Chapter 16

Numerical Differentiation

Estimating the derivative of a function is a common task in scientific computing. The need arises when we have data that represent some quantity $f(x)$, dependent on a variable x, and we would like to know the rate of change $f'(x)$. If the data are obtained from an experiment or a numerical simulation, the function $f(x)$ is only known at discrete values of x. We must resort to numerical techniques to determine its derivative.

16.1 Two–point difference formulas

Our goal is to approximate the derivative of a function $f(x)$ at some point x_0. The only information we have is the value of $f(x)$ at discrete points along the x–axis. To be precise, $f(x)$ is known at x_0 and points separated from x_0 by multiples of h, as shown in Fig 16.1. An approximation to $f'(x_0)$ or $f''(x_0)$ (or higher order derivatives) using the values $f(x_0)$, $f(x_0 \pm h)$, $f(x_0 \pm 2h)$, *etc.* is referred to as a *finite difference formula*.

Let's derive a simple finite difference formula for the first derivative $f'(x_0)$. Start with the Taylor series for $f(x)$ about the point x_0,

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + \cdots \ , \tag{16.1}$$

where $\cdots$ represents terms proportional to $(x - x_0)^3$ and higher powers of $(x - x_0)$. Set $x = x_0 + h$ in this expression to obtain

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2} f''(x_0)h^2 + \cdots \ . \tag{16.2}$$

We can rearrange this relation to find

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{1}{2} f''(x_0)h + \cdots \ . \tag{16.3}$$

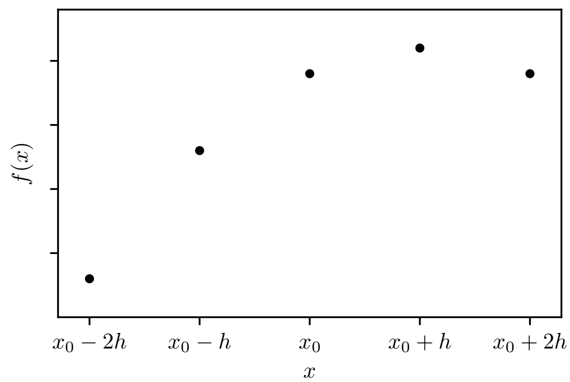

Fig. 16.1: Values of the function $f(x)$ are known at x_0, $x_0 \pm h$, $x_0 \pm 2h$, *etc.* We want to estimate $f'(x_0)$, the derivative of $f(x)$ at the point x_0.

Here, $\cdots$ represents terms proportional to h^2 and higher powers of h. Now, assuming h is small, the terms $-\frac{1}{2}f''(x_0)h + \cdots$ will be small. We can drop these terms and approximate the derivative of $f(x)$ at x_0 by

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h} \; . \tag{16.4}$$

This formula for $f'(x_0)$ uses the values of $f(x)$ at just two points, x_0 and $x_0 + h$. We call this the *two–point forward difference* approximation to the derivative. Geometrically, the two–point forward difference is the slope of a straight line connecting the function values between x_0 and $x_0 + h$.

The error in the two–point forward difference comes from the terms $-\frac{1}{2}f''(x_0)h + \cdots$ that were dropped from Eq. (16.3). For small h, the unwritten terms $\cdots$ are small compared to $-\frac{1}{2}f''(x_0)h$. Thus, the error in the two–point forward difference formula is approximately proportional to h. This implies $|\text{error}| \approx ch$ for some constant c. Taking the logarithm of both sides, we have

$$\log|\text{error}| \approx \log c + \log h \; . \tag{16.5}$$

This result forms the basis of a convergence test for any code that uses the two–point forward difference formula: A plot of $\log|\text{error}|$ versus $\log h$ should approach a straight line with slope 1 as the resolution is increased.

The *two–point backwards difference* approximation is similar. Start with the Taylor expansion (16.1) and let $x = x_0 - h$ to obtain

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h} \ . \tag{16.6}$$

This approximates the derivative by the slope of a line between x_0 and $x_0 - h$. The error in this approximation is proportional to h. Reducing h by a factor of 2 reduces the error by (approximately) a factor of 2.

