CHAPTER II

CHAPTER - II.

NEWTON - COTES INTEGRATION FORMULAE

2.1 INTRODUCTION

There are so many formulae for numerical integration. This is because, there are so many different ways for selecting the base-point spacing, the degree of the polynomial which inter polates the given function or the given data, and the location of base points with respect to the interval of integration. These formulae are sometimes called quadrature or mechanical quadrature. The integration methods, which are commonly used, are classified mainly into two groups :

(1) The Newton-Cotes formulae.

(2) Gaussian quadrature formulae.

In case of the Newton-Cotes formulae, the functional values are taken at equal intervals. And, in case of Gaussian quadrature formulae, functional values are not necessarily equally spaced; but usually are determined by certain properties of orthogonal polynomials. We shall discuss Gaussian quadrature formulae in the chapter III; and here we only discuss the Newton-Cotes integration formulae.

2.2 NEWTON-COTES FORMULAE

Newton-Cotes integration formulae are usually classified into two groups : one group is referred as Newton-Cotes CLOSED integration formulae and the other is referred as Newton-Cotes OPEN integration formulae. In the case of the Newton-Cotes closed integration formulae, the information about f(x) at both limits of integration is required. That is, the end points of the interval or limit points of the integration are also base points. In the case of the Newton-Cotes open integration formulae the information about f(x) at the limit points of the integration is not required.

All these Newton-Cotes integration formulae can be generated by integrating one of the general interpolating polynomials $P_n(x)$, with proper base points and limits of the integration. We have supposed here that f(x) is known (or can be computed) only at the base points $x_0, x_1, \ldots, x_n$; equally spaced by stepsize, say h. Therefore, the logical choice to represent f(x) in the polynomial form is one of the finite difference (forward, backward or central) forms. Suppose the polynomial is represented in the form of the forward finite differences using Newton's forward difference formula,

$$f(x_0+\alpha h) = f(x_0) + \alpha \Delta f(x_0) + \frac{\alpha(\alpha-1)}{2!} \Delta^2 f(x_0) + \ldots$$

$$\ldots + \frac{\alpha(\alpha-1)\ldots(\alpha-n+1)}{n!} \Delta^n f(x_0) + R_n(x_0+\alpha h) \quad (2.1)$$

which can be written as

$$f(x_o+\alpha h) = P_n(x_o+\alpha h) + R_n(x_o+\alpha h),$$

where $\alpha = (x - x_o)/h$, $P_n(x_o+\alpha h)$ is the n-th degree interpolating polynomial and $R_n(x_o+\alpha h)$ is the remainder term , also known as error term. Further this error term $R_n(x_o+\alpha h)$ is given by

$$R_n(x_o+\alpha h) = h^{n+1}\alpha(\alpha-1)(\alpha-2)\ldots(\alpha-n) \frac{f^{(n+1)}(\xi)}{(n+1)\,!},$$

$$\xi \in (x,x_o,\ldots,x_n). \qquad \ldots(2.2)$$

or

$$R_n(x_o+\alpha h) = h^{n+1}\alpha(\alpha-1)(\alpha-2)\ldots(\alpha-n)\ f\,[x,x_n,x_{n-1},\ldots,x_o].$$

The formulae (2.1), (2.2) are used further in the derivation of Newton-Cotes closed as well as open integration formulae.

2.3 NEWTON-COTES CLOSED INTEGRATION FORMULAE

First, we consider very simple case of closed type integration in which the two base points $x_o = a$ and $x_1 = b$ are used. Using these two base points we can determine a first degree polynomial $P_1(x)$, that is, straight line approximation of f(x) as shown in the figure (FIG 2.1). Let us change the independent variable, x to α, by the substitutation,

$$x = x_o + \alpha h \quad \text{or} \quad \alpha = (x - x_o) / h. \qquad \ldots(2.3)$$

Now, for these two base points, equation (2.1) becomes

$$f(x) = f(x_0 + \alpha h)$$

$$= f(x_0) + \alpha \Delta f(x_0) + R_1(x_0 + \alpha h)$$

This can be written as

$$f(x) = P_1(x_0 + \alpha h) + R_1(x_0 + \alpha h),$$

where

$$P_1(x_0 + \alpha h) = f(x_0) + \alpha \Delta f(x_0) \qquad \ldots(2.4)$$

is a first degree polynomial in α. Also, using equation (2.2), the correspondig error term is given by

$$R_1(x_0 + \alpha h) = h^2 \alpha(\alpha - 1) \frac{f''(\xi)}{2!}, \qquad \text{where } \xi = (x_0, x_1)$$

$$\ldots(2.5)$$

Thus using polynomial approximation for f(x) we can write,

$$\int_a^b f(x)dx \doteq \int_{x_0}^{x_1} P_1(x)dx \qquad \text{(polynomial approximation)}$$

$$= h \int_0^1 P_1(x_0 + \alpha h)d\alpha \qquad \text{(by changing the variable x to } \alpha \text{ or by (2.3))}$$

$$= h \int_0^1 [f(x_0) + \alpha \Delta f(x_0)]\, d\alpha \qquad \text{(by 2.4)}$$

$$= h \left[f(x_0) + \frac{\Delta f(x_0)}{2} \right] \qquad \text{(by integrating)}$$

$$\int_a^b f(x)dx = h\left[f(x_0) + \frac{f(x_1) - f(x_0)}{2}\right] \quad \text{(def of forward difference)}$$

$$= \frac{h}{2}\left[f(x_0) + f(x_1)\right]$$

Therefore,

$$\int_a^b f(x)dx \doteq \frac{h}{2}\{f(x_0) + f(x_1)\} \qquad \text{...(2.6)}$$

Equation (2.6) is well-known trapezoidal rule.

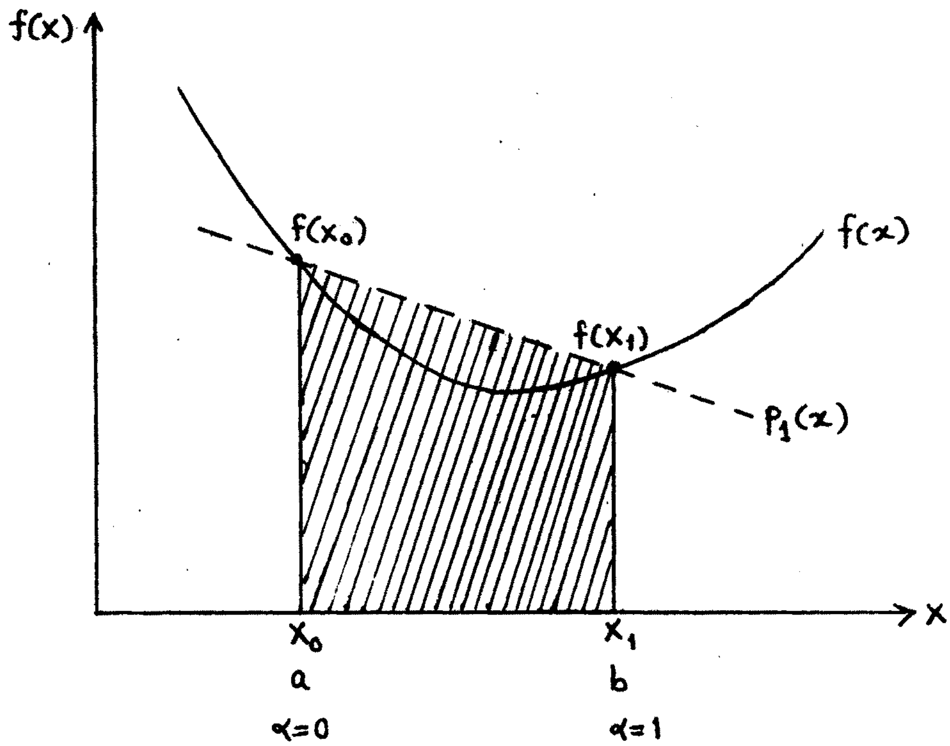

FIG.2.1: The Trapezoidal Rule.

