CHAPTER I

CHAPTER - I

INTRODUCTION AND BASIC CONCEPTS

1.1 INTRODUCTION

Numerical integration is one of the most important and basic topic in numerical analysis. It deals with the study of how the numeric value of an integral can be found. The methods of numerical integration were familiar long before to Archimedes, who tried to calculate the area of a circle. The nature of numerical integration is paradoxically both simple as well as difficult. The study of numerical integration requires, sometimes, a deep knowledge of various branches of pure and applied mathematics. There are so many integration formulae which are simple to use and have much practical value.

Why Numerical Integration Needed ?

There are so many reasons for the need of numerical integration. We discuss some of them here. Usually numerical integration is used when analytic techniques fail. Even, if analytic techniques do work, these may not be sometimes useful, for example, very often the process of integration leads to new transcendental functions like $\int dx/x$ which gives the logarithmic function. Also indefinite integration of a function cannot be expressed in finite terms containing algebraic, logarithmic, or exponential functions. Another important reason is that in many situations, we are confronted with the problem of integrating experimental data, in which case the theoretical devices may be wholly inapplicable.

However, it should be noted that the numerical integration is only complementary analysis to analytic techniques and not a substitute for it. Numerical integration gives the best results if we select the proper formula and corresponding error bounds are taken into the consideration.

Since the computers are now available, these formulae can be easily worked out with greater accuracy and high speed. Some of the integration methods are discussed in this dissertation and computer programs in 'C ' for some of these methods are given.

1.2 THE METHOD OF APPROXIMATE INTEGRATION

Many methods of numerical integration have been devised since the sixteenth century. One of them is of prime importance which is the method of approximate integration. The main concept involved here is as follows:

Suppose we want to find a definite integral,

$$\int_a^b f(x)dx \qquad \ldots(1.1)$$

where, f(x) is a function of x. Then we find a function, say g(x), that is both a suitable approximation of f(x) and also simple to integrate formally. Thus, we can find the value of (1.1) by estimating,

$$\int_a^b g(x)dx \qquad \ldots(1.2)$$

Now, our goal is to obtain such function g(x). For this purpose we consider the interpolating polynomials $P_n(x)$ because several times these produce adequate approximations and also these are simple to integrate. Due to these characteristics the great emphasis is given to polynomials throughout large portion of numerical mathematics. The following figure (FIG. 1.1) illustrates the approximation of f(x) by the polynomial $P_4(x)$.

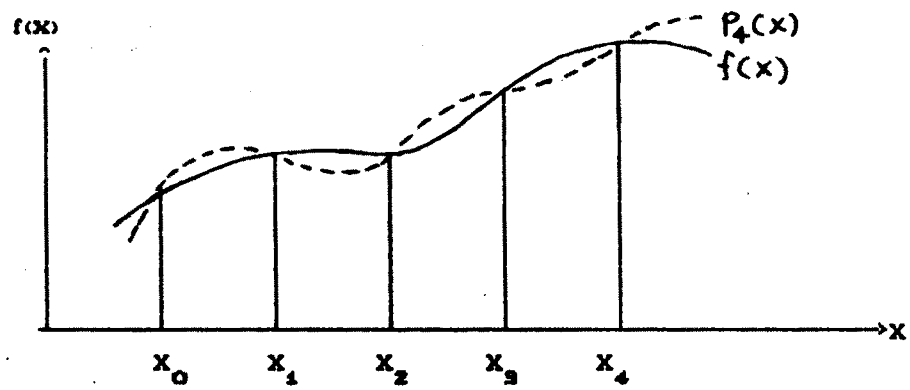

FIG 1.1: A Polynomial Approximation of f(x).