Let's look at a simple example. The data that appear in Fig. 16.1 are: $f(0.8) = 0.8$, $f(2.2) = 1.8$, $f(3.6) = 2.4$, $f(5.0) = 2.6$, and $f(6.4) = 2.4$. The two–point forward and backward difference approximations to $f'(x)$ at $x = 3.6$ are

$$f'(3.6)\big|_{\text{forward}} \approx \frac{f(5.0) - f(3.6)}{5.0 - 3.6} = 0.143 \ ,$$
$$f'(3.6)\big|_{\text{backward}} \approx \frac{f(3.6) - f(2.2)}{3.6 - 2.2} = 0.429 \ .$$

We can apply the difference formulas at other points in the data set as well. For example, the forward difference approximation at $x = 0.8$ is

$$f'(0.8)\big|_{\text{forward}} \approx \frac{f(2.2) - f(0.8)}{2.2 - 0.8} = 0.714 \ ,$$

and the backward difference approximation at $x = 6.4$ is

$$f'(6.4)\big|_{\text{backward}} \approx \frac{f(6.4) - f(5.0)}{6.4 - 5.0} = -0.143 \ .$$

Note that we cannot compute the forward difference approximation at $x = 6.4$, or the backward difference approximation at $x = 0.8$, because we don't have the necessary data.

Exercise 16.1

Consider the function $f(x) = \cos(x) + \sin(3x)$. Find the exact value of the derivative of $f(x)$ at the point $x_0 = 2$. Carry out a convergence test by computing the two–point forward difference approximation to $f'(2)$ with various values of h between 0.001 and 0.0001. Show that the errors are (approximately) proportional to h by plotting $\log|\text{error}|$ versus $\log h$.

16.2 Truncation errors and machine errors

The derivative of a function $f(x)$ at a point x_0 is defined by

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h} \ . \tag{16.7}$$

Apart from the limit symbol, this definition looks like the two–point forward difference formula (16.4). In fact, if we could take the limit as $h \to 0$ in the forward difference formula, the result would be the exact derivative, not just an approximation. Why can't we take the limit $h \to 0$, or at least take h to be very, very small?

In scientific computation, we usually don't have control over h. The value for h is dictated by the practical details of an experiment or a numerical simulation. Even if we could choose h freely, finite difference formulas are subject to machine roundoff error.

Let's look at an example with the function $f(x) = \sin x$, and consider its derivative at $x_0 = 1$. The exact answer is $f'(1) = \cos(1)$. Figure 16.2 shows a graph of $\log|\text{error}|$ versus $\log h$. As h is decreased from 10^{-1}, the error initially decreases. As h is decreased beyond about 10^{-8}, the error begins to grow.

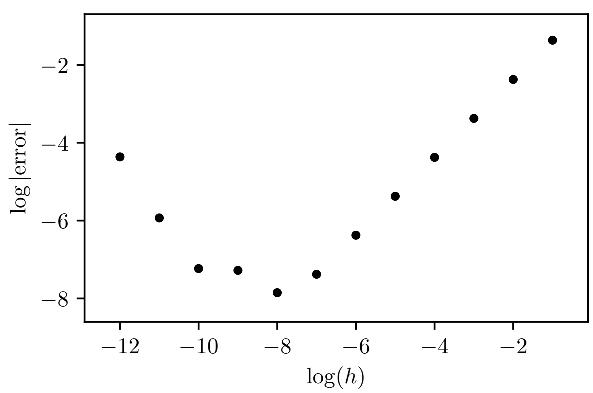

Fig. 16.2: Error as a function of h for the two–point forward difference approximation to $f'(x_0)$ with $f(x) = \sin x$ and $x_0 = 1$.

