UNIT 1 NUMERICAL DIFFERENTIATION

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1.0 INTRODUCTION

Differentiation of a function is a fundamental and important concept in calculus. When the function, say f(x), is given explicitly, its derivatives $f'(x)$, $f''(x)$, $f'''(x)$,… etc. can be easily found using the methods of calculus. For example, if $f(x) = x^2$, we know that $f'(x) = 2x$, $f''(x) = 2$ and all the higher order derivatives are zero. However, if the function is not known explicitly but, instead, we are given a table of values of f(x) corresponding to a set of values of x, then we cannot find the derivatives by using methods of calculus. For instance, if $f(x_k)$ represents distance travelled by a car in time x_k, $k = 0, 1, 2, \ldots$seconds, and we require the velocity and acceleration of the car at any time x_k, then the derivatives $f'(x)$ and $f''(x)$ representing velocity and acceleration respectively, cannot be found analytically. Hence, the need arises to develop methods of differentiation to obtain the derivative of a given function f(x), using the data given in the form of a table, where the data might have been formed as a result of scientific experiments.

Numerical methods have the advantage that they are easily adaptable on calculators and computers. These methods make use of the interpolating polynomials, which we discussed in earlier block. We shall now discuss, in this unit, a few numerical differentiation methods, namely, the method based on undetermined coefficients, methods based on finite difference operators and methods based on interpolation.

1.1 OBJECTIVES

After going through this unit you should be able to:

- explain the importance of the numerical methods over the methods of calculus;
- use the method of undetermined coefficients and methods based on finite difference operators to derive differentiation formulas and obtain the derivative of a function at step points, and
- use the methods derived from the interpolation formulas to obtain the derivative of a function at off step points.

1.2 METHODS BASED ON UNDETERMINED COEFFICIENTS

Earlier, we introduced to you the concepts of round-off and truncation errors. In the derivation of the methods of numerical differentiation, we shall be referring to these errors quite often. Let us first quickly recall these concepts before going further.

Round-off Error

The representation in a computer system, of a non-integer number is generally imprecise. This happens because space allotted to represent a number contains only fixed finite number of bits. But representation may either require more than finite number of allotted bits or even may require infinite number of bits. The situation is similar to the case when we attempt to represent the number 1/3 as a decimal number .333……

Any pre-assigned finite number of digits will fall short for representing 1/3 exactly as a sequence of decimal digits. Suppose, we are allotted 4 digits to represent (the fractional part) of a number, then the error in the representation is .0000333… = 10^{-4} x .3333…

Thus 10^{-4} x .3333 is round-off error in the representation of the number 1/3 using 4 decimal digits on a paper. The numbers in the computer systems are represented in binary form, generally using floating point representation. The error in representation of a number due to fixed finite space allotted to represent it, is called round-off error.

Truncation Error

Truncation error in the values of a function arise due to the method used for computing the values of the function. Generally, the method giving rise to truncation error is a infinite process, i.e., involves steps.

However, as it is impossible to execute infinitely many steps, therefore, the process has to be truncated after finite number of steps. But the truncation of an infinite process of calculation, to finite number of steps, leads to error in the value of the function at a point. Such an error is called truncation error.

For example, a method of computing the value of the function

$$f(x) = e^x$$

at a point x is given by

$$f(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + ...$$

But, as it is impossible to execute the infinitely many steps of computing and adding $\frac{x^n}{n!}$ for all n, the process has to be truncated after finite number of steps say after computing and adding $\frac{x^3}{3!}$. Then the error in the value of f(x) is given by $\frac{x^4}{4!} + \frac{x^5}{5!} + ...$ and is called truncation error.

We may note the difference between round-off error and truncation error

The round-off error in the representation of a number which possibly requires infinite space for its exact representation. On the other hand truncation error in the computed value of a function at a point, is due to the fact that the computation process for computing the value may have infinite steps. But, as infinite number of steps can not be executed, hence we are compelled to stop the process after some finite number of *steps*. But this truncation of an infinite process after finite number of steps leads to an error called truncation error.

Definition: Let f(h) be the exact analytical value of a given function obtained by using an analytical formula and f_h be the approximate value obtained by using a numerical method. If the error $f(h) - f_h = C\,h^{p+1}$, where C is a constant, then p is known as the **order of the numerical method,** and is denoted by $O(h^p)$.

The Method

Let us consider a function f (x), whose values are given at a set of tabular points. For developing numerical differentiation formulas for the derivatives $f'(x)$, $f''(x)$, …at a point $x = x_k$, we express the derivative $f^q(x)$, $q \geq 1$, as a linear combination of the values of f(x) at an arbitrarily chosen set of tabular points. Here, we assume that the tabular points are equally spaced with the step−length h, i.e., various step (nodal) points are $x_m = x_0 \pm mh$, m = 0, 1, … etc. Then we write

$$h^q f^q(x_k) = \sum_{m=-s}^{n} \gamma_m f_{k+m}, \qquad (1)$$

where γ_i for i = −s, −s+1,……,n are the unknowns to be determined and f_{k+m} denotes $f(x_k+mh)$. For example, when s = n = 1 and q = 1, Eqn. (1) reduces to

$$hf'(x_k) = \gamma_{-1}f_{k-1} + \gamma_0 f_k + \gamma_1 f_{k+1}.$$

Similarly, when s =1, n =2 and q = 2, we have

$$h^2 f''(x_k) = \gamma_{-1}f_{k-1} + \gamma_0 f_k + \gamma_1 f_{k+1} + \gamma_2 f_{k+2}.$$

Now suppose we wish to determine a numerical differentiation formula for $f^q(x_k)$ of order p using the method of undetermined coefficients. In other words, we want our formula to give the exact derivative values when f(x) is a polynomial of degree $\leq$ p, that is, for $f(x) = 1, x, x^2, x^3, \ldots, x^p$. We then get p+1 equations for the determination of the unknowns γ_i, i = −s, −s + 1, …, n. You know that if a method is of order p, then its truncation error (TE) is of the form $Ch^{p+1} f^{(p+1)}(\alpha)$, for some constant C. This implies that if $f(x) = x^m$, m = 0, 1, 2, …., p then the method gives exact results since

$$\frac{d^{p+1}}{dx^{p+1}}(x^m) = 0, \text{ for } m = 0, 1, .., p.$$

Let us now illustrate this idea to find the numerical differentiation formula of $O(h^4)$ for $f''(x_k)$.

