Theorem 6.2 (Centered Formula of Order $O(h^4)$). Assume that $f \in C^5[a, b]$ and that $x - 2h, x - h, x, x + h, x + 2h \in [a, b]$. Then

$$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} \tag{10}$$

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

(11)

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + E_{\text{trunc}}(f, h),$$

where

$$E_{\text{trunc}}(f, h) = \frac{h^4 f^{(5)}(c)}{30} = O(h^4).$$

Proof. One way to derive formula (10) is as follows. Start with the difference between the fourth-degree Taylor expansions $f(x) = P_4(x) + E_4(x)$, about x, of $f(x+h)$ and $f(x-h)$:

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{2f^{(3)}(x)h^3}{3!} + \frac{2f^{(5)}(c_1)h^5}{5!} \tag{12}$$

Then use the step size $2h$, instead of h, and write down the following approximation:

$$f(x+2h) - f(x-2h) = 4f'(x)h + \frac{16f^{(3)}(x)h^3}{3!} + \frac{64f^{(5)}(c_2)h^5}{5!}. \tag{13}$$

Next multiply the terms in equation (12) by 8 and subtract (13) from it. The terms involving $f^{(3)}(x)$ will be eliminated and we get

$$\begin{aligned} &-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h) \\ &\qquad = 12f'(x)h + \frac{(16f^{(5)}(c_1) - 64f^{(5)}(c_2))h^5}{120} \end{aligned} \tag{14}$$

If $f^{(5)}(x)$ has one sign and if its magnitude does not change rapidly, we can find a value c that lies in $[x-2h, x+2h]$ so that

$$16 f^{(5)}(c_1) - 64 f^{(5)}(c_2) = -48 f^{(5)}(c). \tag{15}$$

After (15) is substituted into (14) and the result is solved for $f'(x)$, we obtain

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + \frac{f^{(5)}(c)h^4}{30}. \tag{16}$$

The first term on the right side of (16) is the central-difference formula (10), and the second term is the truncation error, the theorem is proved. •

Example 6.2. Let $f(x) = \cos(x)$

(a) Use formulas (3) and (10) with step sizes $h = 0.1, 0.01, 0.001$, and 0.0001, and calculate approximations for $f'(0.8)$. Carry nine decimal places in all the calculations.

(b) Compare with the true value $f'(0.8) = -\sin(0.8)$.

(a) Using formula (3) with $h = 0.01$, we get

$$f'(0.8) \approx \frac{f(0.81) - f(0.79)}{0.02} \approx \frac{0.689498433 - 0.703845316}{0.02} \approx -0.717344150.$$

Using formula (10) with $h = 0.01$, we get

$$\begin{aligned} f'(0.8) &\approx \frac{-f(0.82) + 8f(0.81) - 8f(0.79) + f(0.78)}{0.12} \\ &\approx \frac{-0.682221207 + 8(0.689498433) - 8(0.703845316) + 0.710913538}{0.12} \\ &\approx -0.717356108. \end{aligned}$$

Table 6.2 Numerical Differentiation Using Formulas (3) and (10)

Step size	Approximation by formula (3)	Error using formula (3)	Approximation by formula (10)	Error using formula (10)
0.1	−0.716161095	−0.001194996	−0.717353703	−0.000002389
0.01	−0.717344150	−0.000011941	−0.717356108	0.000000017
0.001	−0.717356000	−0.000000091	−0.717356167	0.000000076
0.0001	−0.717360000	−0.000003909	−0.717360833	0.000004742

(b) The error in approximation for formulas (3) and (10) turns out to be −0.000011941 and 0.000000017, respectively. In this example, formula (10) gives a better approximation to $f'(0.8)$ than formula (3) when $h = 0.01$. The error analysis will illuminate this example and show why this happened . The other calculations are summarized in Table 6.2. ■

Error Analysis and Optimum Step Size

An important topic in the study of numerical differentiation is the effect of the computer's round-off error. Let us examine the formulas more closely. Assume that a computer is used to make numerical computations and that

$$f(x_0 - h) = y_{-1} + e_{-1} \quad \text{and} \quad f(x_0 + h) = y_1 + e_1,$$

where $f(x_0 - h)$ and $f(x_0 + h)$ are approximated by the numerical values y_{-1} and y_1 and e_{-1} and e_1 are the associated round-off errors, respectively. The following result indicates the complex nature of error analysis for numerical differentiation.