The analysis of the preceeding section showed that the error in the two–point forward difference formula is $-\frac{1}{2}f''(x_0)h + \cdots$. We refer to this type of error as *truncation error* because it arises from truncating the infinite series (16.3) to obtain Eq. (16.4). With $f(x) = \sin x$, the truncation error at $x_0 = 1$ is approximately $\frac{1}{2}\sin(1)h$, or

$$\text{truncation error} \approx 0.4207\, h \ . \tag{16.8}$$

Now, the two–point forward difference formula is

$$f'(1) \approx \frac{\sin(1+h) - \sin(1)}{h} \ . \tag{16.9}$$

In addition to the truncation error, this calculation is subject to machine roundoff errors. As discussed in Sec. 4.4, a 64–bit machine can only represent the numerator $\sin(1+h) - \sin(1)$ to an accuracy of about $\pm 10^{-16}$. Thus, there are machine roundoff errors in computing the finite difference formula for $f'(1)$ of roughly $\pm 10^{-16}/h$. The table below compares the truncation error and machine roundoff error for various values of h. (Only the rough "order of magnitude" values are shown.) As h becomes smaller, truncation

h	truncation error	roundoff error
10^{-6}	10^{-6}	10^{-10}
10^{-7}	10^{-7}	10^{-9}
10^{-8}	10^{-8}	10^{-8}
10^{-9}	10^{-9}	10^{-7}
10^{-10}	10^{-10}	10^{-6}
10^{-11}	10^{-11}	10^{-5}

Table 16.1: Truncation error $\approx 0.4207\, h$ and roundoff error $\approx 10^{-16}/h$ for the two–point forward difference approximation to the derivative $f'(1)$, where $f(x) = \sin x$.

error is reduced but machine roundoff error grows. With a two–point forward difference approximation to $d\sin(x)/dx$ at $x = 1$, the best we can do is an overall error of about $\pm 10^{-8}$.

Exercise 16.2

Use the two–point forward difference formula to compute the derivative of the function $f(x) = \cos(x) + \sin(3x)$ at $x_0 = 2$. (See Exercise 16.1.) Plot $\log|\text{error}|$ versus $\log h$ for $h = 10^{-2}$, 10^{-3}, *etc.* Do the errors always decrease as you decrease h?

16.3 Two–point forward difference, again

We can derive the two–point forward difference approximation (16.4) in a different way. Start with a linear combination of the relations

$$f(x_0) = f(x_0) \ , \tag{16.10a}$$

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \cdots \tag{16.10b}$$

with coefficients a and b, which yields

$$af(x_0) + bf(x_0 + h) = (a + b)f(x_0) + bf'(x_0)h + \frac{b}{2}f''(x_0)h^2 + \cdots \ . \tag{16.11}$$

Now ask: What values should we choose for the coefficients a and b such that the right–hand side is as close as possible to $f'(x_0)$? The answer is that the coefficient of $f(x_0)$ should vanish and the coefficient of $f'(x_0)$ should equal 1. That is, a and b should satisfy

$$a + b = 0 \ , \tag{16.12a}$$

$$bh = 1 \ . \tag{16.12b}$$

It would be nice if the coefficient of $f''(x_0)$ vanished, but that would give us a third equation $bh^2/2 = 0$ that is incompatible with Eq. (16.12b). The best we can do with just two unknowns, a and b, is to impose the two conditions (16.12).

The solution to Eqs. (16.12) is $b = 1/h$ and $a = -1/h$. With these values for the coefficients, Eq. (16.11) becomes

$$-\frac{1}{h}f(x_0) + \frac{1}{h}f(x_0 + h) = f'(x_0) + \frac{1}{2}f''(x_0)h + \cdots \ . \tag{16.13}$$

Assuming h is small, we can drop the terms $\frac{1}{2}f''(x_0)h + \cdots$ from the right–hand side. The result is the two–point forward difference formula, Eq. (16.4).

Exercise 16.3

Use the approach of this section to derive the two–point backward difference formula for $f'(x_0)$.