Here, the fourth degree polynomial $P_4(x)$ interpolates a function $f(x)$ at five points, namely X_0, X_1, X_2, X_3, X_4. The true value of the definite integral,

$$\int_{x_0}^{x_4} f(x)dx$$

is given by the area under the solid curve $f(x)$, whereas the approximated value,

$$\int_{x_0}^{x_4} p_4(x)dx$$

is given by the area under the dotted curve. The difference between these two values may be small, even when $P_4(x)$ is not a particularly good approximation, if the difference between $P_4(x)$ and $f(x)$ differs in sign on various segments of the interval of integration. In this situation, positive errors in one segment tend to cancel negative errors in others.Hence many times integration is termed as a "smoothing process."

1.3 THE CONCEPT OF THE DIVIDED DIFFERENCES

Consider a function $f(x)$ whose $(n+1)$ values are given at the given points lying within the interval (a,b). These points may be denoted by $x_0, x_1, \ldots, x_n$ and the values of function corresponding to these points by $f(x_0), f(x_1), \ldots, f(x_n)$. Let us denote the value of the function $f(x)$ at the point x by $[x]$. Thus, we get

$[x_0] = f(x_0)$, $[x_1] = f(x_1), \ldots, [x_n] = f(x_n)$.

Further by $[x_0 x_1]$ we denote the division of the differences, $[x_0] - [x_1]$ by $x_0 - x_1$.

$$\text{i.e. } [x_0 x_1] = \frac{[x_0]-[x_1]}{x_0 - x_1} = \frac{f(x_0) - f(x_1)}{x_0 - x_1}$$

Here $[x_0 x_1]$ is called <u>first divided difference</u>. Other such first divided differences are given as follows:

$$[x_1 x_2] = \frac{[x_1]-[x_2]}{x_1 - x_2}, \quad [x_2 x_3] = \frac{[x_2]-[x_3]}{x_2 - x_3}, \ldots$$

$$\ldots \quad [x_{n-1} x_n] = \frac{[x_{n-1}]-[x_n]}{x_{n-1} - x_n}.$$

Similarly $[x_0 x_1 x_2]$, $[x_1 x_2 x_3], \ldots, [x_{n-2} x_{n-1} x_n]$ denote second divided differences and are defined as

$$[x_0 x_1 x_2] = \frac{[x_0 x_1]-[x_1 x_2]}{x_0 - x_2}, \quad [x_1 x_2 x_3] = \frac{[x_1 x_2]-[x_2 x_3]}{x_1 - x_3}, \ldots$$

and so on. We write above expression in terms of $x_0, x_1, \ldots, x_n$ and the values $f(x_0), f(x_1), \ldots, f(x_n)$ of the function using first divided differences.

Thus,

$$[x_0x_1x_2] = \frac{[x_0x_1]-[x_1x_2]}{x_0 - x_2} = \frac{\dfrac{f(x_0) - f(x_1)}{x_0 - x_1} - \dfrac{f(x_1) - f(x_2)}{x_1 - x_2}}{x_0 - x_2}$$

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

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

In this way we obtain third divided differences, fourth divided differences and so on. In general, we can write n-th divided differences $[x_0x_1x_2...x_n]$ as

$$[x_0x_1...x_n] = \frac{f(x_0)}{(x_0-x_1)(x_0-x_2)...(x_0-x_n)} + \frac{f(x_1)}{(x_1-x_0)(x_1-x_2)...(x_1-x_n)} + \; . \; . \; . \; + \frac{f(x_n)}{(x_n-x_0)(x_n-x_1)...(x_n-x_{n-1})}$$

or $$[x_0x_1...x_n] = \frac{[x_0x_1...x_{n-1}] - [x_1...x_n]}{x_0 - x_n}$$

1.4 FORWARD DIFFERENCES

Suppose values of f(x) at equidistant points, x_0, $x_1 = x_0+h$, $x_2 = x_0+2h$, ... , $x_n = x_0+nh$ are given. Then, the first order forward differences denoted by $\Delta f(x_0)$, $\Delta f(x_1)$, ... , $\Delta f(x_{n-1})$ are defined as

$$\Delta f(x_0) = f(x_1)-f(x_0), \quad \Delta f(x_1) = f(x_2)-f(x_1), \quad \ldots ,$$
$$\Delta f(x_{n-1}) = f(x_n) - f(x_{n-1}).$$