Derivation of $O(h^4)$ formula for $f''(x_k)$

Without loss of generality, let us take $x_k = 0$. We shall take the points symmetrically, that is, $x_m = mh$; m = 0, ± 1, ± 2.

Let $f_{-2}, f_{-1}, f_0, f_1, f_2$ denote the values of f(x) at x = −2h, −h, 0, h, 2h respectively. In this case the formula given by Eqn. (1) can written as

$$h^2 f''(0) = \gamma_{-2}f_{-2} + \gamma_{-1}f_{-1} + \gamma_0 f_0 + \gamma_1 f_1 + \gamma_2 f_2 \qquad (2)$$

As there are five unknown to be determined let us make the formula exact for f(x) = 1, x, x^2, x^3, x^4. Then, we have

$f(x) = 1$, $f''(0) = 0$; $f_{-2} = f_{-1} = f_0 = f_1 = f_2 = 1$

$f(x) = x$, $f''(0) = 0$, $f_{-2} = -2h$; $f_{-1} = -h$; $f_0 = 0$; $f_1 = h$; $f_2 = 2h$;

$f(x) = x^2$, $f''(0) = 2$, $f_{-2} = 4h^2 = f_2$; $f_{-1} = h^2 = f_1$; $f_0 = 0$;

$f(x) = x^3$, $f''(0) = 0$, $f_{-2} = -8h^3$; $f_{-1} = -h^3$; $f_0 = 0$; $f_1 = h^3$, $f_2 = 8h^3$

$f(x) = x^4$, $f''(0) = 0$; $f_{-2} = 16h^4 = f_2$; $f_{-1} = h^4 = f_1$; $f_0 = 0$, (3)

where $f_i = f(ih)$, e.g., if $f(x) = x^3$ then $f_2 = f(2h) = (2h)^3 = 8h^3$.

Substituting these values in Eqn. (2), we obtain the following set of equations for determining γ_m, $m = 0, \pm 1, \pm 2$.

$$\begin{aligned}
&\gamma_{-2} + \gamma_{-1} + \gamma_0 + \gamma_1 + \gamma_2 = 0 \\
&-2\gamma_{-2} - \gamma_{-1} + \gamma_1 + 2\gamma_2 = 2 \\
&4\gamma_{-2} + \gamma_{-1} + \gamma_1 + 4\gamma_2 = 2 \\
&-8\gamma_{-2} - \gamma_{-1} + \gamma_1 + 8\gamma_2 = 0 \\
&16\gamma_{-2} + \gamma_{-1} + \gamma_1 + 16\gamma_2 = 0
\end{aligned} \tag{4}$$

Thus we have a system of five equations for five unknowns. The solution of this system of Eqns. (4) is

$$\gamma_{-2} = \gamma_2 = -1/12;\ \gamma_{-1} = \gamma_1 = 16/12;\ \gamma_0 = 30/12;$$

Hence, the numerical differentiation formula of $O(h^4)$ for $f''(0)$ as given by Eqn. (2) is

$$f''(0) \approx f''_0 = \frac{1}{12h^2}\left[-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2\right] \tag{5}$$

Now, we know that TE of the formula (5) is given by the first non-zero term in the Taylor expression of

$$f''(x_0) - \frac{1}{12h^2}\left[-f(x_0 - 2h) + 16f(x_0 - h) - 30f(x_0) + 16f(x_0 + h) - f(x_0 + 2h)\right] \tag{6}$$

The Taylor series expansions give

$$f(x_0 - 2h) = f(x_0) - 2hf'(x_0) + 2h^2 f''(x_0) - \frac{4h^3}{3}f'''(x_0) + \frac{2h^4}{3}f^{IV}(x_0)$$
$$- \frac{4h^5}{15}f^{V}(x_0) + \frac{4h^6}{45}f^{VI}(x_0) - \ldots..$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f^{IV}(x_0) - \frac{h^5}{120}f^{V}(x_0)$$
$$+ \frac{h^6}{720}f^{VI}(x_0) + \ldots\ldots.$$

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f^{IV}(x_0) + \frac{h^5}{120}f^{V}(x_0)$$
$$+ \frac{h^6}{720}f^{IV}(x_0) + \ldots\ldots$$

$$f(x_0 + 2h) = f(x_0) + 2hf'(x_0) + \frac{2h^2}{2}f''(x_0) + \frac{4h^3}{3}f'''(x_0) + \frac{2h^4}{3}f^{IV}(x_0) + \frac{4h^5}{15}f^{V}(x_0)$$

$$+\frac{4h^6}{45}f^{VI}(x_0)+............$$

Substituting these expansions in Eqn. (6) and simplifying, we get the first non-zero term or the TE of the formula (5) as

$$TE = f''(x_0) - \frac{1}{12h^2}\left[-f(x_0-2h)+16f(x_0-h)-30f(x_{0)}+16f(x_0+h)-f(x_0+2h)\right]$$

$$= -\frac{h^6}{90}f^{VI}(\alpha), 0<\alpha<1.$$

You may now try the following exercise.

