3.1 Numerical differentiation

One basic tool that we will often use in this book is the Taylor expansion of a function $f(x)$ around a point x_0:

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x - x_0)^2}{2!}f''(x_0) + \cdots + \frac{(x - x_0)^n}{n!}f^{(n)}(x_0) + \cdots . \tag{3.1}$$

The above expansion can be generalized to describe a multivariable function $f(x, y, \ldots)$ around the point $(x_0, y_0, \ldots)$:

$$\begin{aligned} f(x, y, \ldots) = {} & f(x_0, y_0, \ldots) + (x - x_0)f_x(x_0, y_0, \ldots) \\ & + (y - y_0)f_y(x_0, y_0, \ldots) + \frac{(x - x_0)^2}{2!}f_{xx}(x_0, y_0, \ldots) \\ & + \frac{(y - y_0)^2}{2!}f_{yy}(x_0, y_0, \ldots) + \frac{2(x - x_0)(y - y_0)}{2!}f_{xy}(x_0, y_0, \ldots) + \cdots , \end{aligned} \tag{3.2}$$

where the subscript indices denote partial derivatives, for example, $f_{xy} = \partial^2 f/\partial x \partial y$.

The first-order derivative of a single-variable function $f(x)$ around a point x_i is defined from the limit

$$f'(x_i) = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \tag{3.3}$$

if it exists. Now if we divide the space into discrete points x_i with evenly spaced intervals $x_{i+1} - x_i = h$ and label the function at the lattice points as $f_i = f(x_i)$, we obtain the simplest expression for the first-order derivative

$$f_i' = \frac{f_{i+1} - f_i}{h} + O(h). \tag{3.4}$$

We have used the notation $O(h)$ for a term on the order of h. Similar notation will be used throughout this book. The above formula is referred to as the *two-point formula* for the first-order derivative and can easily be derived by taking the Taylor expansion of f_{i+1} around x_i. The accuracy can be improved if we expand f_{i+1} and f_{i-1} around x_i and take the difference

$$f_{i+1} - f_{i-1} = 2hf_i' + O(h^3). \tag{3.5}$$

After a simple rearrangement, we have

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2), \tag{3.6}$$

which is commonly known as the *three-point formula* for the first-order derivative. The accuracy of the expression increases to a higher order in h if more points are used. For example, a *five-point formula* can be derived by including the expansions of f_{i+2} and f_{i-2} around x_i. If we use the combinations

$$f_{i+1} - f_{i-1} = 2hf_i' + \frac{h^3}{3} f_i^{(3)} + O(h^5) \tag{3.7}$$

and

$$f_{i+2} - f_{i-2} = 4hf_i' + \frac{8h^3}{3} f_i^{(3)} + O(h^5) \tag{3.8}$$

to cancel the $f_i^{(3)}$ terms, we have

$$f_i' = \frac{1}{12h}(f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}) + O(h^4). \tag{3.9}$$

We can, of course, make the accuracy even higher by including more points, but in many cases this is not good practice. For real problems, the derivatives at points close to the boundaries are important and need to be calculated accurately. The errors in the derivatives of the boundary points will accumulate in other points when the scheme is used to integrate an equation. The more points involved in the expressions of the derivatives, the more difficulties we encounter in obtaining accurate derivatives at the boundaries. Another way to increase the accuracy is by decreasing the interval h. This is very practical on vector computers. The algorithms for first-order or second-order derivatives are usually fully vectorized, so a vector processor can calculate many points in just one computer clock cycle.

Approximate expressions for the second-order derivative can be obtained with different combinations of f_j. The *three-point formula* for the second-order derivative is given by the combination

$$f_{i+1} - 2f_i + f_{i-1} = h^2 f_i'' + O(h^4), \tag{3.10}$$

with the Taylor expansions of $f_{i\pm1}$ around x_i. Note that the third-order term with $f_i^{(3)}$ vanishes because of the cancellation in the combination. The above equation gives the second-order derivative as

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + O(h^2). \tag{3.11}$$

Similarly, we can combine the expansions of $f_{i\pm2}$ and $f_{i\pm1}$ around x_i and f_i to cancel the f_i', $f_i^{(3)}$, $f_i^{(4)}$, and $f_i^{(5)}$ terms; then we have

$$f_i'' = \frac{1}{12h^2}(-f_{i-2} + 16f_{i-1} - 30f_i + 16f_{i+1} - f_{i+2}) + O(h^4) \tag{3.12}$$

as the *five-point formula* for the second-order derivative. The difficulty in dealing with the points around the boundaries still remains. We can use the interpolation formulas that we developed in the Chapter 2 to extrapolate the derivatives to the

Table 3.1. *Derivatives obtained in the example*

x	f'	$\Delta f'$	f''	$\Delta f''$
0	0.999 959	−0.000 041	0.000 004	0.000 004
$\pi/10$	0.951 017	−0.000 039	−0.309 087	−0.000 070
$\pi/5$	0.808 985	−0.000 032	−0.587 736	0.000 049
$3\pi/10$	0.587 762	−0.000 023	−0.809 013	0.000 004
$2\pi/5$	0.309 003	−0.000 014	−0.951 055	0.000 001
$\pi/2$	−0.000 004	−0.000 004	−0.999 980	0.000 020

We have taken a simple function $f(x) = \sin x$, given at 101 discrete points with evenly spaced intervals in the region $[0, \pi/2]$. The Lagrange interpolation is applied to extrapolate the derivatives at the boundary points. The numerical results are summarized in Table 3.1, together with their errors. Note that the extrapolated data are of the same order of accuracy as other calculated values for f' and f'' at both $x = 0$ and $x = \pi/2$ because the three-point Lagrange interpolation scheme is accurate to a quadratic behavior. The functions $\sin x$ and $\cos x$ are well approximated by a linear or a quadratic curve at those two points.

In practice, we may encounter two problems with the formulas used above. The first problem is that we may not have the data given at uniform data points. One solution to such a problem is to perform an interpolation of the data first and then apply the above formulas to the function at the uniform data points generated from the interpolation. This approach can be tedious and has errors from two sources, the interpolation and the formulas above. The easiest solution to the problem is to adopt formulas that are suitable for nonuniform data points. If we use the Taylor expansion

$$f(x_{i\pm1}) = f(x_i) + (x_{i\pm1} - x_i)f'(x_i) + \frac{1}{2!}(x_{i\pm1} - x_i)^2 f''(x_i) + O(h^3) \qquad (3.13)$$

and a combination of f_{i-1}, f_i, and f_{i+1} to cancel the second-order terms, we obtain

$$f'_i = \frac{h_{i-1}^2 f_{i+1} + \left(h_i^2 - h_{i-1}^2\right) f_i - h_i^2 f_{i-1}}{h_i h_{i-1}(h_i + h_{i-1})} + O(h^2), \qquad (3.14)$$

where $h_i = x_{i+1} - x_i$ and h is the larger of $|h_{i-1}|$ and $|h_i|$. This is the three-point formula for the first-order derivative in the case of nonuniform data points. Note that the accuracy here is the same as for the uniform data points. This is a better choice than interpolating the data first because the formula can be implemented in almost the same manner as in the case of the uniform data points. The following method returns the first-order derivative for such a situation.