From figure, FIG 2.1, we see that the required area is the area under a solid curve and the approximated area is the area under the dotted line and is shown by the shaded portion .This approximated area (shaded portion) is a trapezoid. Hence the name of this rule is trapezoidal rule.

The error involved in this case is obtained by the integral of the remainder term given in equation (2.5). Therefore, we get

$$\int_{x_0}^{x_1} R_1(x)dx = h \int_0^1 R_1(x_0+\alpha h)$$

$$= h \int_0^1 h^2\alpha(\alpha - 1) \frac{f''(\xi)}{2!} d\alpha, \quad \xi \in (x_0, x_1)$$

$$= h^3\int_0^1 \alpha (\alpha-1)\frac{f''(\xi)}{2!} d\alpha \qquad \ldots(2.7)$$

If f(x) is continuous function of x then $f''(\xi)$ is also continuous function of x. But $f''(\xi)$ is unknown function of x, therefore, we can't evaluate equation (2.7) further directly. Hence to solve the integration in equation (2.7) we take another approach. Here we see that α is simply a transformed value of x , therefore, $f''(\xi)$ is a continous function of the variable α . Also, the factor α $(\alpha-1)$ is negative for all α in the interval $(\emptyset,1)$. Using these two things we can apply the integral mean value theorem to solve this integration and we can write accordingly, equation (2.7), as

$$\int_{x_0}^{x_1} R_1(x)dx = h^3 \frac{f''(\bar{\xi})}{2!} \int_0^1 \alpha(\alpha-1)d\alpha$$

$$= \frac{h^3}{2!} f''(\bar{\xi}) \left[\frac{\alpha^3}{3} - \frac{\alpha^2}{2} \right]_0^1$$

$$= -\frac{h^3}{12} f''(\bar{\xi}), \qquad \xi, \bar{\xi} \in [x_0, x_1]$$

Therefore, the trapezoidal rule with error term is given by

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\bar{\xi}), \qquad \bar{\xi} \in [x_0, x_1] \qquad \ldots(2.8)$$

Here we observe that if the function f(x) is a linear function, then the trapezoidal rule gives exact approximation to the integral value of the function f(x) over the interval [a,b], because in that case $f''(\xi)$ vanishes.

Now, we consider the more general situation. Here, we consider the interval [a,b], and the (n+1) equally spaced base points

$$a=x_0 < x_1 < x_2 < \ldots < x_{n-1} < x_n$$

as shown in the figure ,(FIG 2.2). Here, the lower limit of integration, a , coincides with the first base point x_0 whereas the upper limit of integration, b, is arbitrary for the moment. Since there are (n+1) base points, the degree of the interpolating polynomial will be n. We denote this n^{th} degree interpolating polynomial by $P_n(x)$. Hence the approximation to the integral $\int_a^b f(x)dx$ is given by

$$\int_a^b f(x)\,dx \doteq \int_a^b P_n(x)\,dx$$

By substituting $x = x_0 + \alpha h$ and assuming $\bar{\alpha} = (b-x_0)/h$, we get

$$\int_a^b f(x)dx = h\int_0^{\bar{\alpha}} P_n(x_0 + \alpha h)d\alpha$$

$$= h\int_0^{\bar{\alpha}} \Big\{ f(x_0) + \alpha \Delta f(x_0) + \frac{\alpha(\alpha-1)}{2!} \Delta^2 f(x_0) +$$

$$\ldots + \frac{\alpha(\alpha-1)\ldots(\alpha-n+1)}{n!} \Delta^n f(x_0)\Big\}\, d\alpha, \quad \text{(by 2.1).}$$

Therefore,

$$\int_a^b f(x)dx \doteq h \Big[\alpha f(x_0) + \frac{\alpha^2}{2} \Delta f(x_0) + \left(\frac{\alpha^3}{6} - \frac{\alpha^2}{4}\right) \Delta^2 f(x_0)$$

$$+ \left(\frac{\alpha^4}{24} - \frac{\alpha^3}{6} + \frac{\alpha^2}{6}\right)\Delta^3 f(x_0)$$

$$+ \left(\frac{\alpha^5}{120} - \frac{\alpha^4}{16} + \frac{11\alpha^3}{72} - \frac{\alpha^2}{8}\right)\Delta^2 f(x_0) + \ldots\Big]_0^{\bar{\alpha}}$$

Therefore,

$$\int_a^b f(x)dx \doteq h \Big[\bar{\alpha} f(x_0) + \frac{\bar{\alpha}^2}{2} \Delta f(x_0) + \left(\frac{\bar{\alpha}^3}{6} - \frac{\bar{\alpha}^2}{4}\right) \Delta^2 f(x_0)$$

$$+\left(\frac{\bar{\alpha}^4}{24} - \frac{\bar{\alpha}^3}{6} + \frac{\bar{\alpha}^2}{6}\right) \Delta^3 f(x_0) + \ldots\ldots \Big]. \quad \ldots(2.9)$$

