Lesson 16: Numerical Differentiation

1 Introduction

Estimating the derivative of a function is a very common task in scientific computing. The need arises, for example, when we have data that represent some dependent variable f as a function of an independent variable x, and we would like to know the rate at which f changes. If the data are generated from a numerical code, or from an experiment, then f is only known at discrete values of x and we cannot differentiate $f(x)$ analytically. We must resort to numerical techniques.

Numerical differentiation can be difficult to do well. We cannot apply the definition

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \tag{1}$$

directly if the data are discrete, because we cannot take the limit $h \to 0$. Even in cases where we can evaluate the function everywhere, this expression for the derivative is prone to an error know as *subtractive cancellation*. Subtractive cancellation occurs if you make h very small, as the definition requires.

Consider for example the function $f(x) = \cos(x)\tanh(x)$. You can verify that it's derivative at $x = 2$ is

$$f'(2) = \cos(2)\mathrm{sech}^2(2) - \sin(2)\tanh(2) \approx -0.905989 \tag{2}$$

However, if we use the definition (1) with $h = 10^{-16}$, the result in double precision is

$$f'(2) = \frac{f(2+h) - f(2)}{h} = 0.0 \tag{3}$$

The answer is wrong because with double precision both $f(2+h)$ and $f(2)$ evaluate to -0.40117702779274822. With single precision, subtractive cancellation occurs for much larger values of h.

2 Forward and Backward Difference Formulas

The definition (1) for the derivative $f'(x)$ requires us to evaluate the function at two points, namely, $x + h$ and x. We need to develop techniques to *approximate* the derivative $f'(x)$ that do not require us to take the limit $h \to 0$. The approximations to $f'(x)$ are constructed from combinations of the function f evaluated at various points surrounding x. We refer to these as *finite difference* formulas.

Let's say we want to approximate $f'(x)$ using the values of f at the points x and $x+h$. That is, we want a formula that says

$$f'(x) \approx af(x+h) + bf(x) \tag{4}$$

for some constants a and b. We can determine a and b by using the Taylor series

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \cdots \tag{5}$$

to expand the right–hand side of Eq. (4). This yields

$$af(x+h) + bf(x) = (a+b)f(x) + af'(x)h + \frac{a}{2}f''(x)h^2 + \cdots \tag{6}$$

The right–hand side of this relation will equal $f'(x)$, approximately, if $a+b=0$ and $a=1/h$. (That is, $a=1/h$ and $b=-1/h$.) With these values for the constants, then

$$\frac{1}{h}f(x+h) - \frac{1}{h}f(x) = f'(x) + \frac{1}{2}f''(x)h + \cdots \tag{7}$$

Equivalently, we can write

$$f'(x) = \frac{f(x+h)-f(x)}{h} - \frac{1}{2}f''(x)h + \cdots \tag{8}$$

Thus, the approximation (4) that we sought is

$$f'(x) \approx \frac{f(x+h)-f(x)}{h} \tag{9}$$

This approximation is called the *forward difference*. It is simply the definition (1) without the limit $h \to 0$. From Eq. (8), we see that the error in the forward difference approximation is

$$\mathcal{E}_F = \frac{1}{2}f''(x)h + \cdots \tag{10}$$

In particular, $\mathcal{E}_F$ is proportional to h.

We can carry out a similar analysis to obtain a finite difference approximation to $f'(x)$ using the points $x-h$ and x. The result is the *backward difference* approximation

$$f'(x) \approx \frac{f(x)-f(x-h)}{h} \tag{11}$$

with error

$$\mathcal{E}_B = -\frac{1}{2}f''(x)h + \cdots \tag{12}$$

Again, the error is proportional to h.

Exercise 1: Write a code to compute the forward and backward difference approximations to $f'(2)$, where $f(x) = \cos(x)\tanh(x)$. Use $h = 10^{-1}, 10^{-2}, \ldots$. For both approximation methods, show that the errors $\mathcal{E}$ are proportional to h. One way to do this is to show that a log–log plot of $\mathcal{E}$ versus h gives a straight line with slope 2. Here is a simpler way. If the error is proportional to h, then $\mathcal{E} = Ch$ for some constant C. Let h_1 and h_2 denote your two smallest h values, and $\mathcal{E}_1$ and $\mathcal{E}_2$ denote the corresponding errors. The relations $\mathcal{E}_1 = Ch_1$ and $\mathcal{E}_2 = Ch_2$ imply $\mathcal{E}_2/\mathcal{E}_1 = h_2/h_1$. If the ratio $\mathcal{E}_2/\mathcal{E}_1$ agrees (approximately) with the ratio h_2/h_1, then the errors are proportional to h.

