Chapter 4

Numerical Differentiation

4.1 INTRODUCTION

Numerical differentiation is useful in estimating the derivatives of a function f(x) when either f(x) is very complicated and is difficult to differentiate easily, or, it is not known as explicit expression in x, but the values of the function are given in a tabular form. We use numerical differentiation only when there is no better alternative method available to compute derivatives analytically or when the analytical solution is rather complicated. Generally, it is considered that numerical differentiation is basically an **unstable process** which means that small values of h can lead to greatly magnified errors in the final result. In fact, we may not always expect reasonable results even when the original data are known to be accurate. In actual practice this operation is avoided altogether if possible because it tends to enhance the effects of rounding errors present in the tabular values. This is particularly true when the $f(x_1)$ values are themselves subject to more error, as they would probably be if determined experimentally. If derivative values are computed in such cases, particularly when the results are to be used in subsequent calculations, it is usually better to consider curve fitting, using least-squares technique and differentiate the formula for the curve.

In this chapter, we shall derive some formulas for estimating derivatives. In spite of some inherent shortcomings, numerical differentiation is useful to derive formulas for solving integrals, ordinary and partial differential equations. Standard examples of numerical differentiation often use known functions so that the numerical approximation can be compared with the exact answer.

4.2 DERIVATION OF DIFFERENTIATION FORMULAS

Formulas for numerical differentiation may easily be obtained by differentiating interpolation polynomials.

In order to derive a differentiation formula, we differentiate a suitable interpolation formula with respect to p.

We shall write, $x = x_0 + ph$. Differentiating this w.r.t.p., we get,

$$\frac{dx}{dp} = h$$

or, $$\frac{dx}{dp} = \frac{1}{h} \qquad \text{... (4.1)}$$

Also, $f_p = f(x) = f(x_0 + ph)$ ... (4.2)

Differentiating (4.2) w.r.t.x., we get,

$$\frac{df_p}{dx} = \frac{d}{dx} f(x_0 + ph)$$

$$= \frac{d}{dp} f(x_0 + ph) \frac{dx}{dp} \qquad \text{(Note the step.)}$$

$$= \frac{1}{h} \frac{d}{dp} f(x_0 + ph)$$

$$= \frac{1}{h} \frac{df_p}{dp}$$

Denoting $\frac{df_p}{dp}$ by f'_p , we get,

$$f'_p = \frac{1}{h} \frac{df_p}{dp} \qquad \text{... (4.3)}$$

4.3 RELATIONSHIP BETWEEN OPERATORS E AND D

Before proceeding further, let us define one more operator D, called the **differential operator,**

$$Df_r = f'(x_r) = f'_r$$

Taylor series may also be written in the following manner:

$$f(r+1) = f(r) + hf'(r) + \frac{h^2}{2!} f''(r) + \frac{h^3}{3!} f'''(r) + \ldots$$

or, $$f_{r+1} = f_r + hf'_r + \frac{h^2}{2!} f''_r + \frac{h^3}{3!} f'''_r + \ldots$$

$$= f_r + hDf_r + \frac{h^2}{2!} D^2 f_r + \frac{h^3}{3!} D^3 f_r + \ldots$$

$$Ef_r = (1 + hD + \frac{h^2}{2!} D^2 + \frac{h^3}{3!} D^3 + \ldots) f_r$$

$$= e^{hD} f_r$$

or, simply, $E = e^{hD}$ ... (4.4)