Ex.1) A differentiation rule of the form
$f'_0 = \alpha_0 f_0 + \alpha_1 f_1 + \alpha_2 f_2$
is given. Find α_0, α_1 and α_2 so that the rule is exact for polynomials of degree 2 or less.

You must have observed that in the numerical differentiation formula discussed above, we have to solve a system of equations. If the number of nodal points involved is large or if we have to determine a method of high order, then we have to solve a large system of linear equations, which becomes tedious. To avoid this, we can use finite difference operators to obtain the differentiation formulas, which we shall illustrate in the next section.

1.3 METHODS BASED ON FINITE DIFFERENCE OPERATORS

Recall that in Unit 4 of Block 2, we introduced the finite difference operators E, ∇, Δ, μ and δ. There we also stated the relations among various operators, e.g.

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

$$\mu = \frac{1}{2}(E^{1/2}+E^{-1/2})$$

$$l_n\ E = \log_e E$$

In order to construct the numerical differentiation formulas using these operators, we shall first derive relations between the differential operator D where Df(x) = f ′(x) and the various difference operators.

By Taylor series, we have

$$f(x+h) = f(x) + hf'(x) + h^2 f''(x) + \ldots..$$

$$= [1 + hD + h^2D^2 + \ldots]\ f(x)$$
$$= e^{hD}\ f(x) \qquad (7)$$

Using, Ef (x) = f (x+h), we obtain from Eqn. (7), the identity

$$E = e^{hD} \tag{8}$$

Taking logrithm of both sides, we get

$$hD = \ln E = \ln\left(1+\Delta\right) = \Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \ldots\ldots. \tag{9}$$

$$hD = \ln E = -\ln(1-\nabla) = \nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} - \frac{\nabla^4}{4} + \ldots \tag{10}$$

We can relate D with δ as follows:

We know that $\delta = E^{1/2} - E^{-1/2}$. Using identity (8), we can write

$$\delta f(x) = \left[e^{hD/2} - e^{-hD/2}\right] f(x) \; +$$

Hence, $\delta = 2\sinh\,(hD/2)$

or $hD = 2\sinh^{-1}(\delta/2)$ (11)

Similarly $\mu = \cosh\,(hD/2)$ (12)

Then, we also have $\mu\,\delta = 2\sinh\,(h\,D/2)\cosh\,(h\,D/2) = \sinh\,(hD)$

or $hD = \sinh^{-1}(\mu\,\delta)$ (13)

and $\mu^2 = \cosh^2(hD/2) = 1 + \sinh^2(hD/2) = 1 + \dfrac{\delta^2}{4}$ (14)

Using the Maclaurin's expansion of $\sinh^{-1}x$, in relation (11), we can express hD as an infinite series in $\delta/2$.

Thus, we have

$$hD = 2\sinh^{-1}(\delta/2)$$

$$= \delta - \frac{1^2.\delta^3}{2^2 3!} + \frac{1^2 3^2.\delta^5}{2^4.5!} + \frac{1^2.3^2.5^2.\delta^7}{2^6.7!} + \ldots.. \tag{15}$$

Notice that this formula involves off-step points when operated on f(x). The formula involving only the step points can be obtained by using the relation (13), i.e.,

$$hD = \sinh^{-1}(\mu\,\delta)$$

$$= \mu\delta - \frac{1^2\mu^3\delta^3}{3!} + \frac{1^2.3^2.\mu^5\delta^5}{5!} - \frac{1^2.3^2.5^2.\mu^7\delta^7}{7!} + \ldots \tag{16}$$

Using relation (14) in Eqn. (16), we obtain

$$hD = \mu\left[\delta - \frac{\delta^3}{6} + \frac{\delta^5}{30} - \frac{\delta^7}{140} + \ldots\right] \tag{17}$$

Thus, Eqns. (9), (10) and (17) give us the relation between hD and various difference operators. Let us see how we can use these relations to derive numerical differentiation formulas for f'_k, f''_k etc.

We first derive formulas for f'_k. From Eqn. (9), we get

$$hDf(x_k) = hf'_k = \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \ldots\right) f_k$$

Thus forward difference formulas of O(h), O (h^2), O (h^3) and $0(h^4)$ can be obtained by retaining respectively 1,2 3, and 4 terms of the relation (9) as follows:

0(h) method : $hf'_k = \Delta f_k = f_{k+1} - f_k$ (18)

$0(h^2)$ method : $hf'_k = \Delta f_k = \frac{1}{2}\left(-f_{k+2} + 4f_{k+1} - 3f_k\right)$ (19)

$0(h^3)$ method : $hf'_k = \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3}\right) f_k = \frac{1}{6}\left(2f_{k+3} - 9f_{k+2} + 18f_{k+1} - 11f_k\right)$ (20)

$0(h^4)$ method :

$hf'_k = \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4}\right) f_k = \frac{1}{12}\left(-3f_{k+4} + 16f_{k+3} - 36f_{k+2} + 48f_{k+1} - 25f_k\right)$ (21)

TE of the formula (18) is

$$TE = f'(x_k) - \frac{1}{h}\left[f(x_{k+1}) - f(x_k)\right] = -\frac{h}{2} f''(\xi) \tag{22}$$

and that of formula (19) is

$$TE = f'(x_k) - \frac{1}{2h}\left[-f(x_{k+2}) + 4f(x_{k+1}) - 3f(x_k)\right]^2 = \frac{h^2}{3} f'''(\xi) \tag{23}$$

Similarly the TE of formulas (20) and (21) can be calculated. Backward difference formulas of 0(h) $0(h^2)$, $0(h^3)$ and $0(h^4)$ for f_k can be obtained in the same way by using the equality (10) and retaining respectively 1,2,3 or 4 terms. We are leaving it as an exercise for you to derive these formulas.