3 Central Difference Formula

Let's derive a finite difference approximation for $f'(x)$ using the *three* points $x - h$, x and $x + h$. That is, we seek a relation

$$f'(x) \approx af(x-h) + bf(x) + cf(x+h) \tag{13}$$

for some constants a, b and c. The contants are determined by expanding $f(x-h)$ and $f(x+h)$ in Taylor series

$$f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(x)h^3 + \cdots \tag{14a}$$

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \cdots \tag{14b}$$

and inserting these into the right–hand side of Eq. (13):

$$\begin{aligned} af(x-h) + bf(x) + cf(x+h) &= (a+b+c)f(x) + (c-a)f'(x)h + \frac{1}{2}(c+a)f''(x)h^2 \\ &\quad + \frac{1}{6}(c-a)f'''(x)h^3 + \cdots \end{aligned} \tag{15}$$

This expression will equal $f'(x)$, approximately, if $(a + b + c) = 0$, $(c - a) = 1/h$, and $(c + a) = 0$. That is, $a = -1/(2h)$, $b = 0$, and $c = 1/(2h)$. With these values for the constants, we have

$$-\frac{1}{2h}f(x-h) + \frac{1}{2h}f(x+h) = f'(x) + \frac{1}{6}f'''(x)h^2 + \cdots \tag{16}$$

This gives us the *central difference* formula for the first derivative:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \tag{17}$$

The error for this method is

$$\mathcal{E}_C = \frac{1}{6}f'''(x)h^2 + \cdots \tag{18}$$

It is proportional to h^2.

The central difference formula is simply the average of the forward and backward difference formulas. In taking the average, the order h terms in the errors $\mathcal{E}_F$ and $\mathcal{E}_B$ cancel. The order h^2 terms, included in the $\cdots$ of Eqs. (10) and (12), do not cancel; rather, they combine to give the central difference error $\mathcal{E}_C$.

> Homework: Compute the derivative of $f(x) = \cos(x)\tanh(x)$ at $x = 2$ using the central difference method. Show that the error $\mathcal{E}$ is proportional to h^2 by using two h values and comparing the ratio $\mathcal{E}_2/\mathcal{E}_1$ to $(h_2/h_1)^2$.

4 Other stencils

The pattern of evaluation points and coefficients is sometimes referred to as the "stencil". For example, the forward difference formula (9) might be called a one–sided, two–point stencil. The central difference formula is a centered, three–point stencil (although the coefficient of one of those points is zero).

The method of the preceeding sections can be used to obtain other stencils for $f'(x)$. For example, we might want to calculate the derivative without any function evaluations at points less than x. For this we can choose a three–point stencil consisting of the points x, $x + h$ and $x + 2h$. Using the Taylor series expressions

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \cdots \tag{19a}$$

$$f(x+2h) = f(x) + 2f'(x)h + \frac{4}{2}f''(x)h^2 + \frac{8}{6}f'''(x)h^3 + \cdots \tag{19b}$$

we have

$$\begin{aligned} af(x) + bf(x+h) + cf(x+2h) &= (a+b+c)f(x) + (b+2c)f'(x)h \\ &\quad + \frac{1}{2}(b+4c)f''(x)h^2 + \frac{1}{6}(b+8c)f'''(x)h^3 + \cdots \end{aligned} \tag{20}$$

This will approximate $f'(x)$ if the coefficients satisfy

$$(a+b+c) = 0 \tag{21a}$$

$$(b+2c)h = 1 \tag{21b}$$

$$(b+4c) = 0 \tag{21c}$$

The solution is $a = -3/(2h)$, $b = 2/h$, $c = -1/(2h)$. This yields the finite difference formula

$$f'(x) \approx \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} \tag{22}$$

The terms $(b+8c)f'''(x)h^3/6 + \cdots$ from Eq. (20), which are order h^2, do not vanish. Thus, the error for this one–sided, three–point stencil is proportional to h^2.

Homework: Find the five–point centered stencil for $f'(x)$. This stencil spans the points $x-2h$, $x-h$, x, $x+h$, $x+2h$. Write a python code using the `linalg` package in `numpy` to solve for the constants. Write a python code using this stencil to compute the derivative of $f(x) = \cos(x)\tanh(x)$ at $x = 2$. Show that the errors scale like h^4.

In general, derivative formulas that use large stencils have higher order error. (That is, the error is a higher power of h.) However, derivative formulas with large stencils are more susceptible to subtractive cancellation errors. Thus, a stencil with a very high order error is not always accurate.

5 Second derivatives

We can apply the same technique to derive finite difference stencils for second derivatives, $f''(x)$, as well as higher order derivatives. For example, consider the three–point centered stencil for $f''(x)$. We can derive this stencil by examining the Taylor expansion from Eq. (15), which is repeated here:

$$\begin{aligned} af(x-h) + bf(x) + cf(x+h) &= (a+b+c)f(x) + (c-a)f'(x)h + \frac{1}{2}(c+a)f''(x)h^2 \\ &\quad + \frac{1}{6}(c-a)f'''(x)h^3 + \cdots \end{aligned} \tag{23}$$

The right–hand side will approximate $f''(x)$ if $(a+b+c) = 0$, $(c-a) = 0$ and $(c+a)h^2/2 = 1$. This gives $a = 1/h^2$, $b = -2/h^2$ and $c = 1/h^2$, so that

$$\frac{1}{h^2}f(x-h) - \frac{2}{h^2}f(x) + \frac{1}{h^2}f(x+h) = f''(x) + \cdots \tag{24}$$

Thus, the centered three–point stencil for the second derivative is

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \tag{25}$$

Note that the term $(c-a)f'''(x)h^3/6$ in Eq. (23) vanishes for the chosen values of a, b and c. The next order term in Eq. (23) is proportional to $(c+a)f''''(x)h^4$. This term does not vanish and is proportional to h^2. Thus, the error for the formula (25) is of order h^2.

Homework: Use the three-point centered stencil to compute the second derivative of $f(x) = \log(x)/\cosh(x)$. Plot a graph of $f''(x)$ for $2.0 \le x \le 5.0$.