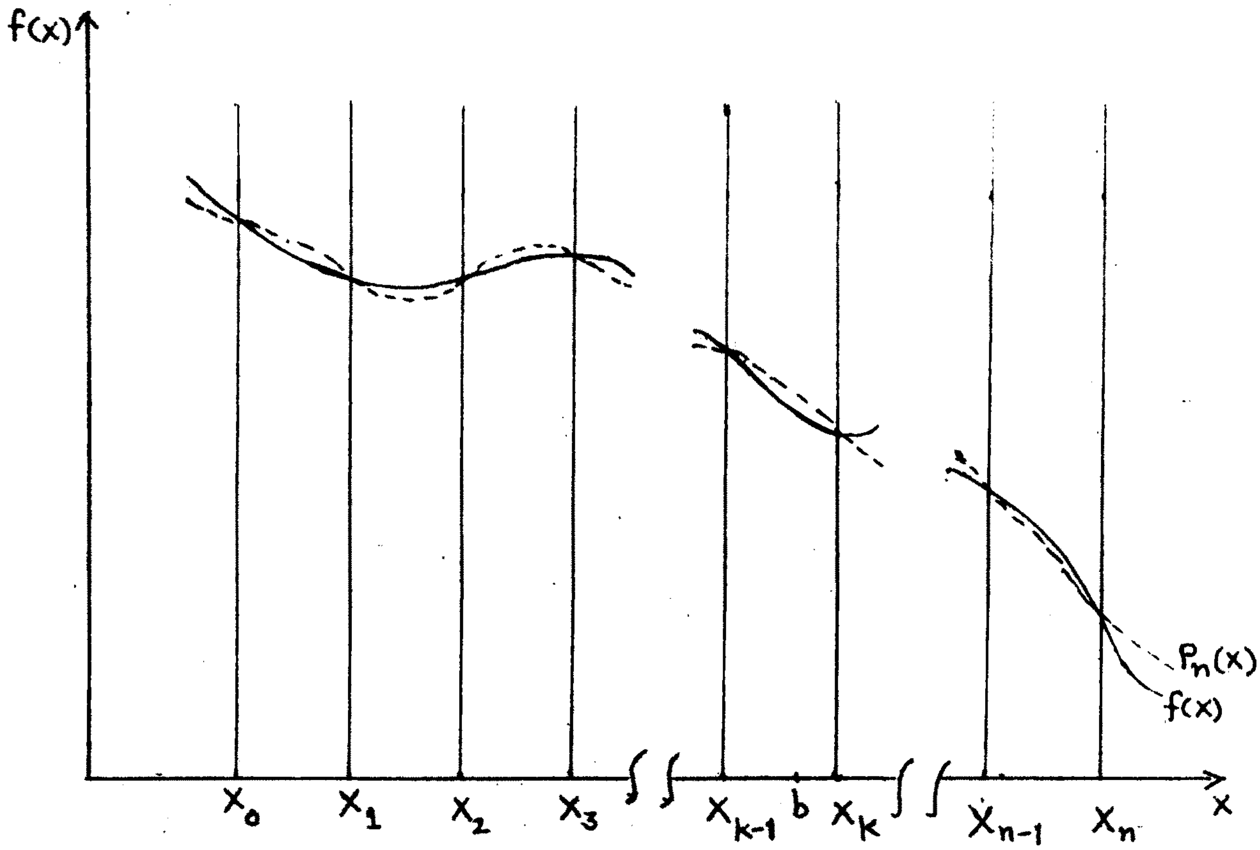

FIG 2.2: General Case For Closed Integration.

The error term, in this case, can be obtained by integrating the equation (2.2). Thus, error term is given by

$$h\int_{0}^{\bar{\alpha}} R_n(x_0+\alpha h)\,d\alpha = h^{n+2}\int_{0}^{\bar{\alpha}}\left[\alpha(\alpha-1)(\alpha-2)\ldots(\alpha-n)\frac{f^{(n+1)}(\xi)}{(\overline{n+1})!}\right]d\alpha, \quad \ldots(2.10)$$

The equations (2.9) and (2.10) represent a family of related integration formulae. If we choose the upper limit b so as to coincide with one of the base points, say x_m , then the integration is across m intervals, that is, between $a = x_0$ and $b = x_m$. Also, in such case $\bar{\alpha}$ assumes an integral value. Thus, if $\bar{\alpha} = 1$, the equations (2.9) and

(2.10) reduce to the trapezoidal rule given by equation (2.8). Hence letting $\bar{\alpha}$ = 2,3,4,...etc in equations (2.9) and (2.10), we can obtain similar formulae for integration across m = 2,3,4 or more intervals. Again the selection of n is still open. It seems the most natural to have the choice n = $\bar{\alpha}$ .This set of formulae are known as Newton-Cotes closed integration formulae.

As a particular case, let us choose $\bar{\alpha}$ = n = 2 . For this choice equation (2.9) can be written as

$$\int_{x_0}^{x_2} f(x)dx \doteq h\int_0^2 f(x_0+\alpha h)\,d\alpha$$

$$= h\left[2f(x_0) + 2\Delta f(x_0) + \frac{1}{3}\Delta^2 f(x_0) + 0\Delta^3 f(x_0) - \frac{1}{90}\Delta^4 f(x_0)+\dots\right] \quad \dots(2.11a)$$

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

(since $\Delta^4 f(x_0)$ = 0 for three values)

Therefore,

$$\int_{x_0}^{x_2} f(x)\,dx \doteq \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] \quad \dots(2.11b)$$

The equation (2.11b) is a famous Simpson's 1/3rd prule or Simpson's first rule. This rule is most frequently used than any other numerical integration formula. Famous numerical mathematician, Milton Abramowitz used to say - somewhat like - that 95% of all pratical work in numerical analysis boiled down to applications of Simpson's rule and linear interpolation.

The calculation of error term in this case is somewhat unexcepting to us in few places. Since the coefficient of $\Delta^3 f(x_0)$ in equation (2.11a) is zero, therefore, by putting n = 2 in the equation (2.1Ø) we can not obtain the required error term. Hence, we put n = 3 (but $\bar{\alpha}$ = 2) in the equation (2.1Ø) and obtain

$$h\int_0^2 R_3(x_0+\alpha h)\,d\alpha = h^5\int_0^2 \alpha(\alpha-1)(\alpha-2)(\alpha-3)\,\frac{f^{(4)}(\xi)}{4\,!}\,d\alpha.$$

$$\xi \in (x_0, x_2).$$

Further, the integration on the right hand side can not be evaluated directly by the application of the integral mean value theorem, as in case of trapezoidal rule. The reason is that the factor $\alpha(\alpha-1)(\alpha-2)(\alpha-3)$ does not have a constant sign over the interval of integration. But Steffensen [3,PP 73] has proved that,this error can be evaluated in the similar fashion. Therefore we can further write,

$$h\int_0^2 R_3(x_0+\alpha h)\,d\alpha = h^5\frac{f^{(4)}(\bar{\xi})}{4\,!}\int_0^2 \alpha(\alpha-1)(\alpha-2)(\alpha-3)\,d\alpha,$$

$$= -h^5 f^{(4)}(\xi)/9\emptyset, \qquad \xi, \bar{\xi} \in (x_0, x_2)$$

Here ξ and $\bar{\xi}$ are simply unknown values, therefore, instead of mentioning both ξ and $\bar{\xi}$, we only write ξ in our further discussion. Now, Simpson's $1/3^{rd}$ rule with the error term is then given by

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3} [f(x_0) + 4 f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi),$$

$$\xi \in (x_0, x_2) \qquad \text{...(2.12)}$$

The following figure, FIG 2.3, illustrates the Simpson's $1/3^{rd}$ rule. Here only three points x_0, x_1, x_2 are used to determine the polynomial. We would obviously expect the integration to be exact for f(x), a polynomial of degree two or less; but equation (2.12) shows that the integration is exact for the function f(x), which is a polynomial of degree three or less.

