

October 5, 2017

5 Lecture 5

5.1 Numerical differentiation

- In this lecture we shall study techniques for the numerical differentiation of functions.
- Suppose we have a function $f(x)$ which is reasonably smooth, i.e. differentiable up to some order that we need.
- Let h be a small number.
- We employ Taylor's theorem (see Lecture 2). We shall use both of the following Taylor series

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \cdots \quad (5.1.1a)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \cdots \quad (5.1.1b)$$

There are remainder terms in both series, but their detailed expressions do not matter here.

- We shall employ eqs. (5.1.1a) and (5.1.1b) to derive numerical formulas to approximate the derivatives of f .

5.2 First derivative: finite difference

- We begin with the first derivative $f'(x)$. Using eq. (5.1.1a), an approximate formula is

$$f'(x) \simeq \frac{f(x+h) - f(x)}{h}. \quad (5.2.1)$$

- The formula eq. (5.2.1) is an example of what is called a **finite difference** formula. All of the formulas we shall see below are finite difference formulas.
- There are several details to note about eq. (5.2.1), which we list below.
- From eq. (5.1.1a), the numerical accuracy of eq. (5.2.1) is $O(h)$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2!} f''(x) + \dots \quad (5.2.2)$$

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- In pure mathematics, to compute the first derivative rigorously, we must take the limit $h \rightarrow 0$:

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}. \quad (5.2.3)$$

However, in numerical analysis, we cannot perform such a limit.

We must employ a **small nonzero value for h** , and we cannot “take the limit” $h \rightarrow 0$.

- **There is a problem with eq. (5.2.1):**

1. In the numerator on the right hand side, we subtract two (possibly large) numbers to obtain a value of small amplitude, then we divide by h , which also has a small amplitude.
2. Hence we **divide two numbers of small amplitude**, but *the ratio may not have a small amplitude*.

- **Numerical differentiation (via finite differences) can be unstable.**

1. We have no choice but to compute differences to obtain a numerator of small amplitude (*and there will be roundoff error in doing so*), and then divide by a denominator of small amplitude.
2. This is an important fact to bear in mind.

- It is therefore important to note that **the value of h must not be too small**.

If the value of h is too small, the answer we compute may be dominated by roundoff error, and will not be accurate.

The numerical accuracy of eq. (5.2.1) will not be $O(h)$.

Instead the answer may be contaminated by “numerical noise” (contributions from roundoff errors).

- How do we know what is a suitable value to choose for h ?

We do NOT know a general procedure to choose a suitable value for h .

As always, we require “background information” about the problem we are studying, to give us context about the function f , to decide what is a reasonable value to use for h .

5.3 First derivative: backward difference

- The formula in eq. (5.2.1) is called a **forward difference** formula.
- There is an obvious **backward difference** formula. Use eq. (5.1.1b) to derive

$$f'(x) \simeq \frac{f(x) - f(x-h)}{h}. \quad (5.3.1)$$

- The numerical accuracy of eq. (5.3.1) is also $O(h)$.
- The backward difference formula has the same limitations as the forward difference formula.

5.4 First derivative: centered finite difference

- Why not average the forward and backward finite difference formulas? This is a good idea.
- The average is

$$\begin{aligned} f'(x) &\simeq \frac{1}{2} \left[\frac{f(x+h) - f(x)}{h} + \frac{f(x) - f(x-h)}{h} \right] \\ &= \frac{f(x+h) - f(x-h)}{2h}. \end{aligned} \tag{5.4.1}$$

- However, this does not tell us the order of accuracy of the result. Since each of the forward and backward finite difference formulas has an accuracy of $O(h)$, adding them will naïvely still yield a formula of accuracy $O(h)$.

- **Hence why is the average a good idea?**

To answer this we must derive eq. (5.4.1) from the original Taylor series in eqs. (5.1.1). Subtract eqs. (5.1.1a) and (5.1.1b) and divide by 2 to obtain

$$\frac{f(x+h) - f(x-h)}{2} = hf'(x) + \frac{h^3}{3!} f'''(x) + \dots \tag{5.4.2}$$

- Notice that $f(x)$ all the even order derivatives f'' etc. cancel out. This is important.
- This is the **centered difference** formula:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!} f'''(x) + \dots \tag{5.4.3}$$

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- The accuracy of the formula eq. (5.4.3) is $O(h^2)$.
This is because the even order term in $f''(x)$ cancelled out. This is important.
We cannot directly deduce this improvement in accuracy from the formula eq. (5.4.1).
- The accuracy of the centered difference formula is much better than that of the single sided forward or backward finite difference formulas.

