\frac{3}{8}$ -rule can now be applied to obtain

$$(iii) I = \frac{0.375}{8}[1.50000 + 3(0.98452 + 0.80000 + 0.56637) + 3(0.94118 + 0.71910) + 2(0.87671 + 0.64000)] = 0.77657.$$

Note that the exact solution correct to 5 places of decimals is $I \approx 0.78540$.

Example 16

Evaluate the integral $I = \int_0^1 e^{-x^2} dx$, using

- (i) Trapezoidal rule with $n = 5$
- (ii) Trapezoidal rule with $n = 10$
- (iii) Simpson's $\frac{1}{3}$ -rule with $n = 10$
- (iv) Simpson's $\frac{3}{8}$ -rule with $n = 10$.

Solution:

n	x_n	x_n^2	$f(x_n) = e^{-x_n^2}$
0	0	0	1.000000
1	0.2	0.04	0.960789
2	0.4	0.16	0.852144
3	0.6	0.36	0.697676
4	0.8	0.64	0.527292
5	1.0	1.00	0.367879
Σ			1.367879 3.037901

- (i) Note that $h = 0.2$, thus

$$I = \frac{0.2}{2} (1.367879 + 2 \times 3.037901) = 0.744368.$$

n	x_n	x_n^2	$f(x_n) = e^{-x_n^2}$
0	0	0	1.000000
1	0.1	0.01	0.99050
2	0.2	0.04	0.960789
3	0.3	0.09	0.913931
4	0.4	0.16	0.852144
5	0.5	0.25	0.778801
6	0.6	0.36	0.697676
7	0.7	0.49	0.612626
8	0.8	0.64	0.527292
9	0.9	0.81	0.444858
10	1.0	1.00	0.367879
Σ			1.367879 6.778167

(ii) Here, $h = 0.1$, thus

$$I = \frac{0.1}{2} (1.367879 + 2 \times 6.778167) = 0.746211.$$

(iii) For Simpson's $\frac{1}{3}$ -rule,

$$I = \frac{0.1}{3} (1.367879 + 4 \times 3.740266 + 2 \times 3.037901) = 0.746825.$$

(iv) Simpson's $\frac{3}{8}$ -rule produces

$$I = \frac{0.3}{8} (1.367879 + 3 \times 2.45482 + 3 \times 2.266882 + 2 \times 2.056465) = 0.736722.$$