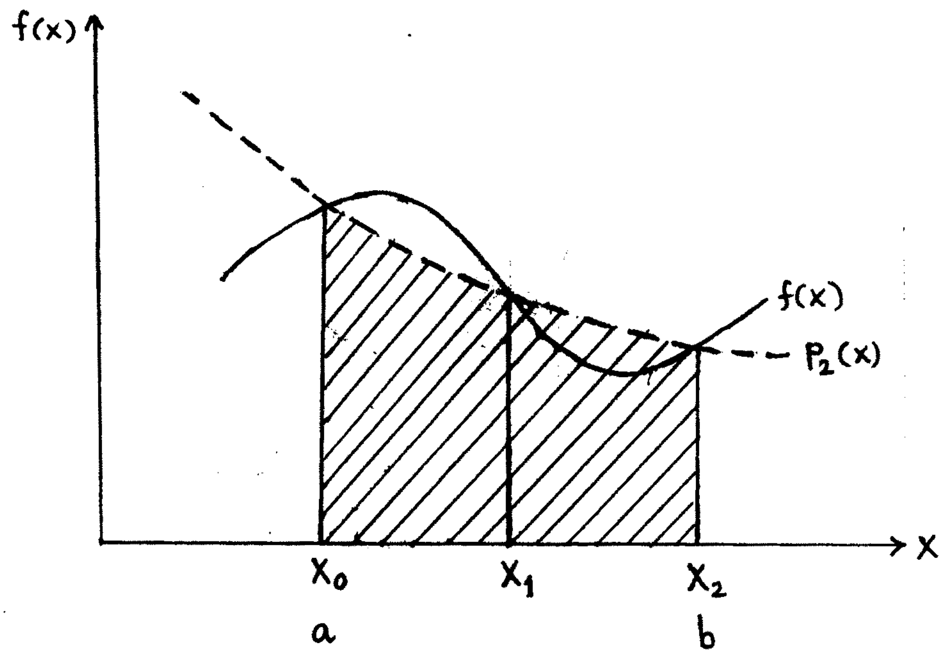

FIG 2.3: Simpson's First Rule.

Here we give the list of Newton-Cotes closed integration formulae corresponding to the values, $\bar{\alpha}$ = 1,2, 3,4,5, as follows:

$\bar{\alpha}$ = 1: Trapezoidal rule -

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi)$$

$\bar{\alpha}$ = 2 : Simpson's 1/3rd rule (or Simpson's first rule) -

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi)$$

$\bar{\alpha}$ = 3 : Simpson's 3/8th rule (or Simpson's second rule) -

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$
$$- \frac{3h^5}{80} f^{(4)}(\xi)$$

$\bar{\alpha}$ = 4 :

$$\int_{x_0}^{x_4} f(x)dx = \frac{2}{45} h [7f(x_0) +32f(x_1) + 12f(x_2) + 32f(x_3)$$
$$+ 7f(x_4)] - \frac{8h^7}{945} f^{(6)}(\xi)$$

$\bar{\alpha}$ = 5 :

$$\int_{x_0}^{x_5} f(x)dx = \frac{5h}{288} [19f(x_0)+75f(x_1)+50f(x_2)+50f(x_3)+75f(x_4)$$
$$+19f(x_5)] - \frac{275h^7}{12096} f^{(6)}(\xi).$$

From this list, we observe that [3,PP 74] when $\bar{\alpha}$ is even, that is when there are odd number of base points, the corresponding formulae are exact for f(x), a polynomial of degree $(\bar{\alpha} + 1)$ or less. While, if $\bar{\alpha}$ is odd, the formulae are exact for f(x), a polynomial of degree $\bar{\alpha}$ or less. Hence the odd-point formulae are more frequently preferred than the even-point formulae. Another thing, we observe here is, that not a single formula requires the calculation of the forward differences or the coefficients of the interpolating polynomial. These involve only the computation of a weighted sum of the base-point functional values. In other words, all formulae in this list can be represented in the form

$$\int_a^b f(x)dx = \sum_{i=0}^{n} w_i f(x_i)$$

where the w_i are referred as the weights assigned to the functional values, $f(x_i)$, $i = \emptyset,1,\ldots n$. Thus we can represent it in terms of Riemann Sums.

2.4 NEWTON COTES OPEN INTEGRATION FORMULAE

Now, we derive general Newton-Cotes integration formulae of open type. As previously said, though these formulae involve equally spaced base points, they do not require the values of the function at one or both of the integration limits. Suppose, we want to evaluate the integration of the function f(x) over the interval of integration [a,b]. Let $x_1, x_2, \ldots, x_{n-1}$ be (n-1) evenly spaced base points and h be the distance between any two consecutive base points. Let a, the lower limit of integration, coincides with $x_0 = x_1 - h$; whereas b, the upper limit of integration, be arbitrary for the moment, as shown in figure, FIG (2.4). Then the interpolating polynomial is of degree (n-2) and the approximation is given by

$$\int_a^b f(x)dx \doteq \int_a^b P_{n-2}(x)dx$$

$$\doteq \int_{x_o}^b P_{n-2}(x)dx$$

$$= h\int_o^{\bar{\alpha}} P_{n-2}(x_o + \alpha h)\, d\alpha \qquad \text{(by putting } x = x_o+\alpha h)$$

...(2.13)

where $\alpha = (x-x_o)/h$ and $\bar{\alpha} = (b-x_o)/h$

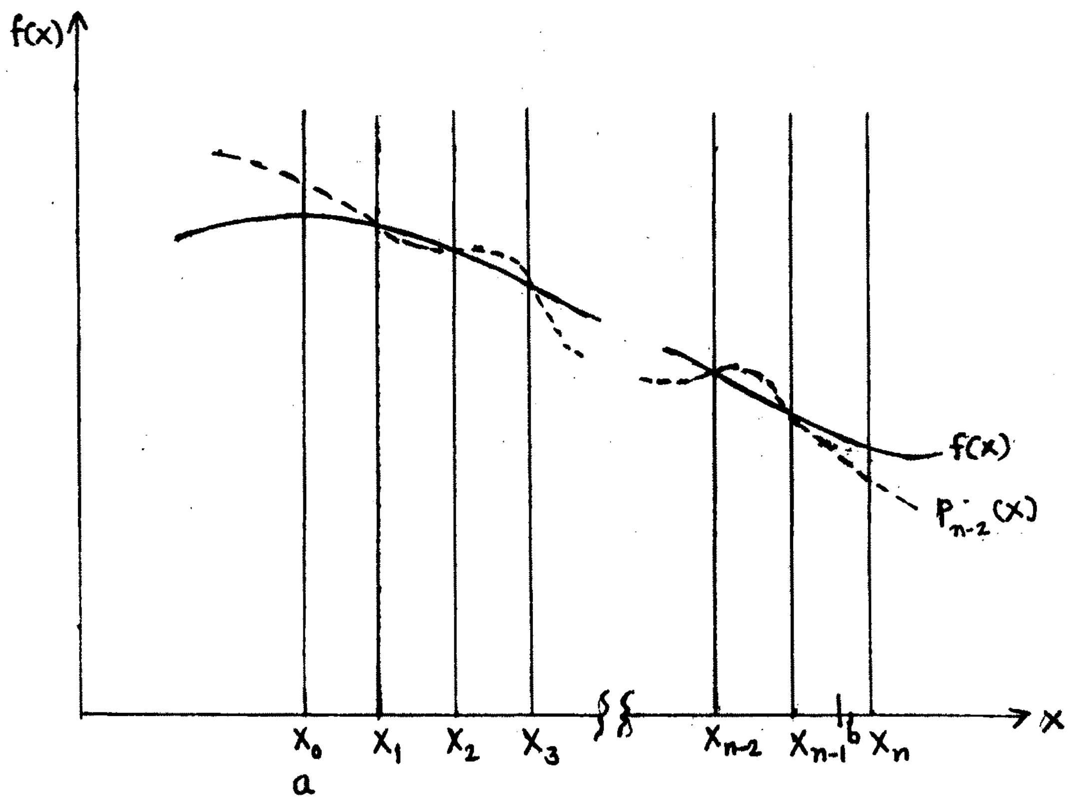

FIG 2.4: Newton-Cotes General Open Integration.

