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 $\boldsymbol{O(h^2)}$). 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

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

where

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

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. •

Suppose that the value of the third derivative $f^{(3)}(c)$ does not change too rapidly; then the truncation error in (4) goes to zero in the same manner as h^2, which is expressed by using the notation $\boldsymbol{O}(h^2)$. When computer calculations are used, it is not desirable to choose h too small. For this reason it is useful to have a formula for approximating $f'(x)$ that has a truncation error term of the order $\boldsymbol{O}(h^4)$.

Theorem 6.2 (Centered Formula of Order $\boldsymbol{O(h^4)}$). 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

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + E_{\text{trunc}}(f, h), \tag{11}$$

where

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

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

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

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

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

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

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

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. •

Suppose that $|f^{(5)}(c)|$ is bounded for $c \in [a, b]$; then the truncation error in (11) goes to zero in the same manner as h^4, which is expressed with the notation $\boldsymbol{O}(h^4)$. Now we can make a comparison of the two formulas (3) and (10). Suppose that $f(x)$ has five continuous derivatives and that $|f^{(3)}(c)|$ and $|f^{(5)}(c)|$ are about the same. Then the truncation error for the fourth-order formula (10) is $\boldsymbol{O}(h^4)$ and will go to zero faster than the truncation error $\boldsymbol{O}(h^2)$ for the second-order formula (3). This permits the use of a larger step size.

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

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

(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. ■

6.2 Numerical Differentiation Formulas

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 $\boldsymbol{O}(h^2)$ and $\boldsymbol{O}(h^4)$ 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 $\boldsymbol{O}(h^2)$ in Table 6.3. Start with the Taylor expansions

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

Table 6.3 Central-Difference Formulas of Order $\boldsymbol{O}(h^2)$

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

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

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

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

Table 6.4 Central-Difference Formulas of Order $\boldsymbol{O}(h^4)$

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

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

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

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

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 $f'(x)$, $f^{(3)}(x)$, $f^{(5)}(x)$, ...:

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

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

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

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

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

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

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

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

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

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

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:

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

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:

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

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 optimal step size will minimize the quantity

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

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:

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

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.

Since the portion of the error due to round off is inversely proportional to the square of h, this term grows when h gets small. This is sometimes referred to as the ***step-size dilemma***. One partial solution to this problem is to use a formula of higher order so that a larger value of h will produce the desired accuracy. The formula for $f''(x_0)$ of order $\boldsymbol{O}(h^4)$ in Table 6.4 is

$$f''(x_0) = \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2} + E(f, h). \tag{12}$$

The error term for (12) has the form

$$E(f, h) = \frac{16\epsilon}{3h^2} + \frac{h^4 f^{(6)}(c)}{90}, \tag{13}$$

where c lies in the interval $[x - 2h, x + 2h]$. A bound for $|E(f, h)|$ is

$$|E(f, h)| \leq \frac{16\epsilon}{3h^2} + \frac{h^4 M}{90}, \tag{14}$$

where $|f^{(6)}(x)| \leq M$. The optimal value for h is given by the formula

$$h = \left(\frac{240\epsilon}{M}\right)^{1/6}. \tag{15}$$

Example 6.5. Let $f(x) = \cos(x)$.

(a) Use formula (12) with $h = 1.0, 0.1,$ and 0.01 and find approximations to $f''(0.8)$. Carry nine decimal places in all the calculations.

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

(c) Determine the optimal step size.

(a) The calculation for $h = 0.1$ is

$$\begin{aligned}
&f''(0.8)\\
&\quad\approx \frac{-f(1.0) + 16f(0.9) - 30f(0.8) + 16f(0.7) - f(0.6)}{0.12}\\
&\quad\approx \frac{-0.540302306 + 9.945759488 - 20.90120127 + 12.23747499 - 0.825335615}{0.12}\\
&\quad\approx -0.696705958.
\end{aligned}$$

(b) The error in this approximation is -0.000000751. The other calculations are summarized in Table 6.6.

(c) When formula (15) is applied, we can use the bound $|f^{(6)}(x)| \leq |\cos(x)| \leq 1 = M$ and the value $\epsilon = 0.5 \times 10^{-9}$. These values give the optimal step size $h = (120 \times 10^{-9}/1)^{1/6} = 0.070231219$. ∎

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