NUMERICAL METHODS

In every scientific investigation, we are confronted with functions, integrals and derivative of functions, transcendental equations, system of linear equations (which are necessarily vast), differential equations (both partial and ordinary), matrices and their eigen values and so on. When solutions of the problems involving these can not be achieved or are difficult to achieve, the only alternative way is to employ numerical methods (which are also known as computational techniques). Particularly after the advent of high speed computers, the subjects Numerical Analysis, computational techniques have gathered immense importance. Even numerical methods have been widely applied in recent times to solve problems arising in economics, sociology, engineering and so on.

The solution obtained by a numerical technique is never exact (or in closed form), rather the numerical solution of the problem under consideration is approximate. It is always hoped that, the approximate solution obtained by a numerical technique should be close to the exact solution of the problem or in other words, the error associated with the numerical method ought to be tolerable. For this, while implementing a numerical method, the error bound is fixed and the magnitude of the error should be less than or equal to the error bound fixed in advance. For this reason, most of the numerical methods are iterative.

Or in other words by executing the method once, which indicated by an index k=1, say the error e_k satisfies the following inequality

$$|e_k| > \varepsilon$$

where ε is the error bound fixed. There the second iteration (k=2), 3rd iteration (k=3) and so on are performed until

$$|e_k| \leq \varepsilon .$$

This will happen if and only if the method employed for the numerical solution of the problem is convergent. This requires analysis of the method and hence the title of the topic is Numerical Analysis where convergence, stability of the method is essential.

We can have the following broad framework which can accommodate most of the numerical methods.

Let $T : X \to Y$ where T is a transformation from the linear space X into Y. Let

$$Tx = y \tag{1}$$

(i) Given T and x, it is required to find y. This constitutes the **direct problem**.

(ii) Given T and y, it is required to find x. This constitutes the **inverse problem**.

(iii) Given x and y, it is required to find T. This constitutes the **identification problem**.

Numerical integration, numerical differentiation come under the category of direct problem; numerical solution of differential equations, numerical solution of integral equations, numerical solution of transcendental equations and linear systems belong to the class of inverse problems and interpolation, approximation of functions, come under the category of identification problems.

Approximation of integrals which is a direct problem heavily relies on interpolation theory which is an identification problem. Thus, for successful solution of a problem of any one of these classes, problems of other classes naturally arise.

The history of numerical integration is very old (Ref. Goldstine (1977)). Numerical integration was first handled by the Greek philosopher Archimedes (300 BC) who could successfully find out the numerical value of the area enclosed by a circle or in other words the approximate value of π. This is known as "Greek Quadrature". For finding out the area of a circle, Archimedes inscribed and circumscribed the circle by regular polygon of *n* sides. Gradually increasing the value of *n*, Archimedes found out the area enclosed by a circle approximately. Since integration and quadrature (finding out the area) from the sequence of areas of inscribed circles or the area of the circumscribed circles are one and the same thing, numerical integration came nearly 2000 years before the inventions of calculus. Further, the ingenious technique employed by Archimedes is in keeping with the modern trends of analysis.

Excellent and extensive research work has been carried out for the numerical approximation of real integrals by eminent and illustrious mathematicians *viz.* Newton, Roger Cotes, Chebysev, Gauss, Hardy, Schenborg, Birkhoff, Sobolov, Rabinowitz, Davis, Lyness, Krylov and so on and the subject *Methods of Numerical Integration* has been immensely enriched by their research.

METHODS OF NUMERICAL INTEGRATION

Let us consider the following definite integral of a function f:**R**→**R** over the interval $a \leq x \leq b$.

$$I(f) = \int_a^b f(x)\, dx \tag{2}$$

The idea behind the approximation of the integral $I(f)$ is essentially the following:

An approximation to the integral of f over $[a,b]$ is the integral of an approximation to the function f i.e.

$$\text{if } P_n(x) \approx f(x), \quad x \in [a,b] \text{ then } I(f) \approx I(P_n).$$

If $P_n(x)$ is the Lagrangian interpolation polynomial of degree$\leq n$ involving $n+1$ nodes inside $[a,b]$, then $R_{n+1}(f)$ given by

$$R_{n+1}(f) = I(P_n) \tag{3}$$

is a $n+1$ point rule meant for the numerical approximation of the integral $I(f)$. The quadrature rule $R_{n+1}(f)$ is also referred to as Lagrange-Newton-Cotes rule. However, if instead of $P_n(x)$, the Hermite interpolation polynomial $H_{2n+1}(x)$ of degree $\leq 2n+1$ would have been used, then the rule would have been the $n+1$ point Gauss-Legendre rule. An exhaustive treatment of Gauss quadrature formulas can be obtained in Stroud and Secrist (1966).

$$R^G_{n+1}(f) = I(H_{2n+1}). \tag{4}$$

provided the coefficients of the derivative terms in $I(H_{2n+1})$ vanish. It is pertinent to note that by using appropriate weight functions and the range of integration, we could have got the other types of Gauss rules *viz.* Gauss-Lobato rules, Gauss-Hermite rules and Gauss-Chebyshev rules.

For the shake of simplicity, we consider the Newton-Cotes rules here. Simplification of equn. (3) leads to

$$R_{n+1}(f) = \sum_{k=0}^{n} c_n f(x_n) \tag{5}$$

where c_n's and x_n's are called the coefficients (or weights) and the nodes (or abscissas) respectively.

It is noteworthy that the n+1 nodes of the Newton-Cotes rule are given as

$$x_k = a + \frac{(b-a)\,k}{n}, \quad k = 0(1)n. \tag{6}$$

For the Newton-Cotes rule $R_{n+1}(f)$ whereas the n+1 coefficients are determined from the following set of n+1 linear equations.

$$\sum_{k=0}^{n} c_k\, x_k^j = \int_a^b x^j dx, \quad j = 0(1)n \tag{7}$$

It is noteworthy that equations (7) are obtained by setting $f(x) = x^j, \quad j = 0(1)n$ in equation $I(f) = R_{n+1}(f)$.

However, for the Gauss type of rule, $R_{n+1}^G(f)$ we can treat the $2n$+2 parameters i.e. the n+1 coefficients as well as the n+1 nodes as unknowns and determine them from the following set of $2n$+2 equations which are linear in w_k and non-linear in x_k.

$$\sum_{k=0}^{n} c_k\, x_k^j = \int_a^b x^j dx, \quad j = 0(1)2n+1 \tag{8}$$

This is precisely the algebraic method of determining the Gauss-Legendre rules. However, the algebraic method is a difficult and unsuitable when $n \geq 4$. Alternative methods using orthogonal polynomials have been devised using which the Gauss techniques can be derived analytically.

The fifth degree 3-point Gauss-Legendre rule is given by

$$R_3^{GL}(f) = [8f(0) + 5\{f(\sqrt{0.6}) + f(-\sqrt{0.6})\}]/9 \tag{9}$$