Corollary 6.1(a). Assume that f satisfies the hypotheses of Theorem 6.1 and use the ***computational formula***

$$f'(x_0) \approx \frac{y_1 - y_{-1}}{2h}. \tag{17}$$

The error analysis is explained by the following equations:

$$f'(x_0) = \frac{y_1 - y_{-1}}{2h} + E(f, h) \tag{18}$$

where

$$\begin{aligned} E(f, h) &= E_{\text{round}}(f, h) + E_{\text{trunc}}(f, h) \\ &= \frac{e_1 - e_{-1}}{2h} - \frac{h^2 f^{(3)}(c)}{6}, \end{aligned} \tag{19}$$

where the ***total error term*** $E(f, h)$ has a part due to round-off error plus a part due to truncation error.

Corollary 6.1(b). Assume that f satisfies the hypotheses of Theorem 6.1 and that numerical computations are made. If $|e_{-1}| \le \epsilon$, $|e_1| \le \epsilon$, and $M = \max_{a \le x \le b}\{|f^{(3)}(x)|\}$, then

$$|E(f,h)| \le \frac{\epsilon}{h} + \frac{Mh^2}{6}, \tag{20}$$

and the value of h that minimizes the right-hand side of (19) is

$$h = \left(\frac{3\epsilon}{M}\right)^{1/3}. \tag{21}$$

Proof. (Paint)

When h is small, the portion of (19) involving $(e_1 - e_{-1})/2h$ can be relatively large. In Example 6.2, when $h = 0.0001$, this difficulty was encountered. The round-off errors are

$$f(0.8001) = 0.696634970 + e_1 \qquad \text{where } e_1 \approx -0.0000000003$$
$$f(0.7999) = 0.696778442 + e_{-1} \qquad \text{where } e_{-1} \approx 0.0000000005.$$

The truncation error term is

$$\frac{-h^2 f^{(3)}(c)}{6} \approx -(0.0001)^2 \left(\frac{\sin(0.8)}{6}\right) \approx 0.000000001.$$

The error term $E(f, h)$ in (19) can now be estimated:

$$\begin{aligned} E(f,h) &\approx \frac{-0.0000000003 - 0.0000000005}{0.0002} - 0.000000001 \\ &= -0.000004001. \end{aligned}$$

Indeed, the computed numerical approximation for the derivative using $h = 0.0001$ is found by the calculation

$$\begin{aligned} f'(0.8) &\approx \frac{f(0.8001) - f(0.7999)}{0.0002} = \frac{0.696634970 - 0.696778442}{0.0002} \\ &= -0.717360000, \end{aligned}$$

and a loss of about four significant digits is evident. The error is -0.000003909 and this is close to the predicted error, -0.000004001.

When formula (21) is applied to Example 6.2, we can use the bound $|f^{(3)}(x)| \leq |\sin(x)| \leq 1 = M$ and the value $\epsilon = 0.5 \times 10^{-9}$ for the magnitude of the round-off error. The optimal value for h is easily calculated: $h = (1.5 \times 10^{-9}/1)^{1/3} \approx 0.001144714$. The step size $h = 0.001$ was closest to the optimal value 0.001144714 and it gave the best approximation to $f'(0.8)$ among the four choices involving formula (3) (see Table 6.2 and Figure 6.3).