16.4 Centered difference formulas

We can use this same strategy to create other finite difference formulas. Start with the Taylor series expansions

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \cdots \ , \tag{16.14a}$$

$$f(x_0) = f(x_0) \ , \tag{16.14b}$$

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \cdots \ , \tag{16.14c}$$

and form a linear combination with coefficients a, b and c. The result is

$$\begin{aligned} af(x_0 - h) + bf(x_0) + cf(x_0 + h) &= (a + b + c)f(x_0) + (c - a)f'(x_0)h \\ &\quad + \frac{c + a}{2}f''(x_0)h^2 + \cdots \ . \end{aligned} \tag{16.15}$$

Choose the coefficients such that the right–hand side is as close to $f'(x_0)$ as possible. We see that the coefficients of $f(x_0)$ and $f''(x_0)$ should vanish, and the coefficient of $f'(x_0)$ should be 1:

$$(a + b + c) = 0 \ , \tag{16.16a}$$

$$(c - a)h = 1 \ , \tag{16.16b}$$

$$(c + a)h^2/2 = 0 \ . \tag{16.16c}$$

The solution is $a = -1/(2h)$, $b = 0$ and $c = 1/(2h)$, and Eq. (16.15) becomes

$$-\frac{1}{2h}f(x_0 - h) + \frac{1}{2h}f(x_0 + h) = f'(x_0) + \cdots \ . \tag{16.17}$$

If we assume h is small and drop the $\cdots$ terms, the result is

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0 - h)}{2h} \ . \tag{16.18}$$

This is a *three–point centered difference* approximation for $f'(x_0)$. (The formula uses only two of the three points, because the coefficient of $f(x_0)$ vanishes.) This approximation to $f'(x_0)$ is simply the average of the two–point forward and backward difference formulas.

Observe that the unwritten terms in Eq. (16.15), the terms represented by $\cdots$, are proportional to h^3 multiplied by some combination of coefficients a, b and c. Since a, b and c are themselves proportional to $1/h$, the unwritten terms are proportional to h^2. It follows that the truncation error in the centered difference formula (16.18) is proportional to h^2. That is, $|\text{error}| = Ch^2$ for some constant C and a plot of $\log|\text{error}|$ versus $\log h$ should be (approximately) a straight line with slope 2.

Geometrically, the three–point centered difference formula (16.18) uses the slope of the line connecting the data points at $x_0 - h$ and $x_0 + h$ to approximate $f'(x_0)$.

Exercise 16.4a

Consider the function $f(x) = \cos(x)\exp(-x^2/2)$. Use the three–point centered difference with $h = 0.1$ to approximate $f'(x)$ at discrete points in the domain $-3 \le x \le 3$. Plot your approximate results for $f'(x)$ and, on the same graph, the exact function $f'(x)$.

Return to the linear combination in Eq. (16.15). We can use this to derive a finite difference formula for the second derivative, $f''(x_0)$, by setting the coefficients of $f(x_0)$ and $f'(x_0)$ equal to zero and the coefficient of $f''(x_0)$ equal to 1. That is,

$$(a + b + c) = 0 \ , \tag{16.19a}$$

$$(c - a)h = 0 \ , \tag{16.19b}$$

$$(c + a)h^2/2 = 1 \ , \tag{16.19c}$$

which has the solution $a = 1/h^2$, $b = -2/h^2$ and $c = 1/h^2$. This gives

$$\frac{1}{h^2} f(x_0 - h) - \frac{2}{h^2} f(x_0) + \frac{1}{h^2} f(x_0 + h) = f''(x_0) + \cdots \ . \tag{16.20}$$

After dropping the $\cdots$ terms, we have the three–point centered difference approximation to the second derivative of $f(x)$:

$$f''(x_0) \approx \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2} \ . \tag{16.21}$$

If we keep track of the unwritten terms in this derivation, we find that the truncation error is proportional to h^2.

Exercise 16.4b

Use the three–point centered difference approximation to compute $f''(x_0)$, where $f(x) = \sin x$ and $x_0 = 1$. Carry out a convergence test with $0.1 \le h \le 0.0001$ to show that the error is (approximately) proportional to h^2. What happens to the error as h decreases below 0.0001?

