Numerical Differentiation

6.1 Approximating The Derivative

The Limit of the Difference Quotient

We now turn our attention to the numerical process for approximating the derivative of $f(x)$:

(1) $$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

The method seems straightforward; choose a sequence $\{h_k\}$ so that $h_k \to 0$ and compute the limit of the sequence:

(2) $$D_k = \frac{f(x+h_k) - f(x)}{h_k} \quad \text{for } k = 1, 2, \ldots, n, \ldots.$$

For example, consider the function $f(x) = e^x$ and use the step sizes $h = 1$, $1/2$, and $1/4$ to construct the secant lines between the points $(0, 1)$ and $(h, f(h))$, respectively. As h gets small, the secant line approaches the tangent line as shown in Figure 6.2. Although Figure 6.2 gives a good visualization of the process described in (1), we must make numerical computations with $h = 0.00001$ to get an acceptable numerical answer, and for this value of h the graphs of the tangent line and secant line would be indistinguishable.

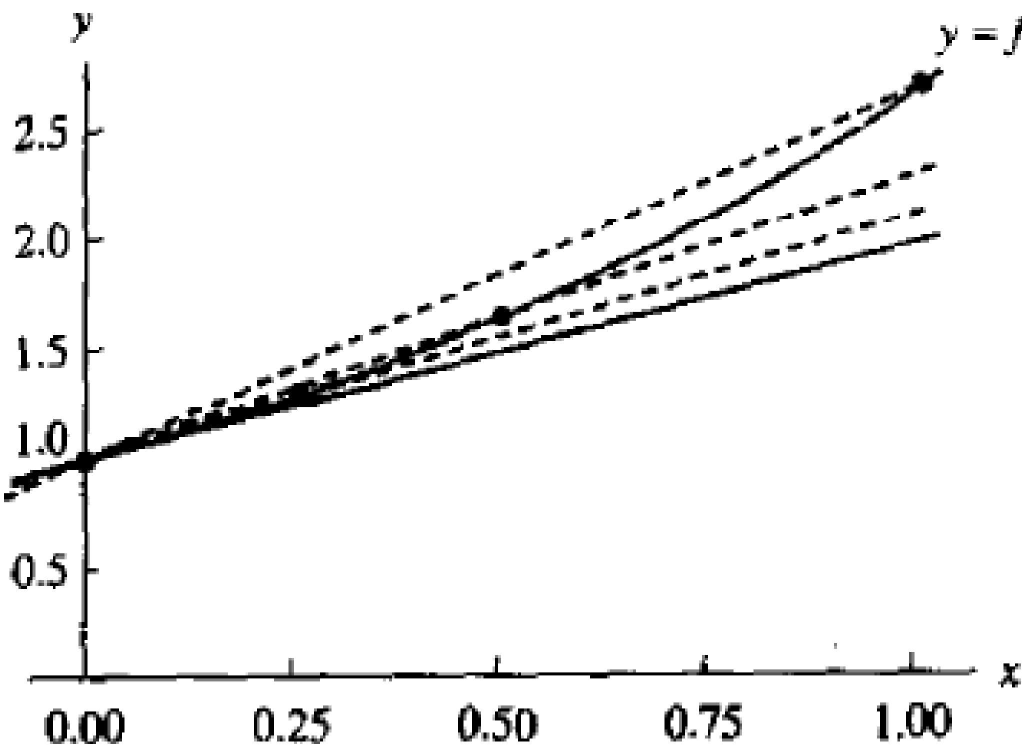

Figure 6.2 Several secant line for $y = e^x$.

Example 6.1. Let $f(x) = e^x$ and $x = 1$. Compute the difference quotients D_k using the step sizes $h_k = 10^{-k}$ for $k = 1, 2, \ldots, 10$. Carry out nine decimal places in all calculations.

A table of the values $f(1 + h_k)$ and $(f(1 + h_k) - f(1))/h_k$ that are used in the computation of D_k is shown in Table 6.1. ■

Table 6.1 Finding the Difference Quotients $D_k = (e^{1+h_k} - e)/h_k$

h_k	$f_k = f(1 + h_k)$	$f_k - e$	$D_k = (f_k - e)/h_k$
$h_1 = 0.1$	3.004166024	0.285884196	2.858841960
$h_2 = 0.01$	2.745601015	0.027319187	2.731918700
$h_3 = 0.001$	2.721001470	0.002719642	2.719642000
$h_4 = 0.0001$	2.718553670	0.000271842	2.718420000
$h_5 = 0.00001$	2.718309011	0.000027183	2.718300000
$h_6 = 10^{-6}$	2.718284547	0.000002719	2.719000000
$h_7 = 10^{-7}$	2.718282100	0.000000272	2.720000000
$h_8 = 10^{-8}$	2.718281856	0.000000028	2.800000000
$h_9 = 10^{-9}$	2.718281831	0.000000003	3.000000000
$h_{10} = 10^{-10}$	2.718281828	0.000000000	0.000000000

The largest value $h_1 = 0.1$ does not produce a good approximation $D_1 \approx f'(1)$, because the step size h_1 is too large and the difference quotient is the slope of the secant line through two points that are not close enough to each other. When formula (2) is used with a fixed precision of nine decimal places, h_9 produced the approximation $D_9 = 3$ and h_{10} produced $D_{10} = 0$. If h_k is too small, then the computed function values $f(x + h_k)$ and $f(x)$ are very close together. The difference $f(x + h_k) - f(x)$ can exhibit the problem of loss of significance due to the subtraction of quantities that are nearly equal. The value $h_{10} = 10^{-10}$ is so small that the stored values of $f(x + h_{10})$ and $f(x)$ are the same, and hence the computed difference quotient is zero.

