6
Differentiation

6.1
Problem 1: Numerical Limits

A particle is moving through space, and you record its position as a function of time $x(t)$ in a table. Your **problem** is to determine its velocity $v(t) = dx/dt$ when all you have is this table of x versus t.

6.2
Method: Numeric

You probably did rather well in your first calculus course and feel competent at taking derivatives. However, you probably did not take derivatives of a table of numbers using the elementary definition:

$$\frac{df(x)}{dx} \stackrel{\text{def}}{=} \lim_{h\to 0} \frac{f(x+h)-f(x)}{h} \tag{6.1}$$

In fact, even a computer runs into errors with this kind of limit because it is wrought with subtractive cancellation; the computer's finite word length causes the numerator to fluctuate between 0 and the machine precision ϵ_m as the denominator approaches zero.

6.3
Forward Difference (Algorithm)

The most direct method for numerical differentiation of a function starts by expanding it in a Taylor series. This series advances the function one small step forward:

$$f(x+h) = f(x) + hf'(x) + \tfrac{h^2}{2}f''(x) + \tfrac{h^3}{6}f^{(3)}(x) + \cdots \tag{6.2}$$

Computationyal Physics. Problem Solving with Computers (2nd edn).
Rubin H. Landau, Manuel José Páez, Cristian C. Bordeianu

ISBN: 978-3-527-40626-5

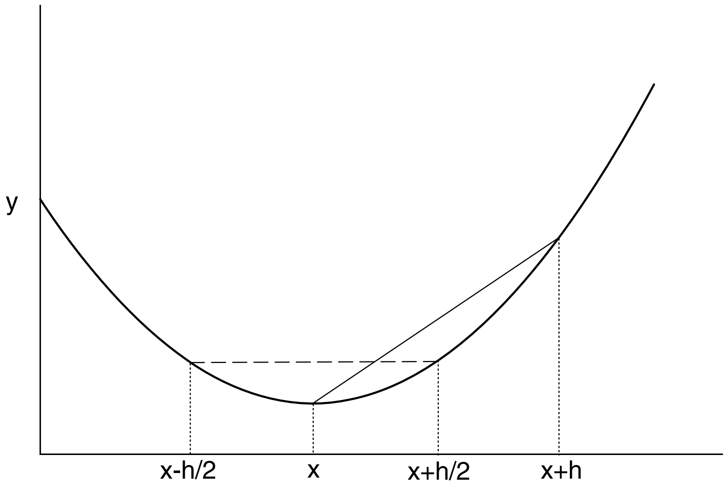

Fig. 6.1 Forward-difference approximation (solid line) and central-difference approximation (dashed line) for the numerical first derivative at point x. The central difference is seen to be more accurate.

where h is the *step size* (Fig. 6.1). We obtain the *forward-difference* derivative algorithm by solving (6.2) for $f'(x)$:

$$f'_{fd}(x) \quad \stackrel{\text{def}}{=} \quad \frac{f(x+h) - f(x)}{h}, \simeq f'(x) + \frac{h}{2} f''(x) + \cdots \tag{6.3}$$

You can think of this approximation as using two points to represent the function by a straight line in the interval from x to $x + h$.

The approximation (6.3) has an error proportional to h (unless the heavens looks down kindly upon you and makes f'' vanish). We can make the approximation error smaller and smaller by making h smaller and smaller. For too small an h, however, precision will be lost through the subtractive cancellation on the LHS of (6.3), and the decreased approximation error becomes irrelevant. As a case in point, let $f(x) = a + bx^2$. The exact derivative is $f' = 2bx$, while the computed derivative is

$$f'_{fd}(x) \approx \frac{f(x+h) - f(x)}{h} = 2bx + bh \tag{6.4}$$

This clearly becomes a good approximation only for small h ($h \ll 2x$).

6.4 Central Difference (Algorithm)

An improved approximation to the derivative starts with the basic definition (6.1). Rather than making a single step of h forward, we form a *central difference* by stepping forward by $h/2$ and backward by $h/2$ (Fig. 6.1):

$$f'_{cd}(x) \stackrel{\text{def}}{=} \frac{f(x+h/2) - f(x-h/2)}{h} = D_{cd}f(x,h) \tag{6.5}$$

where we use the symbol D_{cd} for central difference. When the Taylor series for $f(x \pm h/2)$ are substituted into (6.5), we obtain

$$f'_{cd}(x) \simeq f'(x) + \tfrac{1}{24}h^2 f^{(3)}(x) + \cdots \tag{6.6}$$

The important difference from (6.3) is that when $f(x - h/2)$ is subtracted from $f(x + h/2)$, all terms containing an odd power of h in the Taylor series cancel. Therefore, the central-difference algorithm becomes accurate to one order higher in h, that is, h^2. If the function is well behaved, that is, if $f^{(3)}h^2/24 \ll f^{(2)}h/2$, then you can expect the error with the central-difference method to be smaller than with the forward difference (6.3).