Similarly, the second order forward difference for x_0 is denoted by $\Delta^2 f(x_0)$ and is defined as

$$\Delta^2 f(x_0) = \Delta f(x_0+h)-\Delta f(x_0) = f(x_0+2h) - 2f(x_0+h) + f(x_0).$$

In general, the $(r+1)^{th}$ order forward difference for x_0 is denoted by $\Delta^{r+1} f(x_0)$ and is defined as

$$\Delta^{r+1} f(x_0) = \Delta^r f(x_1) - \Delta^r f(x_0).$$

If (n+1) values of f(x) are given then the n^{th} order forward difference is constant.

1.5 TRUNCATION AND ROUNDING ERRORS

Generally, the process of solving physical problems can be roughly divided into three phases. In the first phase, the construction of mathematical model for the given physical problem is done . In many cases we can not solve this mathematical model analytically and hence we require a numerical solution. Construction of an appropriate numerical model is done in the second phase. And, the actual implementation and solution of the numerical model is done in the third phase.

In the second phase, if the mathematical model is identical to the numerical model,that is, we can solve the mathematical model in a finite number of arithmetic operations then there is no truncation error. However, in most cases numerical model is an approximation to the mathematical model and can't be solved in a finite number of steps. Here error arises, called the truncation error. This error, of course, depends on the mathematical model.

In the third phase, there are actual numerical computations. Here error occurs due to the finite precision with which the calculations can be carried out. Such errors are called the roundoff errors. Here the numbers are usually rounded off to a finite accuracy during the calculation, hence the name is given.

1.6 RELATED DEFINITIONS

Def.1 Continuous Functions:

Let $f(x)$ be a function which is defined for all real numbers x in an interval $[a,b]$. We say that $f(x)$ is continuous at a point x_o if for given any $\epsilon > 0$ (however small), we can find a positive number δ so that

$$|f(x) - f(x_o)| < \epsilon \qquad \text{whenever } |x-x_o| < \delta.$$

If $f(x)$ is continuous at all points in an interval $[a,b]$ then we say that $f(x)$ is continuous in $[a,b]$. The class of all functions which are continuous in $[a,b]$ is denoted by $C[a,b]$. Similarly, the class of all functions which are continuous in $[a,b]$ and whose first k^{th} derivatives are also continuous in $[a,b]$ is denoted by $C^k[a,b]$.

If $f(x)$ is continuous at all points in an interval $[a,b]$, except perhaps at a finite number of points, then we say that $f(x)$ is piecewise continuous in $[a,b]$.

Def.2 The Function $(x-t)_+^k$:

Let x and t be two real numbers and k be a non-negative integer. We define

$$(x-t)_+^k = \begin{cases} (x-t)^k & \text{if } x \geq t \\ 0 & \text{if } x < t \end{cases}$$

This function involves two variables x and t

Def.3 Polynomials:

A function $P_n(x)$ defined by

$$P_n(x) = a_n x^n + a_{n-1}x^{n-1} + \ldots + a_1 x + a_0 , \qquad (a_n \neq 0)$$

is called a polynomial of degree n in x. The constants $a_0, a_1, \ldots, a_n$ are called the coefficients of $P_n(x)$. We always assume $a_n \neq 0$.

If for some value $x_1, P_n(x_1) = 0$ then x_1 is called a root or a zero of $P_n(x)$. If x_1 is a root of $P_n(x)$ then $(x-x_1)$ is a factor of $P_n(x)$ and we can write

$$P_n(x) = (x-x_1)\, Q_{n-1}(x)$$

where $Q_{n-1}(x)$ is a polynomial of degree n-1. Every polynomial of degree n has exactly n roots. The class of all polynomials of degree n in x is denoted by $p_n(x)$.