An obivious representation of $P_{n-2}(x)$ is obtained by the forward finite difference polynomial. Therefore, applying Newton's forward formula and considering forward differences of $f(x_1)$ instead of $f(x_0)$, we get

$$P_{n-2}(x_0 + \alpha h) = f(x_1) + (\alpha-1)\Delta f(x_1) + \frac{(\alpha-1)(\alpha-2)}{2\,!}\Delta^2 f(x_1)$$
$$+ \dots + \frac{(\alpha-1)(\alpha-2)\dots(\alpha-(n-2))}{(n-2)\,!}\Delta^{n-2} f(x_1) \qquad \dots(2.14)$$

Using equation (2.14), the equation (2.13) can be written as

$$\int_a^b f(x)dx \doteq h\int_0^{\alpha} \left[f(x_1) + (\alpha-1)\Delta f(x_1) + \dots + \frac{(\alpha-1)(\alpha-2)\dots(\alpha-n+2)}{(n-2)\,!}\Delta^{n-2} f(x_1)\right] d\alpha$$

$$\doteq h\left[\alpha f(x_1) + \left(\frac{\alpha^2}{2} - \alpha\right)\Delta f(x_1) + \left(\frac{\alpha^3}{6} - \frac{3\alpha^2}{4} + \alpha\right)\Delta^2 f(x_1) + \dots\right]_0^{\bar{\alpha}}$$

Therefore,

$$\int_a^b f(x)dx \doteq h\left[\bar{\alpha} f(x_1) + \left(\frac{\bar{\alpha}^2}{2} - \bar{\alpha}\right)\Delta f(x_1) + \left(\frac{\bar{\alpha}^3}{6} - \frac{3\bar{\alpha}^2}{4} + \bar{\alpha}\right)\Delta^2 f(x_1) + \dots\right] \qquad \dots(2.15)$$

The error term for this case is given by

$$h\int_0^{\bar{\alpha}} R_{n-2}(x_0+\alpha h)d\alpha = h^n\int_0^{\bar{\alpha}} \frac{\alpha(\alpha-1)(\alpha-2)\ldots(\alpha-n+1)}{(n-1)\,!} f^{(n-1)}(\xi)\, d\alpha,$$

$$\text{where } \xi = (x_0, b) \qquad \ldots(2.16)$$

Equations (2.15) and (2.16) describe a family of related Newton-Cotes open integration formulae. Taking different integral values for $\bar{\alpha}$ (=n), we get different Newton-Cotes open integration formulae. A list of few formulae is given below.

$$\bar{\alpha} = 2 : \int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3} f''(\xi)$$

$$\bar{\alpha} = 3 : \int_{x_0}^{x_3} f(x)dx = \frac{3h}{2}\left[f(x_1)+f(x_2) \right] + \frac{3h^3}{4} f''(\xi)$$

$\bar{\alpha} = 4$:

$$\int_{x_0}^{x_4} f(x)dx = \frac{4h}{3}\left[2f(x_1)-f(x_2)+2f(x_3) \right] + \frac{14h^5}{45} f^{(4)}(\xi)$$

$\bar{\alpha} = 5$:

$$\int_{x_0}^{x_5} f(x)dx = \frac{5h}{24}\left[11f(x_1)+f(x_2)+f(x_3)+11f(x_4)\right]+\frac{95h^5}{144} f^{(4)}(\xi)$$

$\bar{\alpha} = 6$:

$$\int_{x_0}^{x_6} f(x)dx = \frac{3h}{10}\left[11f(x_1)-14f(x_2)+26f(x_3)-14f(x_4)+11f(x_5)\right]$$

$$+ \frac{41h^7}{140} f^{(6)}(\xi).$$

As in the case of closed integration formulae, here also we observe that [3,pp 76] when there are odd number of base points, that is, when $\bar{\alpha}$ is even, the corresponding formulae are exact for f(x), a polynomial of degree $(\bar{\alpha}+1)$ or less. While if $\bar{\alpha}$ is odd then the corresponding formulae are exact for f(x), a polynomial of degree $\bar{\alpha}$ or less. For this reason, the odd point formulae are more frequently used than the even point formulae.

2.5 COMPOSITE INTEGRATION FORMULAE

Suppose we subdivide the interval of integration [a,b] into smaller ones and then apply the low order formula separately on each subinterval. Then, the resulting integration formula is called COMPOSITE INTEGRATION FORMULA. In this way, we apply a low order formula repeatedly instead of a single application of a high order formula. This technique became very popular because of the simplicity of the low order formula and also due to lack of computational difficulties associated with the high order formulae. Though we can extend any of the Newton-Cotes low order formulae to its composite form, we especially use closed formulae. The reason is that the base points at the ends of each subinterval, except x = a and x = b, are also base points for adjacent subintervals. Therefore, if we apply an m-point formula n times then we need n(m-1)+1 functional evaluations only instead of nm as one might be expected. Thus, there is a considerable saving especially when m is small.

As an example, we consider a very simple composite formula which is generated by repeated applications of the trapezoidal rule. Let the interval [a,b] be divided into n equal subintervals as shown in figure (for n = 7), FIG 2.5, such that $h = (b-a)/n$.