If we now return to our polynomial example (6.4), we find that for this parabola, the central difference gives the exact answer independent of h:

$$f'_{cd}(x) \approx \frac{f(x+h/2) - f(x-h/2)}{h} = 2bx \tag{6.7}$$

6.5 Extrapolated Difference (Method)

Because a differentiation rule based on keeping a certain number of terms in a Taylor series also provides an expression for the error (the terms not included), we can try to reduce the error by being clever. While the central difference (6.5) makes the error term proportional to h vanish, we can make the term proportional to h^2 also vanish by algebraically *extrapolating* from relatively large h, and thus small roundoff error, to $h \to 0$:

$$f'_{ed}(x) \simeq \lim_{h\to 0} D_{cd}f(x,h) \tag{6.8}$$

We introduce the required, additional information by forming the central difference with step size $h/2$:

$$D_{ed}f(x,h/2) \stackrel{\text{def}}{=} \frac{f(x+h/4) - f(x-h/4)}{h/2} \tag{6.9}$$

$$\approx f'(x) + \frac{h^2 f^{(3)}(x)}{96} + \cdots \tag{6.10}$$

We now eliminate the quadratic error term as well as the linear error term in (6.6) by forming the combination

$$f'_{ed}(x) \stackrel{\text{def}}{=} \frac{4D_{cd}f(x,h/2) - D_{cd}f(x,h)}{3} \tag{6.11}$$

$$\approx f'(x) - \frac{h^4 f^{(5)}(x)}{4 \times 16 \times 120} + \cdots \tag{6.12}$$

If $h = 0.4$ and $f^{(5)} \simeq 1$, then there will be only one place of the roundoff error and the truncation error is approximately machine precision ϵ_m; this is the best you can hope for.

A good way of computing (6.11) is to group the terms as

$$f'_{ed}(x) = \frac{1}{3h}\left\{8\left[f(x+\tfrac{h}{4}) - f(x-\tfrac{h}{4})\right] - \left[f(x+\tfrac{h}{2}) - f(x-\tfrac{h}{2})\right]\right\} \tag{6.13}$$

The advantage to (6.13) is that it may reduce the loss of precision that occurs when large and small numbers are added together, only to be subtracted from other large numbers; it is better to first subtract the large numbers from each other and then add the difference to the small numbers.

When working with these and similar higher order methods, it is important to remember that while they may work as designed for well-behaved functions, they may fail badly for functions containing noise, as may result from computations or measurements. If noise is large, it may be better to first fit the data with some analytic function using the techniques of Chap. 8 and then differentiate the fit.

Regardless of the algorithm, the point to remember is that evaluating the derivative of $f(x)$ at x requires you to know the values of f surrounding x. We shall use this same idea when we solve ordinary and partial differential equations.

6.6 Error Analysis (Assessment)

The approximation errors in numerical differentiation decrease with decreasing step size h, while roundoff errors increase with decreasing step size (you have to take more steps and do more calculations). Recall from our discussion in Chap. 3 that the least overall approximation occurs for an h that makes the total error $\epsilon_{\text{approx}} + \epsilon_{\text{ro}}$ a minimum, and that a rough guide this occurs when $\epsilon_{\text{ro}} \approx \epsilon_{\text{approx}}$.