Ex. 2) Derive backward difference formulas for f'_k of 0(h), $0(h^2)$, $0(h^3)$ and $0(h^4)$.

Central difference formulas for f'_k can be obtained by using the relation (17), i.e.,

$$hf'_k = \mu\left(\delta - \frac{\delta^3}{6} + \ldots\right) f_k$$

Note that relation (17) gives us methods of $0(h^2)$ and $0(h^4)$, on retaining respectively 1 and 2 terms, as follows:

$0(h^2)$ method : $hf'_k = \frac{1}{2}\left(f_{k+1} - f_{k-1}\right)$ (24)

$0(h^4)$ method : $hf'_k = \frac{1}{12}\left(-f_{k-2} + 8f_{k-1} + 8f_{k+1} + f_{k+2}\right)$ (25)

We now illustrate these methods through an example.

Example 1: Given the following table of values of f(x) = e^x, find $f'(0.2)$ using formulas (18), (19), (24) and (25).

x :	0.0	0.1	0.2	0.3	0.4
f(x) :	1.000000	1.105171	1.221403	1.349859	1.491825

Using $(18), f'(0.2) = \dfrac{f(0.3) - f(0.2)}{0.1}$

or $$f'(0.2) = \frac{1.349859 - 1.221403}{0.1}$$

$$= 1.28456$$

$$TE = -\frac{h}{2} f''(0.2) = -\frac{1}{2} e^{0.2} = -0.061070$$

Actual error = 1.221402758 − 1.28456 = − 0.063157

Using $(19), f'(0.2) = \dfrac{1}{0.2}\left[-f(0.4) + 4f(0.3) - 3f(0.2)\right] = 1.21701$

$$TE = \frac{h^2}{3} f'''(0.2) = \frac{0.01}{3} e^{0.2} = 0.004071;$$

Actual error = 0.004393

Using $(24), f'(0.2) = \dfrac{1}{0.2}\left[f(0.3) - f(0.1)\right] = 1.22344$

$$TE = -\frac{h^2}{6} f'''(0.2) = -\frac{0.01}{6} e^{0.2} = -0.0020357$$

Actual error $= -0.002037$

Using $(25), f'(0.2) = \dfrac{1}{12}\left[-f(0.0) + 8f(0.1) - 8f(0.3) + f(0.4)\right] = 1.221399167$

$$TE = \frac{h^4 f^{VI}(0.2)}{30} = \frac{0.0001}{30} e^{0.2} = 0.4071 \times 10^{-5};$$

Actual error $= 0.3591 \times 10^{-5}$

Numerical differentiation formulas for f''_k can be obtained by considering

$$h^2 D^2 = \Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 - \frac{2}{3}\Delta^5 + \ldots \tag{26}$$

$$= \nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \frac{2}{3}\nabla^5 + \ldots \tag{27}$$

$$= \delta^2 - \frac{\delta^4}{12} + \frac{\delta^6}{90} - \ldots \tag{28}$$

We can write the forward difference methods of 0(h), 0(h^2), 0(h^3) and 0(h^4) for f''_k using Eqn. (26) and retaining 1,2,3 and 4 terms respectively as follows:

$$0(h) \text{ method: } h^2 f''_k = f_{k+2} - 2f_{k+1} + f_k \quad (29)$$

$$0(h^2) \text{ method: } h^2 f''_k = -f_{k+3} + 4f_{k+2} - 5f_{k+1} + 2f_k \quad (30)$$

$$0(h^3) \text{ method: } h^2 f''_k = \frac{1}{12}\left(11f_{k+4} - 56 f_{k+3} + 114f_{k+2} - 104f_{k+1} + 35f_k\right) \quad (31)$$

$$0(h^4) \text{ method: } h^2 f''_k = \frac{1}{12}\left(-8f_{k+5} + 51f_{k+4} - 136f_{k+3} + 194f_{k+2} - 144f_{k+1} + 43f_k\right) \quad (32)$$

Backward difference formulas can be written in the same way by using Eqn. (27). Central difference formulas of 0(h^2) and 0(h^4) for f''_k are obtained by using Eqn. (28) and retaining 1 or 2 terms respectively as follows:

$$0(h^2) \text{ method: } h^2 f''_k = \left(f_{k-1} - 2f_k + f_{k+1}\right) \quad (33)$$

$$0(h^4) \text{ method: } h^2 f''_k = \frac{1}{12}\left(-f_{k-2} + 16f_{k-1} - 30f_k + 16f_{k+1} - f_{k+2}\right) \quad (34)$$

Let us consider an example,

Example 2: For the table of values of $f(x) = e^x$, given in Example 1, find $f''(0.2)$ using the formulas (33) and (34).

Solution: Using (33), $f''(0.2) = \frac{1}{0.01}\left[f(0.1) - 2f(0.2) + f(0.3)\right] = 1.2224$

$$TE = \frac{-h^2 f^{IV}(0.2)}{12} = \frac{-(0.01)e^{0.2}}{12} = -0.0010178$$

Actual error = − 0.0009972

Using Eqn. (34),

$$f''(0.2) = \frac{\left[-f(0.0) + 16f(0.1) - 30f(0.2) + 16f(0.3) - f(0.4)\right]}{0.12} = 1.221375$$

$$TE = \frac{h^4 f^{VI}(0.2)}{90} = 0.13571 \times 10^{-5}$$

Actual error = 0.27758×10^{-4}

And now the following exercises for you.