5.5 Second derivative

- We shall require both eqs. (5.1.1a) and (5.1.1b) to obtain a finite difference formula for the second derivative $f''(x)$.
- Add eqs. (5.1.1a) and (5.1.1b) and divide by 2 to obtain

$$\frac{f(x+h) + f(x-h)}{2} = f(x) + \frac{h^2}{2!} f''(x) + O(h^4) \quad (5.5.1)$$

- Notice that all the odd order derivatives $f'(x)$, $f'''(x)$, etc. cancel out. This is important.
- This is the finite difference formula for $f''(x)$ (it is also a centered difference):

$$f''(x) = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} - \frac{h^2}{4!} f''''(x) + \dots \quad (5.5.2)$$

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- The accuracy of the formula is also $O(h^2)$.
This is because the odd order term in $f''''(x)$ cancelled out. This is important.
- Notice that eq. (5.5.2) can be derived by taking a finite difference of the forward and backward finite difference formulas for f' :

$$f''(x) \simeq \frac{1}{h} \left[\frac{f(x+h) - f(x)}{h} - \frac{f(x) - f(x-h)}{h} \right]. \quad (5.5.3)$$

Each of the forward and backward finite difference formulas has an accuracy of only $O(h)$, but the subtraction yields a formula with an accuracy of $O(h^2)$. However, to see this one must use the derivation of eq. (5.5.2).

- Notice that the denominator in eq. (5.5.2) is h^2 . Since h is a small amplitude, therefore h^2 will have a very small amplitude. This illustrates the problem, that computing numerical derivatives using finite differences can be inaccurate if the value of h is too small.

5.6 Third and higher derivatives

- Most textbooks stop with the finite difference formula for the second derivative, and with good reason.
- A finite difference formula for the third derivative will require division by h^3 , which will have a very small amplitude. The numerator will also require multiple subtractions to compute the finite difference. It can be very difficult to obtain a numerically accurate result.
- The obvious procedure is to perform a numerical finite difference by subtraction of two finite difference formulas for the second derivative:

$$\begin{aligned} f'''(x) &\simeq \frac{1}{h} \left[\frac{f(x+2h) + f(x) - 2f(x+h)}{h^2} - \frac{f(x) + f(x-2h) - 2f(x-h)}{h^2} \right] \\ &= \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{h^3}. \end{aligned} \tag{5.6.1}$$

- To derive the order of accuracy of this formula, one must write the Taylor series for $f(x \pm 2h)$ in addition to the Taylor series for $f(x \pm h)$.
- One can proceed in this way to obtain finite difference formulas for higher derivatives. In fact the finite difference formula for $f'''(x)$ can also be obtained using the function values $f(x)$, $f(x \pm h)$ and $f(x \pm 2h)$.

5.7 Symbolic differentiation

- There are numerous mathematical software packages which have libraries of standard mathematical functions. The packages can perform many operations of numerical analysis.
- These packages can symbolically determine the derivative of numerous standard mathematical functions.
- Hence, for example, given $f(x) = \sin(x)$, they can return that $f'(x) = \cos(x)$.
- Hence one can enter an expression such as

$$f(x) = \frac{\ln(x) + \sin(x)}{e^x + \cos(x)}. \quad (5.7.1)$$

The package will return a symbolic expression for $f'(x)$, such as

$$f'(x) = \frac{(1/x) + \cos(x)}{e^x + \cos(x)} - \frac{(\ln(x) + \sin(x))(e^x - \sin(x))}{(e^x + \cos(x))^2}. \quad (5.7.2)$$

- The packages can also return symbolic expressions for the integrals of functions.
- We shall not discuss symbolic differentiation and integration in these lectures.