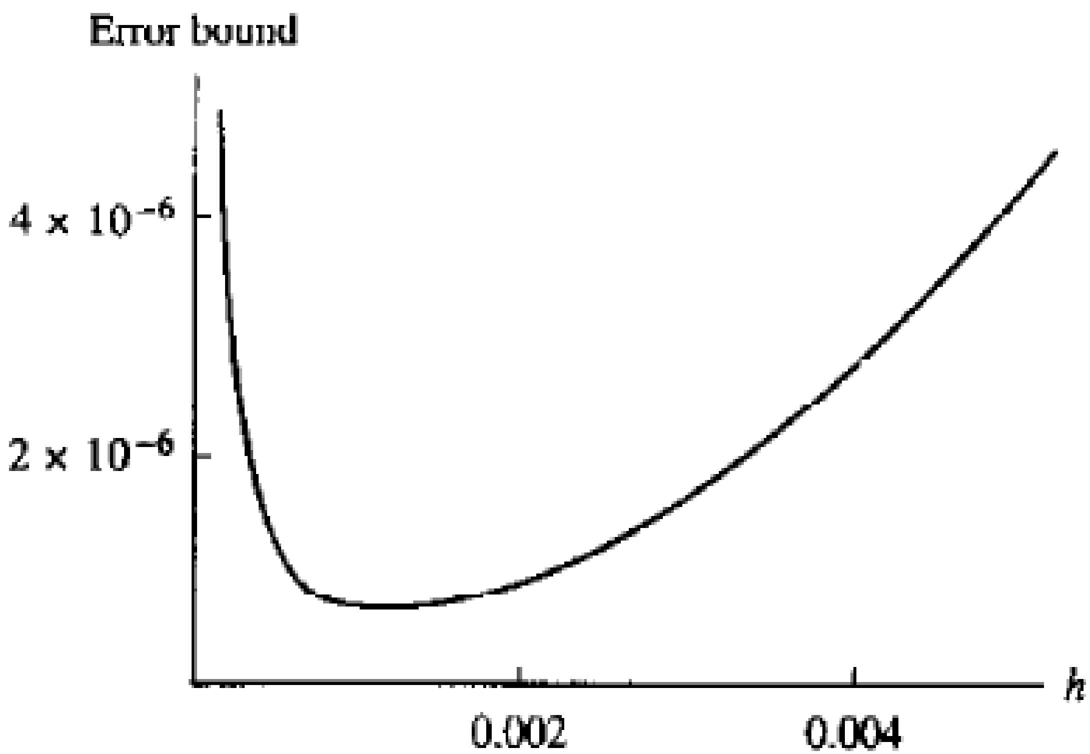

Figure 6.3 Finding the optimum step size $h \approx 0.001144714$ when formula (21) is applied to $f(x) = \cos(x)$ in Example 6.2.

More Central-difference Formulas

The formulas for $f'(x_0)$ in the preceding section required that the function can be computed at abscissas that lie on both sides of x, and they were referred to as central-difference formulas. Taylor series can be used to obtain central-difference formulas for the higher derivatives. The popular choices are those of order $O(h^2)$ and $O(h^4)$ and are given in Tables 6.3 and 6.4. In these tables we use the convention that $f_k = f(x_0+kh)$ for $k = -3, -2, -1, 0, 1, 2, 3$.

For illustration, we will derive the formula for $f''(x)$ of order $O(h^2)$ in Table 6.3 Start with the Taylor expansions

$$(1) \qquad f(x+h) = f(x) + hf'(x) + \frac{h^2 f''(x)}{2} + \frac{h^3 f^{(3)}(x)}{6} + \frac{h^4 f^{(4)}(x)}{24} + \cdots$$

and

$$(2) \qquad f(x-h) = f(x) - hf'(x) + \frac{h^2 f''(x)}{2} - \frac{h^3 f^{(3)}(x)}{6} + \frac{h^4 f^{(4)}(x)}{24} - \cdots .$$

Adding equations (1) and (2) will eliminate the terms involving the odd derivatives $f'(x), f^{(3)}(x), f^{(5)}(x), \ldots$:

$$f(x+h) + f(x-h) = 2f(x) + \frac{2h^2 f''(x)}{2} + \frac{2h^4 f^{(4)}(x)}{24} + \cdots. \tag{3}$$

Solving equation (3) for $f''(x)$ yields

$$\begin{aligned} f''(x) = {} & \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{2h^2 f^{(4)}(x)}{4!} \\ & - \frac{2h^4 f^{(6)}(x)}{6!} - \cdots - \frac{2h^{2k-2} f^{(2k)}(x)}{(2k)!} - \cdots. \end{aligned} \tag{4}$$

If the series in (4) is truncated at the fourth derivative, there exists a value c that lies in $[x-h, x+h]$ so that

$$f''(x_0) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} - \frac{h^2 f^{(4)}(c)}{12}. \tag{5}$$

This gives us the desired formula for approximating $f''(x)$:

$$f''(x_0) \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}. \tag{6}$$

Error Analysis

Let $f_k = y_k + e_k$, where e_k is the error in computing $f(x_k)$, including noise in measurement and round-off error. Then formula (6) can be written

(7) $$f''(x_0) = \frac{y_1 - 2y_0 + y_{-1}}{h^2} + E(f, h).$$

The error term $E(h, f)$ for the numerical derivative (7) will have a part due to round-off error and a part due to truncation error:

(8) $$E(f, h) = \frac{e_1 - 2e_0 + e_{-1}}{h^2} - \frac{h^2 f^{(4)}(c)}{12}.$$

If it is assumed that each error e_k is of the magnitude ϵ, with signs that accumulate errors, and that $|f^{(4)}(x)| \le M$, then we get the following error bound:

(9) $$|E(f, h)| \le \frac{4\epsilon}{h^2} + \frac{Mh^2}{12}.$$

If h is small, then the contribution $4\epsilon/h^2$ due to round-off error is large. When h is large, the contribution $Mh^2/12$ is large. The optimum step size will minimize the quantity

(10) $$g(h) = \frac{4\epsilon}{h^2} + \frac{Mh^2}{12}.$$

Setting $g'(h) = 0$ results in $-8\epsilon/h^3 + Mh/6 = 0$, which yields the equation $h^4 = 48\epsilon/M$, from which we obtain the optimal value:

(11) $$h = \left(\frac{48\epsilon}{M}\right)^{1/4}$$

Example 6.4. Let $f(x) = \cos(x)$.