Ex. 3) From the following table of values find $f'(6.0)$ using an 0(h) formula and $f''(6.3)$ using an 0(h^2) formula.

x	:	6.0	6.1	6.2	6.3	6.4
f(x)	:	0.1750	− 0.1998	− 0.2223	− 0.2422	−0.2596

Ex. 4) Calculate the first and second derivatives of $1_n x$ at x = 500 from the following table. Use $0(h^2)$ forward difference method. Compute TE and actual errors.

x	:	500	510	520	530
f(x)	:	6.2146	6.2344	6.2538	6.2729

In Secs. 5.2 and 5.3, we have derived numerical differentiation formulas to obtain the derivative values at **nodal** points or **step points**, when the function values are given in the form of a table. However, these methods cannot be used to find the derivative values at off-step points. In the next section we shall derive methods which can be used for finding the derivative values at the off-step points as well as at steps points.

1.4 METHODS BASED ON INTERPOLATION

In these methods, given the values of f(x) at a set of points $x_0, x_1, \ldots x_n$ the general approach for deriving numerical differentiation formulas is to obtain the unique interpolating polynomial $P_n(x)$ fitting the data. We then differentiate this polynomial q times ($q \le n$), to get $P_n{}^q(x)$. The value $P_n{}^q(x_k)$ then gives us the approximate value of $f^{(q)}(x_k)$ where x_k may be a step point or an off-step point. We would like to point out here that even when the original data are known to be accurate i.e. $P_n(x_k), = f(x_k)$, k = 0, 1, 2, …, n, yet the derivative values may differ considerably at these points. The approximations may further deteriorate while finding the values at off-step points or as the order of the derivative increases. However, these disadvantages are present in every numerical differentiation formula, as in general, one does not know whether the function representing a table of values has a derivative at every point or not.

We shall first derive differentiation formulas for the derivatives using non-uniform nodal points. That is, when the difference between any two consecutive points is not uniform.

Non-Uniform Nodal Points

Let the data (x_k, f_k), k = 0,1, …, n be given at n+1 points where the step length $x_i - x_{i-1}$ may not be uniform.

In Unit 4 you have seen that the Lagrange interpolating polynomial fitting the data (x_k, f_k), k = 0, 1, …, n is given by

$$P_n(x) = \sum_{k=0}^{n} L_k(x) f_k \tag{35}$$

where L_k (x) are the fundamental Lagrange polynomials given by

$$L_k(x) = \frac{\pi(x)}{(x - x_k)\,\pi'(x_k)} \tag{36}$$

and $\pi(x) = (x - x_0)(x - x_1)\ldots(x - x_n)$ (37)

$$\pi'(x_k) = (x_k - x_0)(x_k - x_1)\ldots(x_k - x_{k-1})(x_k - x_{k+1})\ldots(x_k - x_n) \tag{38}$$

The error of interpolation is given by

$$E_n(x) = f(x) - P_n(x) = \frac{\pi(x)}{(n+1)!} f^{(n+1)}(\alpha), \quad x_0 < \alpha < x_n$$

Differentiating $P_n(x)$ = w.r.t. x, we obtain

$$P'_n(x) = \sum_{k=0}^{n} L'_k(x) f_k \tag{39}$$

and the error is given by

$$E'_n(x) = \frac{1}{(n+1)!}\left\{\pi'(x) f^{(n+1)}(\alpha) + \pi(x)\left(f^{(n+1)}(\alpha)\right)'\right\} \tag{40}$$

Since in Eqn. (40), the function $\alpha(x)$ is not known in the second term on the hand side, we cannot evaluate $E'_n(x)$ directly. However, since at a nodal point $\pi(x_k) = 0$, we obtain

$$E'_n(x_k) = \frac{\pi'(x_k)}{(n+1)!} f^{(n+1)}(\alpha) \tag{41}$$

If we want to obtain the differentiation formulas for any higher order, say qth $(1 \le q \le n)$ order derivative, then we differentiate $P_n(x)$, q times and get

$$f^{(q)}(x) \approx P_n^{(q)}(x) = \sum_{k=0}^{n} L_k^{(q)}(x) f_k \tag{42}$$

Similarly, the error term is obtained by differentiating $E_n(x)$, q times.
Let us consider the following examples.

Example 3: Find f′(x) and the error of approximation using Lagrange Interpolation for the data (x_k, f_k), k = 0, 1.

Solution: We know that $P_1(x) = L_0(x) f_0 + L_1(x) f_1$

Where $L_0(x) = \frac{x - x_1}{x_0 - x_1}$ and $L_1(x) = \frac{x - x_0}{x_1 - x_0}$

Now,

$$P'_1(x) = L'_0(x) f_0 + L'_1(x) f_1$$

and $L'_0(x) = \frac{1}{x_0 - x_1}, L'_1(x) = \frac{1}{x_1 - x_0}$

Hence, $$f'(x) = P'_1(x) = \frac{f_0}{x_0 - x_1} + \frac{f_1}{x_1 - x_0} = \frac{(f_1 - f_0)}{(x_1 - x_0)} \tag{43}$$

$$E'_1(x_0) = \frac{(x_0 - x_1)}{2} f''(\alpha) \text{ and } E'_1(x_1) = \frac{(x_1 - x_0)}{2} f''(\alpha), \ x_0 < \alpha < x_1.$$

Example 4: Find f ′ (x) and f″(x) given f_0, f_1, f_2 at x_0, x_1, x_2 respectively, using Lagrange interpolation.