Def.4 Interpolating polynomials:

Suppose a function f(x) is defined on the real line and we are given any n distinct points $x_0, x_1, x_2, \ldots, x_n$. Then there exists a unique polynomial $P_n(x)$ of degree n which has the same value as f(x) at each of these points, that is, $P_n(x)$ satisfies

$$P_n(x_k) = f(x_k), \; k = 0,1,2,\ldots,n.$$

This unique polynomial $P_n(x)$ is said to interpolate to the function f(x) at the points $x_0, x_1, \ldots, x_n$.

Def.5 Inner product of two functions:

Let $w(x) \geq 0$ be a fixed weight function defined on $[a,b]$. Let $f(x)$ and $g(x)$ be two continuous functions defined on $[a,b]$. Then the integral

$$\int_a^b w(x)\, f(x)\, g(x)\, dx.$$

is known as the inner product of the functions $f(x)$ and $g(x)$ over the interval $[a,b]$ with respect to the weight $w(x)$. We denote the inner product by (f,g).

Def.6 Orthogonal polynomials:

Two polynomials $g_n(x)$ and $g_m(x)$ taken from a family of related polynomials $g_k(x)$ are said to be orthogonal with respect to a weight function $w(x)$ on the interval $[a,b]$ if their inner product

$$\langle g_n(x), g_m(x) \rangle = \begin{cases} 0 & n \neq m \\ c(n) \neq 0 & n = m \end{cases}$$

In general, c depends on n. If such relationship holds for all n, the family of polynomials $\{g_k(x)\}$ is said to constitute a set of orthogonal polynomials. Some common families of orthogonal functions are the sets $\{\sin kx\}$ and $\{\cos kx\}$.

Further by multiplying each $g_n(x)$ by an appropriate constant we can form a set of polynomials $\{g_k^*(x)\}$ which is said to be orthonormal, where

$$\langle g_n^*(x), g_m^*(x) \rangle = \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n. \end{cases}$$

The zeros of (real) orthogonal polynomials are real, simple and located in the interior of [a,b]. The proof of this statement is given by Stroud [10, pp 130].

Def.7 Riemann Sums and Definite Integrals:

Let a function f(x) be defined for all x in the finite interval [a,b]. Take (n+1) arbitrary points $\xi_{j,n}$, j=0,1,...,n, in this interval such that

$$a = \xi_{0,n} < \xi_{1,n} < \xi_{2,n} < \dots < \xi_{n-1,n} < \xi_{n,n} = b.$$

We take further a point $x_{j,n}$ in the interval $[\xi_{j-1,n}, \xi_{j,n}]$ for all j=1,2,...,n. Then we define the Riemann Sum for f(x) based on the points $\xi_{j,n}$, j = 0,1,2,...,n and $x_{j,n}$, j = 1,2,...,n as

$$S_n(f) = (\xi_{1,n} - \xi_{0,n})\, f(x_{1,n}) + (\xi_{2,n} - \xi_{1,n})\, f(x_{2,n}) + \dots$$

$$+ \dots + (\xi_{n,n} - \xi_{n-1,n})\, f(x_{n,n})$$

$$= \sum_{i=1}^{n} (\xi_{i,n} - \xi_{i-1,n})\, f(x_{i,n})$$

Further, let L_n denote the maximum length of the subintervals. If $\lim_{n\to\infty} S_n(f)$ exists and is independent of the choice of the points $\xi_{j,n}$, $x_{j,n}$ and assuming only that $\lim_{n\to\infty} L_n = 0$ then we define

$$\int_a^b f(x)dx = \lim_{n\to\infty} S_n(f)$$

Def.8 Degree of precision :

If a quadrature formula gives exact results when f(x) is an arbitrary polynomial of degree r or less, but fails to give exact results for at least one polynomial of degree (r+1), then the quadrature formula is said to possess a degree of precision equal to r.

1.7 LAGRANGE'S INTERPOLATION FORMULA

Given (x_i, y_i), $i = 0, \ldots, n$ where x_i may or may not be equally spaced, suppose we have to obtain an n^{th} degree polynomial $L_n(x)$ that passes through all the points (x_i, y_i). This polynomial is an approximation to the function f(x), which coincides with the polynomial at each (x_i, y_i).