(**a**) Use formula (6) with $h = 0.1$, 0.01, and 0.001 and find approximations to $f''(0.8)$. Carry nine decimal places in all calculations.

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

(**a**) The calculation for $h = 0.01$ is

$$\begin{aligned} f''(0.8) &\approx \frac{f(0.81) - 2f(0.80) + f(0.79)}{0.0001} \\ &\approx \frac{0.689498433 - 2(0.696706709) + 0.703845316}{0.0001} \\ &\approx -0.696690000. \end{aligned}$$

(**b**) The error in this approximation is -0.000016709. The other calculations are summarized in Table 6.5. The error analysis will illuminate this example and show why $h = 0.01$ was best. ■

Table 6.5 Numerical Approximations to $f''(x)$ for Example 6.4

Step size	Approximation by formula (6)	Error using formula (6)
$h = 0.1$	-0.696126300	-0.000580409
$h = 0.01$	-0.696690000	-0.000016709
$h = 0.001$	-0.696000000	-0.000706709

When formula (11) is applied to Example 6.4, use the bound $|f^{(4)}(x)| \le |\cos(x)| \le 1 = M$ and the value $\epsilon = 0.5 \times 10^{-9}$. The optimal step size is $h = (24 \times 10^{-9}/1)^{1/4} = 0.01244666$, and we see that $h = 0.01$ was closest to the optimal value.

Table 6.3 Central-difference Formulas of Order $O(h^2)$

$$f'(x_0) \approx \frac{f_1 - f_{-1}}{2h}$$

$$f''(x_0) \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}$$

$$f^{(3)}(x_0) \approx \frac{f_2 - f_1 + 2f_{-1} - f_{-2}}{2h^3}$$

$$f^{(4)}(x_0) \approx \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4}$$

Table 6.4 Central-difference Formulas of Order $O(h^4)$

$$f'(x_0) \approx \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}$$

$$f''(x_0) \approx \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2}$$

$$f^{(3)}(x_0) \approx \frac{-f_3 + 8f_2 - 13f_1 + 13f_{-1} - 8f_{-2} + f_{-3}}{8h^3}$$

$$f^{(4)}(x_0) \approx \frac{-f_3 + 12f_2 - 39f_1 + 56f_0 - 39f_{-1} + 12f_{-2} - f_{-3}}{6h^4}$$

Table 6.7 Forward- and Backward-difference Formulas of Order $O(h^2)$

$f'(x_0) \approx \dfrac{-3f_0 + 4f_1 - f_2}{2h}$	$\begin{pmatrix}\text{forward}\\ \text{difference}\end{pmatrix}$
$f'(x_0) \approx \dfrac{3f_0 - 4f_{-1} + f_{-2}}{2h}$	$\begin{pmatrix}\text{backward}\\ \text{difference}\end{pmatrix}$
$f''(x_0) \approx \dfrac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2}$	$\begin{pmatrix}\text{forward}\\ \text{difference}\end{pmatrix}$
$f''(x_0) \approx \dfrac{2f_0 - 5f_{-1} + 4f_{-2} - f_{-3}}{h^2}$	$\begin{pmatrix}\text{backward}\\ \text{difference}\end{pmatrix}$

Exercises for Numerical Differentiation Formulas

1. Let $f(x) = \ln(x)$ and carry eight or nine decimal places.
   (a) Use formula (6) with $h = 0.05$ to approximate $f''(5)$.
   (b) Use formula (6) with $h = 0.01$ to approximate $f''(5)$.
   (c) Use formula (12) with $h = 0.1$ to approximate $f''(5)$.
   (d) Which answer, (a), (b), or (c), is most accurate?
2. Let $f(x) = \cos(x)$ and carry eight or nine decimal places.
   (a) Use formula (6) with $h = 0.05$ to approximate $f''(1)$.
   (b) Use formula (6) with $h = 0.01$ to approximate $f''(1)$.
   (c) Use formula (12) with $h = 0.1$ to approximate $f''(1)$.
   (d) Which answer, (a), (b), or (c), is most accurate?
3. Consider the table for $f(x) = \ln(x)$ rounded to four decimal places.

x	$f(x) = \ln(x)$
4.90	1.5892
4.95	1.5994
5.00	1.6094
5.05	1.6194
5.10	1.6292

   (a) Use formula (6) with $h = 0.05$ to approximate $f''(5)$.
   (b) Use formula (6) with $h = 0.01$ to approximate $f''(5)$.
   (c) Use formula (12) with $h = 0.05$ to approximate $f''(5)$
   (d) Which answer, (a), (b), or (c), is most accurate?