Solution: By Language's interpolation formula

$$f(x) \approx P_2(x) = L_0(x) f_0 + L_1(x) f_1 + L_2(x) f_2$$

where,

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}; \qquad L'_0(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}; \qquad L'_1(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}; \qquad L'_2(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

$$\text{Hence, } f'(x) = P'_2(x) = L'_0(x) f_0 + L'_1(x) f_1 + L'_2(x) f_2$$

$$\text{and } P''_2(x) = L''_0(x) f_0 + L''_1(x) f_1 + L''_2(x) f_2$$
$$= \frac{2f_0}{(x_0-x_1)(x_0-x_2)} + \frac{2f_1}{(x_1-x_0)(x_1-x_2)} + \frac{2f_2}{(x_2-x_1)}$$

Example 5: Given the following values of f(x) = In x, find the approximate value of $f'(2.0)$ and $f''(2.0)$. Also find the errors of approximations.

x	:	2.0	2.2	2.6
f(x)	:	0.69315	0.78846	0.95551

Solution: Using the Lagrange's interpolation formula, we have

$$f'(x_0) = P'_2(x_0) = \frac{2x_0-x_1-x_2}{(x_0-x_1)(x_0-x_2)} f_0 + \frac{x_0-x_2}{(x_1-x_0)(x_1-x_2)} f_1 + \frac{x_0-x_1}{(x_2-x_0)(x_2-x_1)} f_2$$

$\therefore$ we get

$$f'(2.0) = \frac{4-2.2-2.6}{(2-2.2)(2-2.6)}(0.69315) + \frac{2-2.6}{(2.2-2)(2.2-2.6)}(0.78846)$$

$$+ \frac{2-2.2}{(2.6-2)(2.6-2.2)}(0.95551) = 0.49619$$

The exact value of $f'(2.0) = 0.5$

Error is given by

$$E'_2(x_0) = \frac{1}{6}(x_0-x_1)(x_0-x_2) f'''(2.0)$$

$$= \frac{1}{6}(2.0-2.2)(2.0-2.6)(-0.25) = -0.005$$

Similarly,

$$f''(x_0)=2\left[\frac{f_0}{(x_0-x_1)(x_0-x_2)}+\frac{f_1}{(x_1-x_0)(x_1-x_2)}+\frac{f_2}{(x_2-x_0)(x_2-x_1)}\right]$$

$$\therefore f''(2.0)=2\left[\frac{0.69315}{(2-2.2)(2-2.6)}+\frac{0.78846}{(2.2-2)(2.2-2.6)}+\frac{0.95551}{(2.6-2)(2.6-2.2)}\right]$$

$$= -\ 0.19642$$

The exact value of $f''(2.0) = -\ 0.25$.

Error is given by

$$E''_2(x_0)=\frac{1}{3}(2x_0-x_1-x_2)f'''(2.0)+\frac{1}{6}(x_0-x_1)(x_0-x_2)\left[f^{IV}(2.0)+f^{IV}(2.0)\right]$$
$$= -\ 0.05166$$

You may now try the following exercise.

Ex.5) Use Lagrange's interpolation to find $f'(x)$ and $f''(x)$ at each of the values $x = 2.5; 5.0$ from the following table

x	:	1	2	3	4
f(x)	:	1	16	81	256

Next, let us consider the case of uniform nodal points.

Uniform Nodal Points

When the difference between any two consecutive points is the same, i.e., when we are given values of f(x) at equally spaced points, we can use Newton's forward or backward interpolation formulas to find the unique interpolating polynomial $P_n(x)$. We can then differentiate this polynomial to find the derivative values either at the nodal points or at off-step points.

Let the data (x_k, f_k), $k = 0, 1, \ldots, n$ be given at $(n+1)$ points where the step points x_k, $k = 0, 1, \ldots, n$ are equispaced with step length h. That is, we have $x_k = x_0 + kh$, $k = 1, 2, \ldots, n$.

You know that by Newton's forward interpolation formula

$$f(x)=P_n(x)=f_0+\frac{(x-x_0)}{h}\Delta f_0+\frac{(x-x_0)(x-x_1)}{2!h^2}\Delta^2 f_0+\ldots$$

$$+\frac{(x-x_0)(x-x_1)\ldots(x-x_{n-1})\Delta^n f_0.}{n!h^n} \tag{44}$$

with error

$$E_n(x)=\frac{(x-x_0)(x-x_1)\ldots(x-x_n)}{(n+1)!h^{n+1}}\Delta^{n+1} f(\alpha),\quad x_0<\alpha<x_n. \tag{45}$$

If we put $\frac{x - x_0}{h} = s$ or $x = x_0 + sh$, then Eqns. (44) and (45) reduce respectively to

$$f(s) = P_n(s) = f_0 + \frac{s\Delta f_0}{1!} + \frac{s(s-1)\Delta^2 f_0}{2!} + \frac{s(s-1)(s-2)\Delta^3 f_0}{3!} + \ldots$$

$$+ \frac{s(s-1)\ldots(s-n+1)\Delta^n f_0}{n!} \tag{46}$$

and

$$E_n(x) = \frac{s(s-1)\ldots(s-n)}{(n+1)!} h^{(n+1)} f^{(n+1)}(\alpha) \tag{47}$$

$$\frac{dP}{dx} = \frac{dp}{ds} \times \frac{ds}{dx} = \frac{1}{h} \cdot \frac{dP(s)}{ds}$$

$$\because\ dx = 0 + h\,ds \text{ or } \frac{ds}{dx} = \frac{1}{h}.$$

Now from (46) we get,

Differentiation of $P_n(x)$ w.r.t. x gives us

$$P'_n(x) = \frac{1}{h}\left[\Delta f_0 + \frac{(2s-1)}{2}\Delta^2 f_0 + \frac{(3s^2 - 6s + 2)}{6}\Delta^3 f_0 + \ldots\right] \tag{48}$$

At $x = x_0$, we have $s = 0$ and hence

$$f'(x_0) = \frac{1}{h}\left[\Delta f_0 - \frac{\Delta^2 f_0}{2} + \frac{\Delta^3 f_0}{3} + \frac{\Delta^4 f_0}{4} + \ldots\right]$$

which is same as formula (9) obtained in Sec. 5.3 by difference operator method. We can obtain the derivative at any step or off-step point by finding the value of s and substituting the same in Eqn. (48). The formula corresponding to Eqn. (48) in backward differences is

$$P'_n(x) = \frac{1}{h}\left[\nabla f_n + \frac{(2s+1)}{2}\nabla^2 f_n + \frac{(2s^2 + 6s + 2)}{6}\nabla^3 f_n + \ldots\right] \tag{49}$$

where $x = x_n + sh$.