Because differentiation subtracts two numbers close in value, we will assume that the roundoff error for differentiation is machine precision:

$$\begin{aligned} f' &\approx \frac{f(x+h)-f(x)}{h} \approx \frac{\epsilon_m}{h} \\ \Rightarrow \qquad \epsilon_{\text{ro}} &\approx \frac{\epsilon_m}{h} \end{aligned} \tag{6.14}$$

The approximation error with the forward-difference algorithm (6.3) is $\mathcal{O}(h)$, while that with the central-difference algorithm (6.6) is $\mathcal{O}(h^2)$:

$$\epsilon_{\text{approx}}^{\text{fd}} \approx \frac{f^{(2)}h}{2}, \qquad \epsilon_{\text{approx}}^{\text{cd}} \approx \frac{f^{(3)}h^2}{24} \tag{6.15}$$

Consequently, roundoff and approximation errors become equal when

$$\begin{aligned} &\tfrac{\epsilon_m}{h} \approx \epsilon_{\text{approx}}^{\text{fd}} = \tfrac{f^{(2)}h}{2} && \tfrac{\epsilon_m}{h} \approx \epsilon_{\text{approx}}^{\text{cd}} = \tfrac{f^{(3)}h^2}{24} \\ &\Rightarrow \quad h_{\text{fd}}^2 = \tfrac{2\epsilon_m}{f^{(2)}} && \Rightarrow \quad h_{\text{cd}}^3 = \tfrac{24\epsilon_m}{f^{(3)}} \end{aligned} \tag{6.16}$$

We take $f' \approx f^{(2)} \approx f^{(3)}$ (which may be crude in general, though not bad for e^x or $\cos x$), and assume double precision, $\epsilon_m \approx 10^{-15}$:

$$\begin{aligned} &h_{\text{fd}} \approx 4 \times 10^{-8} && h_{\text{cd}} \approx 3 \times 10^{-5} \\ \Rightarrow \quad &\epsilon_{\text{fd}} \simeq \tfrac{\epsilon_m}{h_{\text{cd}}} \simeq 3 \times 10^{-8}, && \Rightarrow \quad \epsilon_{\text{cd}} \simeq \tfrac{\epsilon_m}{h_{\text{cd}}} \simeq 3 \times 10^{-11} \end{aligned} \tag{6.17}$$

This may seem backward because the better algorithm leads to a larger h value. It is not. The ability to use a larger h means that the error in the central-difference method is some 1000 times smaller than the error in the forward-difference method here.

6.7
Error Analysis (Implementation and Assessment)

1. Use forward-, central-, and extrapolated-difference algorithms to differentiate the functions $\cos x$ and e^x at $x = 0.1, 1.,$ and 100.
   (a) Print out the derivative and its relative error $\mathcal{E}$ as functions of h. Reduce the step size h until it equals machine precision $h \approx \epsilon_m$.
   (b) Plot $\log_{10} |\mathcal{E}|$ versus $\log_{10} h$ and check whether the number of decimal places obtained agrees with the estimates in the text.
   (c) See if you can identify regions where truncation error dominate at large h and the roundoff error at small h in your plot. Do the slopes agree with our predictions?

6.8
Second Derivatives (Problem 2)

Let us say that you have measured the position $x(t)$ versus time for a particle. Your **problem** is to determine the force on the particle. Newton's second law tells us that the force and acceleration are linearly related:

$$F = ma = m\frac{d^2x}{dt^2} \tag{6.18}$$

where F is the force, m is the particle's mass, and a is the acceleration. So if we can determine the acceleration $a(t) = d^2x/dt^2$ from the $x(t)$ values, we can determine the force.

The concerns we expressed about errors in first derivatives are even more valid for second derivatives where additional subtractions may lead to additional cancellations. Let us look again at the central-difference method:

$$f'(x) \simeq \frac{f(x+h/2) - f(x-h/2)}{h} \tag{6.19}$$

This algorithm gives the derivative at x by moving forward and backward from x by $h/2$. We take the second derivative $f^{(2)}(x)$ to be the central difference of the first derivative:

$$f^{(2)}(x) \simeq \frac{f'(x+\frac{h}{2}) - f'(x-\frac{h}{2})}{h}, \tag{6.20}$$

$$\simeq \frac{[f(x+h) - f(x)] - [f(x) - f(x-h)]}{h^2} \tag{6.21}$$

$$\simeq \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} \tag{6.22}$$

As was true for first derivatives, we can determine the second derivative at x by evaluating the function in the region surrounding x. Although the form (6.22) is more compact and requires fewer steps than (6.21), it may increase subtractive cancellation by first storing the "large" number $f(x+h) + f(x-h)$, and then subtracting another large number $2f(x)$ from it. We ask you to explore this difference as an exercise.

6.8.1
Second Derivative Assessment

Write a program to calculate the second derivative of $\cos x$ using the central-difference algorithms (6.21) and (6.22). Test it over four cycles. Start with $h \approx \pi/10$ and keep reducing h until you reach machine precision.