Then

$$x_i = x_o + ih \qquad (i = 1,\ldots,n)$$

Further,

$$\int_a^b f(x)dx = \int_{x_o}^{x_n} f(x)dx = \int_{x_o}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \ldots + \int_{x_{n-1}}^{x_n} f(x)dx$$

$$= \frac{h}{2}\Big\{[f(x_o)+f(x_1)] + [f(x_1)+f(x_2)] + \ldots +$$

$$+ [f(x_{n-1})+f(x_n)]\Big\} - \frac{h^3}{12}\sum_{i=1}^{n} f''(\xi_i)$$

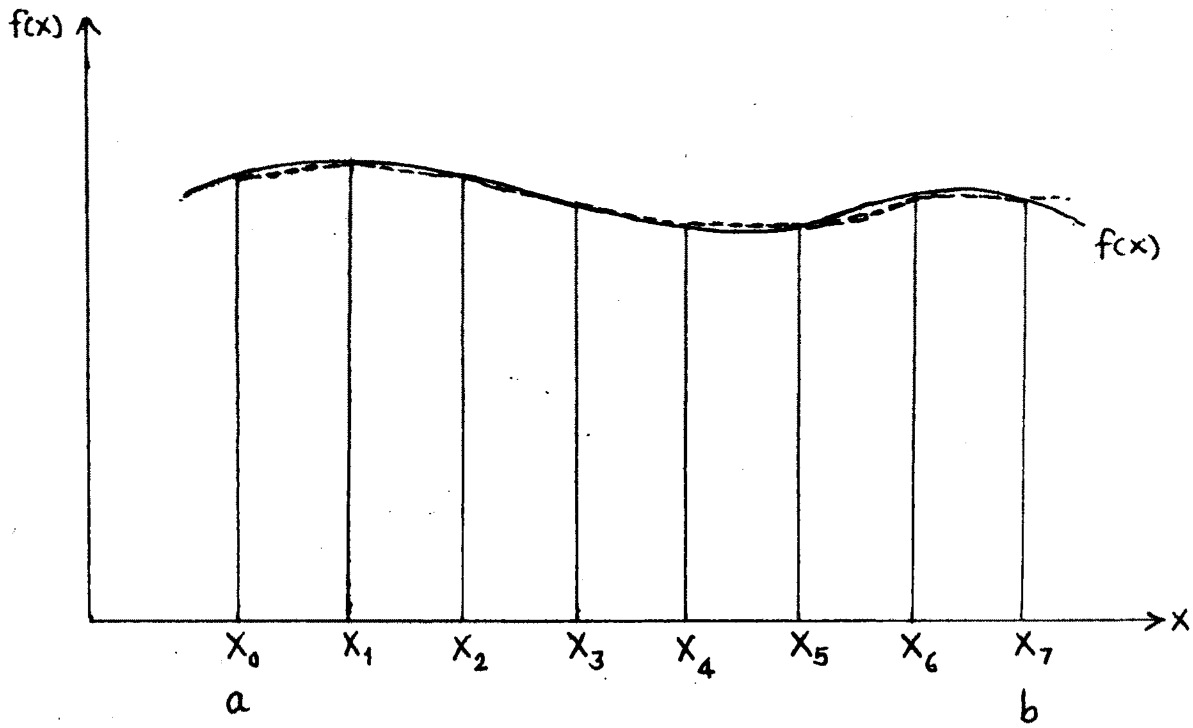

FIG 2.5: The Composite Trapezoidal Rule.

$$\int_a^b f(x)dx = \frac{h}{2}[f(x_0) + f(x_n)] + h\sum_{i=1}^{n-1} f(x_i) - \frac{h^3}{12}\sum_{i=1}^{n} f''(\xi_i),$$

$$\xi_i \in [x_{i-1}, x_i] \qquad \ldots(2.17)$$

In terms of n,a and b, this formula is written as

$$\int_a^b f(x)dx = \frac{(b-a)}{n}\left[\frac{1}{2} f(a) + \frac{1}{2} f(b) + \sum_{i=1}^{n-1} f(a + \frac{(b-a)}{n} i)\right]$$

$$- \frac{(b-a)^3}{12n^2} f''(\xi), \qquad a \le \xi \le b. \qquad \ldots(2.18)$$

The equation (2.17) or (2.18) is the extended or composite form of the trapezoidal rule.

Similarly we can obtain composite Simpson's rule. For n applications of Simpson's 1/3rd rule we require functional values of (2n+1) base points: $x_0, x_1, \ldots, x_{2n}$. The composite form of the Simpson's rule is

$$\int_a^b f(x)dx = \int_{x_0}^{x_{2n}} f(x)dx$$

$$= \frac{h}{3}[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)+\ldots+$$

$$+2f(x_{2n-2})+4f(x_{2n-1})+f(x_{2n})] - \frac{h^5}{90} 4\sum_{i=1}^{n} f^{(4)}(\xi_i)$$

$$\ldots(2.19)$$

where, $h = (b-a)/2n$,

$$x_{2i-2} < \xi_i < x_{2i}\ , \quad x_i = x_0 + ih\ , \quad i = 0,1,2,3\ldots,2n.$$

In terms of a,b and n , it is written as

$$\int_a^b f(x)dx = \frac{(b-a)}{6n}\Big[f(a) + f(b) + 2\sum_{i=1}^{n-1} f(a + \frac{(b-a)}{n} i) +$$

$$+ 4\sum_{\substack{i=1 \\ \triangle i=2}}^{2n-1} f(a+\frac{(b-a)}{2n} i)\Big] - \frac{(b-a)^5}{2880n^4} f^{(4)}(\xi) \qquad \ldots(2.20)$$

where $a < \xi < b$. The second sum involves $\triangle i = 2$ which indicates that the index i should take only odd values.

In this way we can generate the composite formula similar to (2.17) and (2.19) for any of the low order integration formulae. There are several theoretical facts about the effectiveness of a family of composite rules as $n \to \infty$. One, which is very important [4,pp 57] is that, if the low order rule integrates the constant 1 exactly, then its composite rule will converge to $\int_a^b f(x)dx$. as $n \to \infty$.

2.6 REMARKS ON NEWTON-COTES FORMULAE

First of all, we should note that the Newton-Cotes formulae are equispaced points formulae. Therefore, if the given data is not equispaced then these formulae are wholly inapplicable.

If we compare both groups (open as well as closed) of Newton-Cotes formulae for the same number of functional values, then we observe that [3,pp 76] the open formulae are slightly better when two or three points are used. But, for more than three points the closed formulae are more accurate. For this conclusion, of course, we have assumed that the derivative terms $f^{(k-1)}(\xi)$ are roughly the same for the two corresponding formulae. Hence it is beneficial to use closed type formula rather than open type formula where it can apply. Again, we should take a note of caution for the use of formulae of open type, because, the error estimates given in these formulae are valid only if the integrands f(x) are in classes of type $C^2[a,b]$,(for two-points formula), $C^4[a,b]$ (for three and four points formula) etc.

Further, if the value of the function at an end point of the interval cannot be computed because of a singularity then the use of open type formulae lead to serious error. On the other hand, there are some advantages also in using open type formulae in some cases. [4,pp 71]. In particular, for functions whose derivatives have singularities at the end points, it is observed that,the open type formulae rather than the corresponding closed formulae are more effective. This is one example of the principle of "avoiding the singularity." We cannot restrict open type formula for equidistance points. For example, the Gauss formulae are also of open type.

A formula is said to have degree of precision m if it is exact for all polynomials of degree m or less. e.g Simpson's first rule has degree of precision three because it produces exactly the integral of all polynomials of degree three or less. Since the degree of precision of the Newton-Cotes formulae increases with the number of points we might guess that a very high order formula would be more exact than a low order formula. But, unfortunately, this is not the case [3,pp 77] because high order formulae have some very undesirable properties from the view of the computation such as large weight factors with alternating sign and which lead to serious rounding errors. Moreover, there are so many functions for which the magnitude of the derivative increases without bound when order of derivative increases. Thus, we conclude that high order Newton-Cotes formula can produce large error than a low order one. Therefore, we should use low order formulae and formulae having more than eight points are never used. Again we can reduce error associated with low order formulae by applying its corresponding composite formulae.