Formulas for higher order derivatives can be obtained by differentiating $P'_n(x)$ further and the corresponding error can be obtained by differentiating $E'_n(x)$.

Let us illustrate the method through the following examples:

Example 6: Find the first and second derivatives of f(x) at x = 1.1 from the following tabulated values.

x :	1.0	1.2	1.4	1.6	1.8	2.0
f(x) :	0.0000	0.1280	0. 5440	1.2960	2.4320	4.0000

Table 1

x	f(x)	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$	$\Delta^5 f(x)$
1.0	0.0					
		0.1280				
1.2	0.1280		0.2880			
		0.4160		0.0480		
1.4	0.5440		0.3360		0.0000	
		0.7520		0.0480		0.0000
1.6	1.2960		0.3840		0.0000	
		1.1360		0.0480		
1.8	2.4320		0.4320			
		1.5680				
2.0	4.0000					

Since, $x = x_0 + s\,h$, $x_0 = 1$, $h = 0.2$ and $x = 1.1$, we have $s = \frac{1.1-1}{0.2} = 0.5$

Substituting the value of s in formula (48), we get

$$f'(1.1) = \frac{1}{h}\left[\Delta f_0 - \frac{0.25}{6}\Delta^3 f_0\right] \tag{50}$$

Substituting the values of Δf_0 and $\Delta^3 f_0$ in Eqn. (50) from Table 1, we get

$$f'(1.1) = 0.63$$

To obtain the second derivative, we differentiate formula (48) and obtain

$$f''(x) = P''(x) = \frac{1}{h}\left[\Delta^2 f_0 + (s-1)\Delta^3 f_0\right]$$

Thus $f''(1.1) = 6.6$

Note: If you construct a forward difference interpolating polynomial P(x), fitting the data given in Table 1, you will find that $f(x) = P(x) = x^3 - 3x + 2$. Also, $f'(1.1) = 6.3$, $f''(1.1) = 6.6$. The values obtained from this equation or directly as done above have to be same as the interpolating polynomial is unique.

Example 7: Find $f'(x)$ at $x = 0.4$ from the following table of values.

x	:	0.1	0.2	0.3	0.4	0.5
f(x)	:	1. 10517	1.22140	1.34986	1.49182	256

Solution: Since we are required to find the derivative at the right-hand end point, we will use the backward difference formula. The backward difference table for the given data is given by

Table 2

X	f(x)	$\nabla f(x)$	$\nabla^2 f(x)$	$\nabla^3 f(x)$
0.1	1.10517			
		0.11623		
0.2	1.22140		0.01223	
		0.12846		0.00127
0.3	1.34986		0.01350	
		0.14196		
0.4	1.49182			

Since $x_n = 0.4$, $h = 0.1$, $x = 0.4$, we get $s = 0$

Substituting the value of s in formula (49), we get

$$f'(0.4) = \frac{1}{4}\left[\Delta f_3 + \frac{1}{2}\Delta^2 f_3 + \Delta^3 f_3\right]$$

$$= \frac{1}{0.1}\left[0.14196 + \frac{0.0135}{2} + \frac{0.00127}{3}\right]$$

$$= 1.14913$$

How about trying a few exercises now ?

Ex.6) The position f(x) of a particle moving in a line at different point of time x_k is given by the following table. Estimate the velocity and acceleration of the particle at points x = 15 and 3.5

x	:	0	1	2	3	4
f(x)	:	−25	−9	0	7	15

Ex.7) Construct a difference table for the following data

x	:	1.3	1.5	1.7	1.9	2.1	2.3	2.5
f(x)	:	3.669	4.482	5.474	6.686	8.166	9.974	12.182

Taking h = 0.2, compute $f'(1.5)$ and the error, if we are given $f(x) = e^x$

Ex.8) Compute $f''(0.6)$ from the following table using $0(h^2)$ central difference formula with step lengths h = 0.4, 0.2, 0.1.

x	:	0.2	0.4	0.5	0.6	0.7	0.8	1.0
f(x)	:	1.420072	1.881243	2.128147	2.386761	2.657971	2.942897	3.559753

Ex. 9) Using central difference formula of $0(h^2)$ find $f''(0.3)$ from the given table

x	:	01	0.2	0.3	0.4	0.5
f(x)	:	0.091	0.155	0.182	0.171	0.130

1.5 SUMMARY

In this unit we have covered the following:

1) If a function f(x) is not known explicitly but is defined by a table of values of f(x) corresponding to a set of values of x, then its derivatives can be obtained by numerical differentiation methods.

2) Numerical differentiation formulas using

   (i) the method of undetermined coefficients and
   (ii) methods based on finite difference operators can be obtained for the derivatives of a function at nodal or step points when the function is given in the form of table.

3) When it is required to find the derivative of a function at off-step points then the methods mentioned in (2) above cannot be used. In such cases, the methods derived from the interpolation formulas are useful.