In Example 6.1 the mathematical value for the limit is $f'(1) \approx 2.718281828$. Observe that the value $h_5 = 10^{-5}$ gives the best approximation, $D_5 = 2.7183$.

Example 6.1 shows that it is not easy to find numerically the limit in equation (2). The sequence starts to converge to e, and D_5 is the closest; then the terms move away from e. In Program 6.1 it is suggested that terms in the sequence $\{D_k\}$ should be computed until $|D_{N+1} - D_N| \geq |D_N - D_{N-1}|$. This is an attempt to determine the best approximation before the terms start to move away from the limit. When this criterion is applied to Example 6.1, we have $0.0007 = |D_6 - D_5| > |D_5 - D_4| = 0.00012$; hence D_5 is the answer we choose. We now proceed to develop formulas that give a reasonable amount of accuracy for larger values of h.

The Central-difference Formulas

If the function $f(x)$ can be evaluated at values that lie to the left and right of x, then the best two-point formula will involve abscissas that are chosen symmetrically on both sides of x.

Theorem 6.1 (Centered Formula of Order $O(h^2)$). Assume that $f \in C^3[a, b]$ and that $x - h, x, x + h \in [a, b]$. Then

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}. \tag{3}$$

Furthermore, there exists a number $c = c(x) \in [a, b]$ such that

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} + E_{\text{trunc}}(f, h), \tag{4}$$

where

$$E_{\text{trunc}}(f, h) = -\frac{h^2 f^{(3)}(c)}{6} = O(h^2).$$

The term $E(f, h)$ is called the ***truncation error***.

Proof. Start with the second-degree Taylor expansions $f(x) = P_2(x) + E_2(x)$, about x, for $f(x+h)$ and $f(x-h)$:

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(c_1)h^3}{3!} \tag{5}$$

and

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(c_2)h^3}{3!}. \tag{6}$$

After (6) is subtracted from (5), the result is

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{((f^{(3)}(c_1) + f^{(3)}(c_2))h^3}{3!}. \tag{7}$$

Since $f^{(3)}(x)$ is continuous, the intermediate value theorem can be used to find a value c so that

$$\frac{f^{(3)}(c_1) + f^{(3)}(c_2)}{2} = f^{(3)}(c). \tag{8}$$

This can be substituted into (7) and the terms rearranged to yield

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f^{(3)}(c)h^2}{3!}. \tag{9}$$

The first term on the right side of (9) is the central-difference formula (3), the second term is the truncation error, and the proof is complete. •

1. Let $f(x) = \sin(x)$, where x is measured in radians.

   (a) Calculate approximations to $f'(0.8)$ using formula (3) with $h = 0.1$, $h = 0.01$, and $h = 0.001$. Carry eight or nine decimal places.

   (b) Compare with the value $f'(0.8) = \cos(0.8)$.

   (c) Compute bounds for the truncation error (4). Use

$$|f^{(3)}(c)| \leq \cos(0.7) \approx 0.764842187$$

   for all cases.

2. Let $f(x) = e^x$.

   (a) Calculate approximations to $f'(2.3)$ using formula (3) with $h = 0.1$, $h = ($ and $h = 0.001$. Carry eight or nine decimal places.

   (b) Compare with the value $f'(2.3) = e^{2.3}$.

   (c) Compute bounds for the truncation error (4). Use

$$|f^{(3)}(c)| \leq e^{2.4} \approx 11.02317638$$

3. Let $f(x) = \sin(x)$, where x is measured in radians.

(a) Calculate approximations to $f'(0.8)$ using formula (10) with $h = 0.1$ and $h = 0.01$, and compare with $f'(0.8) = \cos(0.8)$.

(b) Use the extrapolation formula in (29) to compute the approximations to $f'(0.8)$ in part (a).

(c) Compute bounds for the truncation error (11). Use

$$|f^{(5)}(c)| \le \cos(0.6) \approx 0.825335615$$

for both cases.

4. Let $f(x) = e^x$.

(a) Calculate approximations to $f'(2.3)$ using formula (10) with $h = 0.1$ and $h = 0.01$, and compare with $f'(2.3) = e^{2.3}$.

(b) Use the extrapolation formula in (29) to compute the approximations to $f'(2.3)$ in part (a).

(c) Compute bounds for the truncation error (11). Use

$$|f^{(5)}(c)| \le e^{2.5} \approx 12.18249396$$

for both cases.