Let the n-th degree polynomials $P_k(x)$, $k=0,1,\ldots,n$ be

$$P_k(x) = (x-x_o)(x-x_1)\ldots(x-x_{k-1})(x-x_{k+1})\ldots(x-x_n)$$
$$= \prod_{\substack{i=o \\ i\neq k}}^{n} (x-x_i)$$

Then the coefficient A_k in the equation,

$$L_n(x) = \sum_{k=o}^{n} A_k P_k(x) \qquad \ldots(1.3)$$

can be determined so that equation (1.3) is satisfied by each (x_i, y_i). For, if $x = x_k$ then equation (1.3) gives

$$L_n(x_k) = \sum_{k=o}^{n} A_k P_k(x_k)$$

Therefore, $y_k = A_k P_k(x_k)$ [since $P_k(x_i)=0$, if $i \neq k$]

Therefore, $A_k = \dfrac{y_k}{P_k(x_k)}$

Using these values in equations (1.3), we get

$$L_n(x) = \sum_{k=o}^{n} \frac{y_k P_k(x)}{P_k(x_k)}$$

This gives the required n^{th} degree polynomial. This equation is called the Lagrange's interpolation formula.

This formula can be put in the form

$$L_n(x) = \sum_{k=o}^{n} \frac{y_k P\ (x)}{(x-x_k)P'(x_k)} \quad ,$$

where $P(x) = \prod_{i=o}^{n} (x-x_i) = (x-x_k)P_k(x),$

$$P'(x) = (x-x_k)P_k'(x)+P_k(x)$$

or $$L_n(x) = \sum_{i=o}^{n} f(x_i) \prod_{\substack{j=c \\ j\neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)} \quad .$$

1.8 SPLINE

For the interpolation of (n+1) data points, usually we use n-th order polynomial. But in many cases these higher order polynomials tend to swing through wild oscillations in a very small interval. Therefore, another approach is to apply lower order polynomials to subsets of data points. Such connecting polynomials are called SPLINES. Splines provide superior approximations to the functions. The formal definition of spline is as follows:

Let the interval [a, b] be divided into n subintervals,

$$a=x_0 < x_1 < \dots < x_{n-1} < x_n=b$$

not necessarily of equal length. By a spline S(x) of degree m we shall mean a function defined on [a,b] which

(a) Coincides with a polynomial of class p_m on each subinterval, $\Delta_i = [x_{i-1}, x_i]$, $i = 1,2,\dots,n$.

(b) is of class $C^{m-1}[a,b]$.

A spline of degree three is called a cubic spline. A spline S(x) is said to interpolate to the data points $(x_0,y_0),\dots,(x_n,y_n)$ if

$$S(x_i) = y_i, \quad i = 0,1,2,\dots n.$$

A cubic spline is called periodic { of period (b - a) }, if

$$S(a^+) = S(b^-), \quad S'(a^+) = S'(b^-), \quad S''(a^+) = S''(b^-).$$

A cubic spline with end conditions, $S''(a) = S''(b) = 0$, is called the natural spline.

1.9 RELATED THEOREMS

We shall use the following theorems for the purpose of further discussion.

Thm 1: Integral mean - value theorem .

If two functions, $f(x)$ and $g(x)$, are continuous for $a \le x \le b$ and $g(x)$ is of constant sign for $a < x < b$, then

$$\int_a^b f(x)\, g(x)\, dx = f(\xi)\int_a^b g(x)\, dx,$$

where $a < \xi < b$.

Thm 2: The Weierstrass Approximation Theorem

Let $f(x)$ be continuous function on a finite interval $[a,b]$. Given any $\varepsilon > 0$, there exists an integer $N = N(\varepsilon)$ and a polynomial $P_N(x)$ of this degree so that

$$| f(x) - P_N(x) | < \varepsilon$$

for all x in $[a,b]$.