2.7 SPLINE INTERPOLATION

The spline, especially cubic spline proves to be an efficient device for approximation as well as interpolation. Naturally, the cubic spline replaces the spline of draughtsman by a set of cubic polynomials, using a new cubic in each interval of points Hence we study cubic spline in somewhat detail.

In order to match with the idea of the draughtsman's spline, it is necessary that both the slope (dy/dx) and the curvature (d^2y/dx^2) are the same for the adjacent pairs of cubics. We shall derive the cubic spline equation as follows.

2.7.1 Derivation of Cubic Spline Equation

This derivation is mostly based on the derivation of cubic spline equation given by Davis and Rabinowitz [4,pp,51]. Let, as usual, the points $a=x_0<x_1<x_2<\ldots<x_n=b$ be the points of division of the interval $[a,b]$. Let the j-th interval be

$$\Delta_j = [x_{j-1}, x_j] \quad \text{and} \quad h_j = x_j - x_{j-1} \qquad (j = 1,2,\ldots n), \qquad \ldots(2.21)$$

As $s(x)$ is piecewise cubic, therefore, $s'(x)$ is piecewise quadratic and $s''(x)$ is piecewise linear and continuous. Therefore, we can write for the interval Δ_j , $(j = 1,2,\ldots,n)$.

$$s''_j(x) = M_{j-1}\frac{x_j - x}{h_j} + M_j\frac{x - x_{j-1}}{h_j} \qquad \ldots(2.22)$$

where M_j and M_{j-1} are certain constants. in fact,if we put

$x = x_j$ in (2.22), we get

$$s''_j(x_j) = M_j\ , \qquad j= 0,1,2,3,\ldots,n \qquad \ldots(2.23)$$

Now integrating equation (2.22) twice on Δ_j w r t x, we get

$$s'_j(x) = M_{j-1}\frac{(x_j-x)^2}{(-2)h_j} + M_j\frac{(x-x_{j-1})^2}{2h_j} + a_j$$

and $$s_j(x) = M_{j-1}\frac{(x_j-x)^3}{6h_j} + M_j\frac{(x-x_{j-1})^3}{6h_j} + a_jx + b_j$$

where a_j, b_j are constants of integration. This equation can be written in the form

$$s_j(x) = M_{j-1}\frac{(x_j-x)^3}{6h_j} + M_j\frac{(x-x_{j-1})^3}{6h_j} + A_j(x_j-x)+B_j(x-x_{j-1}) \quad ...(2.24)$$

For the determination of A_j and B_j, put $x = x_{j-1}$ in equation (2.24) to get

$$y_{j-1}= s_j(x_{j-1}) = M_{j-1}\frac{(x_j-x_{j-1})^3}{6h_j} + A_j(x_j - x_{j-1})$$

or $$A_j = \frac{1}{h_j}\left[y_{j-1}- \frac{M_{j-1}h_j^2}{6}\right] \quad ...(2.25)$$

Similarly putting $x = x_j$ in equation (2.24), we get

$$B_j = \frac{1}{h_j}\left[y_j- \frac{M_jh_j^2}{6}\right] \quad ...(2.26)$$

Using the values of A_j and B_j in equation (2.24), we obtain

$$s_j(x) = M_{j-1}\frac{(x_j-x)^3}{6h_j} + M_j\frac{(x-x_{j-1})^3}{6h_j} +$$

$$+ \left(y_{j-1} - \frac{M_{j-1}h_j^2}{6}\right)\left(\frac{x_j-x}{h_j}\right) + \left(y_j - \frac{M_jh_j^2}{6}\right)\left(\frac{x-x_{j-1}}{h_j}\right) \quad \ldots(2.27)$$

Differentiating equation (2.27) we get

$$s'_j(x) = -M_{j-1}\frac{(x_j-x)^2}{2h_j} + M_j\frac{(x-x_{j-1})^2}{2h_j} + \frac{y_j-y_{j-1}}{h_j}$$

$$- \frac{M_j-M_{j-1}}{6}h_j \quad \ldots(2.28)$$

for the interval Δ_j

Taking limit of equation (2.28) as $x \to x_j-$ we get

$$s'_j(x_j-) = \frac{h_j}{6}M_{j-1} + \frac{h_j}{3}M_j + \frac{y_j - y_{j-1}}{h_j} \quad \ldots(2.29)$$

Writing equation (2.28) for the interval Δ_{j+1} we get

$$s'_{j+1}(x) = -M_j\frac{(x_{j+1}-x)^2}{2h_{j+1}} + M_{j+1}\frac{(x-x_j)^2}{2h_{j+1}} + \frac{y_{j+1}-y_j}{h_{j+1}} -$$

$$- \frac{M_{j+1}-M_j}{6}h_{j+1}$$

Taking limit of this equation as $x \to x_j+$ we get

$$S'_{j+1}(x_j+) = -M_j\frac{h_{j+1}}{3} - \frac{h_{j+1}}{6}M_{j+1} + \frac{y_{j+1}-y_j}{h_{j+1}} \quad \ldots(2.30)$$

Now, since $s'(x)$ is required to be continous, we should have

$$S'_j(x_j-) = S'_{j-1}(x_j+)$$

Putting values from (2.29) and (2.30) and rearranging terms we get,

$$\frac{h_j}{6} M_{j-1} + \frac{h_j + h_{j+1}}{3} M_j + \frac{h_{j+1}}{6} M_{j+1} = \frac{y_{j+1} - y_j}{h_{j+1}} - \frac{y_j - y_{j-1}}{h_j}$$

$$[j = 1,2,\ldots,(n-1)] \qquad \ldots(2.31)$$

Equation (2.31) produces a set of (n-1) linear equations in $M_0, M_1, \ldots, M_n$. To obtain the unique solution for this system, we require two more equations. After the determination of values of all M_i's, we can determine the interpolation spline completely through equation (2.27). Now, we shall abbreviate these equations (2.31) by using following notations:

$$\lambda_j = \frac{h_{j+1}}{h_j + h_{j+1}}, \quad \mu_j = 1 - \lambda_j = \frac{h_j}{h_j + h_{j+1}}, \quad \sigma_j = \frac{y_j - y_{j-1}}{h_j}$$

$$d_j = \frac{6(\sigma_{j+1} - \sigma_j)}{h_j + h_{j+1}}, \qquad j = 1,2,\ldots,(n-1).$$

Then equation (2.31) reduces to

$$\mu_j M_{j-1} + 2M_j + \lambda_j M_{j+1} = d_j, \quad j = 1,2,\ldots(n-1) \qquad \ldots(2,32)$$