Exercise 16.4c

The data file *ToDifferentiateData.txt* (see the Appendix) contains two columns, x and $f(x)$, with x values equally spaced. Use the three–point centered difference formulas to approximate the first and second derivatives of $f(x)$ at each of the data points, excluding the endpoints. Graph your results.

16.5 Other stencils

The pattern of evaluation points for a finite difference formula is sometimes referred to as a *stencil*. For the two–point forward difference formula, the stencil consists of the points x_0 and $x_0 + h$. For the three–point centered difference formulas, the stencil consists of $x_0 - h$, x_0 and $x_0 + h$.

We can use various stencils to derive more finite difference formulas for approximating derivatives. For example, with the three–point stencil x_0, $x_0 + h$, $x_0 + 2h$ we have

$$f(x_0) = f(x_0) \ , \tag{16.22a}$$

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \cdots \ , \tag{16.22b}$$

$$f(x_0 + 2h) = f(x_0) + 2f'(x_0)h + 2f''(x_0)h^2 + \cdots \ . \tag{16.22c}$$

A linear combination yields

$$\begin{aligned} af(x_0) + bf(x_0 + h) + cf(x_0 + 2h) = (a + b + c)f(x_0) + (b + 2c)f'(x_0)h \\ + (b/2 + 2c)f''(x_0)h^2 + \cdots \ . \end{aligned} \tag{16.23}$$

To approximate the first derivative, $f'(x_0)$, choose

$$(a + b + c) = 0 \ , \tag{16.24a}$$

$$(b + 2c)h = 1 \ , \tag{16.24b}$$

$$(b/2 + 2c)h^2 = 0 \ , \tag{16.24c}$$

with the solution $a = -3/(2h)$, $b = 2/h$, $c = -1/(2h)$. This leads to the three–point, one sided approximation

$$f'(x_0) \approx \frac{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h} \ . \tag{16.25}$$

In this case the truncation error is proportional to h^2.

We can also approximate the second derivative $f''(x_0)$ using the stencil x_0, $x_0 + h$, $x_0 + 2h$. Choose

$$(a + b + c) = 0 \ , \tag{16.26a}$$

$$(b + 2c)h = 0 \ , \tag{16.26b}$$

$$(b/2 + 2c)h^2 = 1 \ . \tag{16.26c}$$

which has the solution $a = 1/h^2$, $b = -2/h^2$, $c = 1/h^2$. The resulting approximation is

$$f''(x_0) \approx \frac{f(x_0) - 2f(x_0 + h) + f(x_0 + 2h)}{h^2} \; , \tag{16.27}$$

with truncation error proportional to h.

Exercise 16.5a

Show that the finite difference approximations for first and second derivatives with stencil $x_0 - 2h$, $x_0 - h$, x_0 are

$$f'(x_0) \approx \frac{f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)}{2h} \; ,$$
$$f''(x_0) \approx \frac{f(x_0 - 2h) - 2f(x_0 - h) + f(x_0)}{h^2} \; .$$

These are three–point one sided approximations for $f'(x_0)$ and $f''(x_0)$, with stencil points in the backward direction. The approximations Eq. (16.25) and (16.27) are one sided with stencil points in the forward direction.

Exercise 16.5b

Sample the function $f(x) = \sin(x + 2\sin(x))$ at N points in the domain $0 \le x \le 2\pi$, then use the data to compute the first derivative $f'(x)$ at each of the sample points. Use the three–point centered stencil for the interior points (the points between 0 and 2π), and use the three–point one sided stencils at the endpoints 0 and 2π. (See Eq. (16.25) and Exercise 16.5a.) Plot your finite difference approximation along with the actual expression for $f'(x)$ on a single graph. Experiment with different values of N.

Exercise 16.5c

Show that the five–point centered difference formula for the first derivative is

$$f'(x_0) \approx \frac{-f(x_0 + 2h) + 8f(x_0 + h) - 8f(x_0 - h) + f(x_0 - 2h)}{12h} \; .$$

(Suggestion: Use SymPy to solve the system of 5 equations for the 5 coefficients.)

Exercise 16.5d

Derive the five–point centered difference formula for the second derivative, $f''(x_0)$.