addition to the truncation error introduced by the methods themselves. Therefore, we also discuss the errors and ways to minimise them.

11.2 DIFFERENTIATING CONTINUOUS FUNCTIONS

We discuss here the numerical process of approximating the derivative $f'(x)$ of a function $f(x)$, when the function itself is available.

Forward Difference Quotient

Consider a small increment $\Delta x = h$ in x. According to Taylor's theorem, we have

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\theta) \tag{11.1}$$

for $x \leq \theta \leq x + h$. By rearranging the terms, we get

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\theta) \tag{11.2}$$

Thus, if h is chosen to be sufficiently small, $f'(x)$ can be approximated by

F.

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h}} \tag{11.3}$$

with a truncation error of

$$\boxed{E_t(h) = -\frac{h}{2} f''(\theta)} \tag{11.4}$$

Equation (11.3) is called the first order *forward difference quotient*. This is also known as *two-point formula*. The truncation error is in the order of h and can be decreased by decreasing h.

Similarly, we can show that the first-order *backward difference quotient* is

B

$$\boxed{f'(x) = \frac{f(x) - f(x-h)}{h}} \tag{11.5}$$

Example 11.1

Estimate approximate derivative of $f(x) = x^2$ at $x = 1$, for $h = 0.2, 0.1, 0.05$ and 0.01 using the first-order forward difference formula.

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

Therefore,

$$f'(1) = \frac{f(1+h) - f(1)}{h}$$

Derivative approximations are tabulated below:

h	$f'(1)$	*Error*
0.2	2.2	0.2
0.1	2.1	0.1
0.05	2.05	0.05
0.01	2.01	0.01

Note that the correct answer is 2. The derivative approximation approaches the exact value as h decreases. The truncation error decreases proportionally with decrease in h. There is no roundoff error.

Central Difference Quotient

Note that Eq. (11.3) was obtained using the linear approximation to $f(x)$. This would give large truncation errors if the functions were of higher order. In such cases, we can reduce truncation errors for a given h by using a quadratic approximation, rather than a linear one. This can be achieved by taking another term in Taylor's expansion, i.e.,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(\theta_1) \tag{11.6}$$

Similarly,

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(\theta_1) \tag{11.7}$$

Subtracting Eq. (11.7) from Eq. (11.6), we obtain

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3!}[f'''(\theta_1) + f'''(\theta_2)] \tag{11.8}$$

Thus, we have

$$\boxed{f'(x) = \frac{f(x+h) - f(x-h)}{2h}} \tag{11.9}$$

with the truncation error of

$$E_t(h) = -\frac{h^2}{12}[f'''(\theta_1) + f'''(\theta_2)] = -\frac{h^2}{6}f'''(\theta)$$

which is of order h^2. Equation (11.9) is called the second-order *central difference quotient*. Note that this is the average of the forward difference quotient and the backward difference quotient. This is also known as *three-point formula*. The distinction between the two-point and three-point formulae is illustrated in Fig. 11.1(a) and Fig. 11.1(b). Note that the approximation is better in the case of three-point formula.