1.6 SOLUTIONS/ANSWERS

E1) Let $f'(x) = \alpha_0 f_0 + \alpha_1 f_1 + \alpha_2 f_2$. Setting $f(x) = 1, x, x^2$ we obtain

$$\alpha_0 + \alpha_1 + \alpha_2 = 0$$

For f(x) = x, $f_0 = 0$, $f_1 = h$ and $f_2 = 2h$, therefore,

$$(\alpha_1 + 2\alpha_2)h = 1$$

For $f(x) = x^2$, $f_0 = 0$, $f_1 = h^2$ and $f_2 = 4h^2$ therefore,

$$(\alpha_1 + 4\alpha_2)h^2 = 0, \text{ hence, } \alpha_1 + 4\alpha_2 = 0$$

Solving we obtain $\alpha_0 = -\frac{3}{2h}$, $\alpha_1 = \frac{2}{h}$ and $\alpha_2 = -\frac{1}{2h}$.

Hence, $f'_0 = \left(\frac{-3f_0 + 4f_1 - f_2}{2h}\right)$

E2) 0(h) method: $hf'_k = (f_k - f_{k-1})$

$0(h^2)$ method: $hf'_k = \left(\frac{3f_k - 2f_{k-1} + f_{k-2}}{2}\right)$

$0(h^3)$ method: $hf'_k = \left(\frac{11f_k - 22f_{k-1} + 9f_{k-2} - 6f_{k-3}}{6}\right)$

$0(h^4)$ method: $hf'_k = \left(\frac{25f_k - 56f_{k-1} + 36f_{k-2} - 24f_{k-3} + 3f_{k-4}}{12}\right)$

E3) Using formula (18), we have

$$f'(6.0) = \left[\frac{f(6.1) - f(6.0)}{0.1}\right] = -3.7480$$

Using formula (33).

$$f''(6.3) = \left[\frac{f(6.4) - 2f(6.3) + f(6.2)}{(0.1)^2}\right] = 0.25$$

E4) Using formula (19), we have

$$f'(500) = \left[\frac{-3f(500) + 4f(510) - f(520)}{2h}\right] = 0.002$$

Using (30), we have

$$f''(500) = \left[\frac{2f(500) - 5f(510) + 4f(520) - f(530)}{h^2}\right] = -0.5 \times 10^{-5}$$

Exact value $f'(x) = 1/x = 0.002$; $f'''(x) = -1/x^2 = -0.4 \times 10^{-5}$

Actual error in $f'(500)$ is 0, whereas in $f''(500)$ it is 0.1×10^{-5}. Truncation error in $f'(x)$ is $\dfrac{-h^2 f'''}{3} = -5.33 \times 10^{-7}$ and in $f''(x)$ it is $\dfrac{11h^2 f^{IV}}{12} = 8.8 \times 10^{-9}$

E5) In the given problem $x_0 = 1$, $x_1 = 2$, $x_2 = 3$, $x_3 = 4$ and $f_0 = 1$, $f_1 = 16$, $f_2 = 81$ and $f_3 = 256$.

Constructing the Lagrange fundamental polynomials, we get

$$L_0(x) = -\left(\frac{x^3 - 9x^2 + 26x - 24}{6}\right); L_1(x) = \left(\frac{x^3 - 8x^2 + 19x - 12}{2}\right)$$

$$L_2(x) = -\left(\frac{x^3 - 7x^2 + 14x - 8}{2}\right); L_3(x) = \left(\frac{x^3 - 6x^2 + 11x - 6}{6}\right)$$

$$P_3(x) = L'_0(x)f_0 + L'_1(x)f_1 + L'_2(x)f_2 + L'_3(x)f_3$$

$$P'_3(x) = L'_0(x)f_0 + L'_1(x)f_1 + L'_2(x)f_2 + L'_3(x)f_3$$

$$P''_3(x) = L''_0(x)f_0 + L''_1(x)f_1 + L''_2(x)f_2 + L''_3(x)f_3$$

We obtain after substitution,

$$P'_3(2.5) = 62.4167; P''_3(2.5) = 79; P'_3(5) = 453.667; P''_3(5) = 234.$$

The exact values of $f'(x)$ and $f''(x)$ are (from $f(x) = x^4$)

$f'(2.5) = 62.5$, $f'(5) = 500$; $f''(2.5) = 75$; $f''(5) = 300$.

E6) We are required to find $f'(x)$ and $f''(x)$ at $x = 1.5$ and 3.5 which are off-step points. Using the Newton's forward difference formula with $x_0 = 0$, $x = 1.5$, $s = 1.5$, we get $f'(1.5) = 8.7915$ and $f''(1.5) = -4.0834$.

Using the backward difference formula with $x_n = 4$, $x = 3.5$, $s = -0.5$, we get $f'(3.5) = 7.393$ and $f''(3.5) = 1.917$.

E7) The difference table for given problem is:

X	f(x)	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
1.3	3.669				
		0.813			
1.5	4.482		0.179		
		0.992		0.41	
1.7	5.474		0.220		0.007
		1.212		0.48	
1.9	6.686		0.268		0.012
		1.480		0.060	
2.1	8.166		0.328		0.012
		1.8.08		0.072	
2.3	9.974		0.400		
		2.208			
2.5	12.182				

Taking $x_0 = 1.5$ we see that s = 0 and we obtain from the interpolation formula

$$f'(1.5) = \frac{1}{h}\left[\Delta f_0 - \frac{\Delta^2 f_0}{2} + \frac{\Delta^3 f_0}{3} - \frac{\Delta^4 f_0}{4} + \ldots\right]$$

$$= \left[0.992 - \frac{0.220}{2} + \frac{0.048}{3} - \frac{0.012}{4}\right] = 4.475$$

Exact value is $e^{1.5} = 4.4817$ and error is = 0.0067

E8) Use the $0(h^2)$ formula (33). With h = 0.1 $f''(0.6) = 1.2596$, h = 0.2, $f''(0.6) = 1.26545$, h = 0.4, $f''(0.6) = 1.289394$.

E9) Using (24) with h = 0.1, we have $f'(0.3) = -3.8$

and with h = 0.2, $f''(0.3) = -3.575$