We shall take two additional equations in the form

$$2M_o + \lambda_o M_1 = d_o$$

and $$\mu_n M_{n-1} + 2M_n = d_n$$

and obtain several possible choices of the constants λ_o, d_o, μ_n, d_n and their interpretation. The combined system in the tridiagonal matrix form, thus, we obtain is

$$\begin{bmatrix} 2 & \lambda_o & \emptyset & \cdots\cdots & \emptyset & \emptyset & \emptyset \\ \mu_1 & 2 & \lambda_1 & \cdots\cdots & \emptyset & \emptyset & \emptyset \\ \emptyset & \mu_2 & 2 & \cdots\cdots & \emptyset & \emptyset & \emptyset \\ \cdot\cdot & \cdots & & & & \cdots & \\ \cdot\cdot & \cdots & & & & \cdots & \\ \emptyset & \emptyset & \emptyset & & 2 & \lambda_{n-2} & \emptyset \\ \emptyset & \emptyset & \emptyset & & \mu_{n-1} & 2 & \lambda_{n-1} \\ \emptyset & \emptyset & \emptyset & & \emptyset & \mu_n & 2 \end{bmatrix} \begin{bmatrix} M_o \\ M_1 \\ M_2 \\ \cdot \\ \cdot \\ M_{n-2} \\ M_{n-1} \\ M_n \end{bmatrix} = \begin{bmatrix} d_o \\ d_1 \\ d_2 \\ \cdot \\ \cdot \\ d_{n-2} \\ d_{n+1} \\ d_n \end{bmatrix}$$

Special cases -(i) if we choose $\lambda_o = \mu_n = d_o = d_n = \emptyset$ then equation (2.33) yields $M_o = M_n = \emptyset$ and then by equation (2.23) we have $s''(a) = s''(b) = \emptyset$. If we consider a spline to be a thin beam, then this corresponds to simple support at both the ends and gives the natural spline.

(ii) We can also specify the slope of the spline at the endpoints. We use here the conditions

$$s'(a) = y'_o \quad \text{and} \quad s'(b) = y'_n$$

Further, from (2.29) thses conditions are equivalent to the selection

$$\lambda_0 = \mu_n = 1, \; d_0 = \frac{6}{h_1}\left(\frac{y_1 - y_0}{h_1} - y'_0\right),$$

$$d_n = \frac{6}{h_n}\left(y'_n - \frac{y_n - y_{n-1}}{h_n}\right)$$

In case, y'_0 and y'_n are unknown, their values are approximated using finite difference formula.

2.8 SPLINE INTEGRATION

Many times we require to integrate a function which is given by scattered data. At this situation, we can fit the data by means of splines, the fit being made in the sense of least squares or any other criteria of minimality. Thus, fit the data (x_j, y_j) by a spline and then integrate it formally. From equation (2.27) we have on the interval Δ_j ,

$$\int_{x_{j-1}}^{x_j} s(x)dx = \frac{y_{j-1} + y_j}{2} h_j - \frac{M_{j-1} + M_j}{24} h_j^3$$

Thus, adding all these integrals for all subintervals of (a,b), we get

$$\int_a^b s(x)dx = \sum_{j=1}^{n} \frac{y_{j-1} + y_j}{2} h_j - \sum_{j=1}^{n} \frac{M_{j-1} + M_j}{24} h_j^3$$

This formula is nothing but the trapezoidal rule with a correction. The computer programm in 'C ' for spline integration is given in the chapter IV.

2.9 ERROR ANALYSIS

It is possible to determine the appropriate high order derivative and study its behaviour on the interval [a,b] to find an error bound for the particular selected formula, if function f(x) is known analytically. But, in practice, the error formula is of less importance because an expression for the derivative can not be available. In some of these cases, it may be possible to estimate the derivative value from high order finite divided differences of the functional values.

However it can be possible to find the error even when information about higher order derivatives is not available, if the integral is computed using two different integration formulae with comparable degrees of precision. As an example, let us consider the evaluation of

$$I^* = \int_a^b f(x)dx.$$

by using Simpson's first and second rules. Each of these rules have degree of precision three. Let the estimation of I^* and the error using Simpson's first rule be I_1 and E_1 respectively; and using Simpson's second rule be I_2 and E_2 respectively. Then we have

$$I^* = I_1 + E_1 = I_2 + E_2 \qquad \ldots(2.34)$$

Now, in terms of the integration limits a and b the values of E_1 and E_2 are

$$E_1 = -\frac{(b-a)^5}{2880} f^{(4)}(\xi_1) \quad \text{and} \quad E_2 = -\frac{(b-a)^5}{6480} f^{(4)}(\xi_2)$$

where ξ_1 and ξ_2 are different and $\xi_1, \xi_2 \in (a,b)$. Therefore

$$\frac{E_1}{E_2} = \frac{9}{4} \quad \frac{f^{(4)}(\xi_1)}{f^{(4)}(\xi_2)}$$

If we suppose that $f^{(4)}(\xi_2) \approx f^{(4)}(\xi_2)$. then above equation reduces to

$$E_1 = \frac{9}{4} E_2$$

With this relation, equation (2.34) becomes,

$$I^* = \frac{9}{5} I_2 - \frac{4}{5} I_1$$

This equation is valid if and only if $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_2)$ are equal.

There is one theorem [10,pp 114] which gives an expression for the error in the n-point Newton-Cotes formula. Here $Q_n(x)$ is the polynomial,

$$Q_n(x) = (x-x_1)(x-x_2)\ldots(x-x_n).$$

where the x_k's are the points in the formula. The statement of this therorem is : If $f^{(n+1)}(x)$ is continuous on [a,b] and n is odd then there exists a point ξ_n, where $\xi_n \in$ (a,b), so that

$$E\,[f] = e_{n+1}\, f^{(n+1)}(\xi_n)$$

where $$e_{n+1} = \frac{1}{(n+1)!} \int_a^b x\, Q_n(x)dx.$$

If $f^{(n)}(x)$ is continous on [a,b] and n is even then there exists a point ξ_n where $\xi_n \in$ (a,b), so that

$$E\,[f] = e_n f^{(n)}(\xi_n)$$

where, $$e_n = \frac{1}{n\,!} \int_a^b Q_n(x)dx.$$

In section 3.10, we will state some additional expressions for E[f] using Peano's kernel theorem and also discuss the bounds on roundoff errors.

The following result [4,pp 58] is also useful in case of composite rules. Let R be a fixed m-point integration rule defined over an interval $[\alpha, \beta]$. Suppose the error, E_R, corresponding to rule R is given by an expression,

$$E_R(f) = c(\beta - \alpha)^{k+1} f^{(k)}(\xi), \qquad \xi \in (\alpha,\beta)$$

provided $f \in C^k[\alpha,\beta]$. Here the constant c may depend on R but it is independent of α,β and f. Let n * R designate the composite rule formed from R which results from dividing the interval of integration into n equal subintervals and applying R to each of them. Let $E_{n\times R}$ denotes the corresponding error. Then this error is given by the expression,

$$\lim_{n\to\infty} n^k E_{n\times R}(f) = c(b-a)^k \left(f^{(k-1)}(b) - f^{(k-1)}(a)\right)$$

provided, $f \in C^k[a,b]$.

Besides this, we have also derived an error term in each Newton-Cotes integration formula studied so far, from the remainder term of the approximation formula.