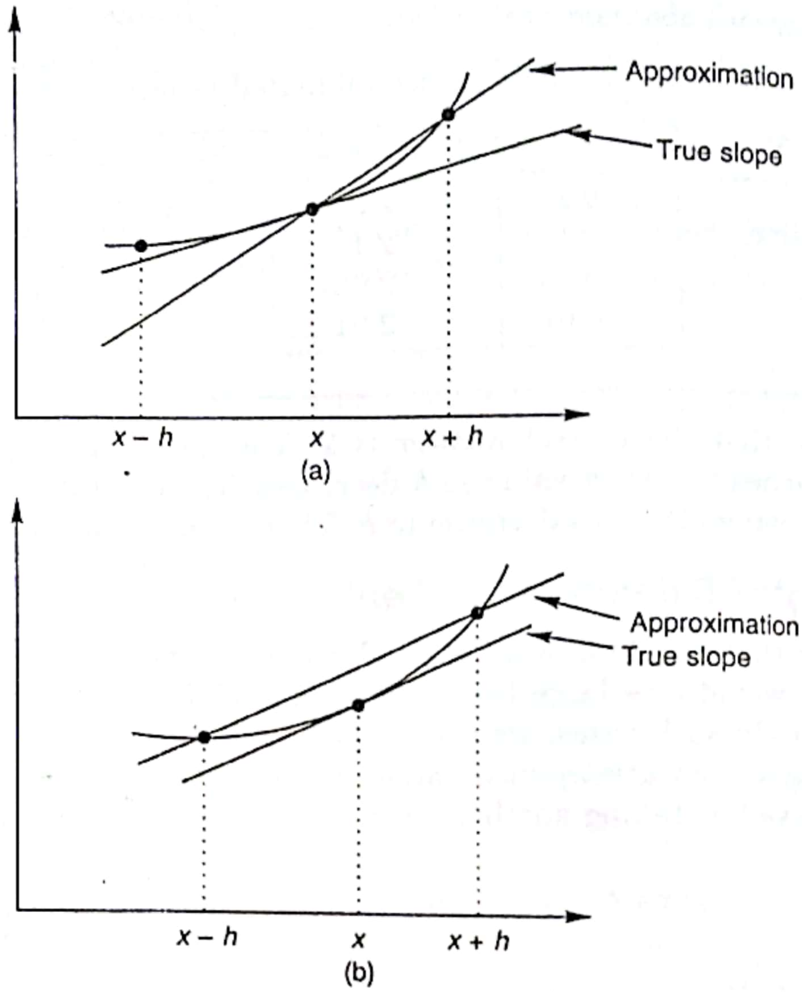

Fig. 11.1 Illustration of (a) Two-point formula and (b) Three-point formula

Example 11.2

Repeat the exercise given in Example 11.1 for the three-point formula.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

Therefore,

$$f'(1) = \frac{f(1+h) - f(1-h)}{2h}$$

The derivative approximations are tabulated below:

h	$f'(1)$	*Error*
0.2	2.0	0
0.1	2.0	0
0.05	2.0	0

The derivative is exact for all values of h. This is because we have used quadratic approximation for a quadratic function. We can also derive further higher-order derivatives by using more points in the formula. For example, the *five-point central difference formula* is given by

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} \tag{11.10}$$

This is a fourth-order approximation and the truncation error is of order h^4. In this case, the truncation error will approach zero much faster compared to the three-point approximation. The derivation of Eq. (11.10) is left to the reader as an exercise. (*Hint: use step size 2h instead of h in Eq. (11.8) and use up to fifth derivative of Taylor's expansion*).

Error Analysis

As mentioned earlier, numerical differentiation is very sensitive to roundoff errors. If $E_r(h)$ is the roundoff error introduced in an approximate derivative, then the total error is given by

$$E(h) = E_r(h) + E_t(h)$$

Let us consider the two-point formula for the purpose of analysis. That is,

$$f'(x) = \frac{f(x+h) - f(x)}{h} = \frac{f_1 - f_0}{h}$$

If we assume the roundoff errors in f_1 and f_0 as e_1 and e_0, respectively, then

$$f'(x) = \frac{(f_1 + e_1) - (f_0 + e_0)}{h}$$

$$= \frac{f_1 - f_0}{h} + \frac{e_1 - e_0}{h}$$

If the errors e_1 and e_0 are of the magnitude e and of opposite sign (i.e., the worst case) then we get the bound for roundoff error as

$$|E_r(h)| \le \frac{2e}{h}$$

We know that the truncation error for two-point formula is

$$|E_t(h)| = -\frac{h}{2} f''(\theta)$$

or

$$|E_t(h)| \le \frac{M_2 h}{2}$$

where M_2 is the bound given by

$$M_2 = \max_{x \le \theta \le x+h} |f''(\theta)|$$

Thus, the bound for total error in the derivative is

$$\boxed{|E(h)| \le \frac{M_2 h}{2} + \frac{2e}{h}} \tag{11.11}$$

Note that when the step size h is increased, the truncation error increases while the roundoff error decreases. This is illustrated in Fig. 11.2. For small values of h, roundoff error has an overriding influence on the total error. Therefore, while reducing the step size, we should exercise proper judgement in choosing the size. This argument applies to all the formulae discussed here.

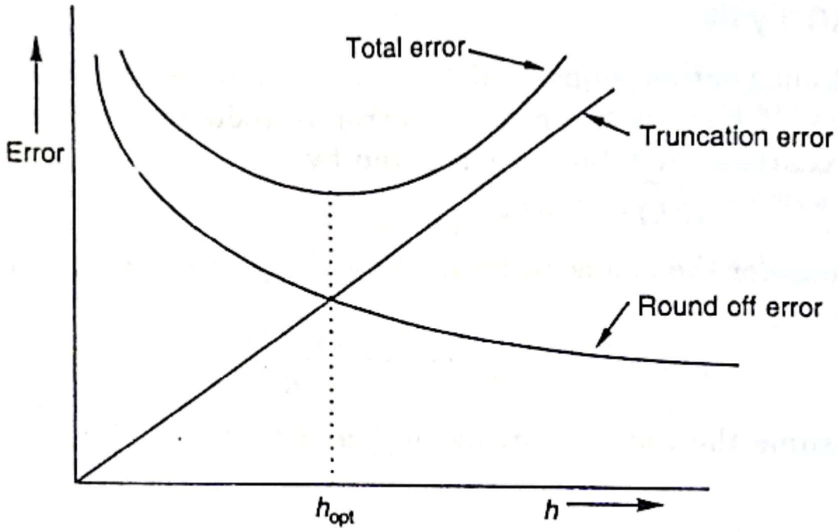

Fig. 11.2 Error in derivatives as a function of h

We can obtain a rough estimate of h that gives the minimum error. By differentiating Eq. (11.11) with respect to h, we obtain

$$E'(h) = \frac{M_2}{2} - \frac{2e}{h^2}$$

We know that $E(h)$ is minimum when $E'(h) = 0$. That is,

$$\frac{M_2}{2} - \frac{2e}{h^2} = 0$$

Solving for h, we obtain

$$h_{opt} = 2\sqrt{\frac{e}{M_2}} \tag{11.12}$$

Substituting this in Eq. (11.11), we get

$$E(h_{opt}) = 2\sqrt{eM_2} \tag{11.13}$$

Example 11.3

Compute the approximate derivatives of $f(x) = \sin x$, at $x = 0.45$ radians, at increasing values of h from 0.01 to 0.04, with a step size of 0.005. Analyse the total error. What is the optimum step size?

$$f(x) = \sin x$$

Using two-point formula

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

Given

$$x = 0.45 \text{ radians}$$

So, $f(x) = \sin(0.45) = 0.4350$ (rounded to four digits). Exact $f'(x) = \cos x = \cos(0.45) = 0.9004$.

Table below gives the approximate derivatives of $\sin x$ at $x = 0.45$ using various values of h.

h	$f(x+h)$	$f'(x)$	*Error*
0.010	0.4439	0.8900	0.0104
0.015	0.4484	0.8933	0.0071
0.020	0.4529	0.8950	0.0054
0.025	0.4573	0.8935	0.0069
0.030	0.4618	0.8933	0.0071
0.035	0.4662	0.8914	0.0090
0.040	0.4706	0.8900	0.0104

The table shows that the total error decreases from 0.0104 (at $h = 0.01$) till $h = 0.02$ and again increases when h is increased as illustrated in Fig. 11.2.

Since we have used four significant digits, the bound for roundoff error e is 0.5×10^{-4}. For the two-point formula, the bound M_2 is given by

$$M_2 = \max |f''(\theta)|$$

$$0.41 \le \theta \le 0.49$$

$$= |\sin(0.49)| = 0.4706$$

Therefore, the optimum step size is

$$h_{\text{opt}} = 2\sqrt{\frac{e}{M_2}} = 2\sqrt{\frac{0.5 \times 10^{-4}}{0.4706}}$$

$$= 0.0206$$

This agrees very closely with our results.

Higher-order Derivatives

We can also obtain approximations to higher-order derivatives using Taylor's expansion. To illustrate this, we derive here the formula for $f''(x)$. We know that

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + R_1$$

and

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + R_2$$

Adding these two expansions gives

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + R_1 + R_2$$

Therefore

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{(R_1 + R_2)}{h^2}$$

Thus, the approximation to second derivative is

$$\boxed{f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}} \qquad (11.14)$$

The truncation error is

$$E_t(h) = -\frac{R_1 + R_2}{h^2}$$

$$= -\frac{1}{h^2}\cdot\frac{h^4}{4!}\left(f^{(4)}(\theta_1) + f^{(4)}(\theta_2)\right)$$

$$= -\frac{h^2}{12}f^{(4)}(\theta)$$

The error is of order h^2.

Similarly, we can obtain other higher-order derivatives with the errors of order h^3 and h^4.

Example 11.4

Find approximation to second derivative of cos (x) at $x = 0.75$ with $h = 0.01$. *Compare with the* true value.

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

$$f''(0.75) = \frac{f(0.76) - 2f(0.75) + f(0.74)}{0.0001} \quad (\text{at } h = 0.01)$$

$$= \frac{0.7248360 - 2(0.7316888) + 0.7384685}{0.0001}$$

$$= \frac{1.4633046 - 1.4633776}{0.0001}$$

$$= -0.7300000$$

Exact value of $f''(0.75) = -\cos(0.75)$

$$= -0.7316888$$

Error $= -0.0016888$

This error includes roundoff error as well.

11.3 DIFFERENTIATING TABULATED FUNCTIONS

Suppose that we are given a set of data points (x_i, f_i), $i = 0, 1, \ldots n$ which correspond to the values of an unknown function $f(x)$ and we wish to estimate the derivatives at these points. Assume that the points are equally spaced with a step size of h.

When function values are available in tabulated form, we may approximate this function by an interpolation polynomial $p(x)$ discussed in Chapter 9 and then differentiate $p(x)$. We will use here Newton's divided difference interpolation polynomial.

Let us first consider the linear equation

$$p_1(x) = a_0 + a_1(x - x_0) + R_1$$

where R_1 is the remainder term used for estimation. Upon differentiation of this formula, we obtain

$$p_1'(x) = a_1 + \frac{dR_1}{dx}$$

Then the approximate derivative of the function $f(x)$ is given by

$$f'(x) = p_1'(x) = a_1$$

We know that

$$a_1 = f[x_0, x_1]$$

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

On substituting

$$h = x_1 - x_0$$

$$x_1 = x + h$$

$$x_0 = x$$

we get

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h}} \qquad (11.15)$$