5.8 Partial derivatives

- There are obviously also numerical finite difference formulas for the partial derivatives of functions of more than one variable. They are also important.
- Let us consider a function of two variables $f(x, y)$.
- The step sizes in x and y are h and k , respectively.
- *The values of h and k need not be equal.*
- To avoid cumbersome notation, we adopt the following notation for the partial derivatives:

$$f_x = \frac{\partial f}{\partial x}, \quad f_y = \frac{\partial f}{\partial y}, \quad f_{xx} = \frac{\partial^2 f}{\partial x^2}, \quad f_{yy} = \frac{\partial^2 f}{\partial y^2}, \quad f_{xy} = \frac{\partial^2 f}{\partial x \partial y}. \quad (5.8.1)$$

The notation for the higher partial derivatives is obvious.

- We require multiple Taylor series. The first four Taylor series are

$$f(x + h, y) = f(x, y) + hf_x + \frac{h^2}{2!} f_{xx} + \cdots \quad (5.8.2a)$$

$$f(x - h, y) = f(x, y) - hf_x + \frac{h^2}{2!} f_{xx} + \cdots \quad (5.8.2b)$$

$$f(x, y + k) = f(x, y) + kf_y + \frac{k^2}{2!} f_{yy} + \cdots \quad (5.8.2c)$$

$$f(x, y - k) = f(x, y) - kf_y + \frac{k^2}{2!} f_{yy} + \cdots \quad (5.8.2d)$$

- These are essentially Taylor series in only one variable. We obtain the obvious formulas

$$\frac{\partial f}{\partial x} \simeq \frac{f(x + h, y) - f(x - h, y)}{2h}, \quad (5.8.3a)$$

$$\frac{\partial f}{\partial y} \simeq \frac{f(x, y + k) - f(x, y - k)}{2k}, \quad (5.8.3b)$$

$$\frac{\partial^2 f}{\partial x^2} \simeq \frac{f(x + h, y) + f(x - h, y) - 2f(x, y)}{h^2}, \quad (5.8.3c)$$

$$\frac{\partial^2 f}{\partial y^2} \simeq \frac{f(x, y + k) + f(x, y - k) - 2f(x, y)}{k^2}. \quad (5.8.3d)$$

- The partial derivative $\partial^2 f / \partial x \partial y$ cannot be obtained from the above Taylor series. We require a Taylor series where both h and k appear

$$\begin{aligned} f(x + h, y + k) &= f(x, y) + hf_x + kf_y \\ &\quad + \frac{h^2}{2!} f_{xx} + hk f_{xy} + \frac{k^2}{2!} f_{yy} \\ &\quad + \frac{h^3}{3!} f_{xxx} + \frac{3h^2k}{3!} f_{xxy} + \frac{3hk^2}{3!} f_{xyy} + \frac{k^3}{3!} f_{yyy} + \cdots \end{aligned} \quad (5.8.4)$$

Note that the coefficient of f_{xy} is hk not $hk/2!$. See also the pattern of the coefficients for the third derivatives (look up Pascal's triangle).

- The four Taylor series are as follows, up to second derivatives only

$$f(x+h, y+k) = f(x, y) + hf_x + kf_y + \frac{h^2}{2!} f_{xx} + hk f_{xy} + \frac{k^2}{2!} f_{yy} + \cdots \quad (5.8.5a)$$

$$f(x-h, y+k) = f(x, y) - hf_x + kf_y + \frac{h^2}{2!} f_{xx} - hk f_{xy} + \frac{k^2}{2!} f_{yy} + \cdots \quad (5.8.5b)$$

$$f(x+h, y-k) = f(x, y) + hf_x - kf_y + \frac{h^2}{2!} f_{xx} - hk f_{xy} + \frac{k^2}{2!} f_{yy} + \cdots \quad (5.8.5c)$$

$$f(x-h, y-k) = f(x, y) - hf_x - kf_y + \frac{h^2}{2!} f_{xx} + hk f_{xy} + \frac{k^2}{2!} f_{yy} + \cdots \quad (5.8.5d)$$

- The finite difference formula for $\partial^2 f / \partial x \partial y$ is

$$\frac{\partial^2 f}{\partial x \partial y} \simeq \frac{f(x+h, y+k) - f(x-h, y+k) - f(x+h, y-k) + f(x-h, y-k)}{4hk}. \quad (5.8.6)$$

This is a centered finite difference formula, where the four points are at the vertices of the rectangle, located at $(x+h, y+k)$, $(x-h, y+k)$, $(x+h, y-k)$ and $(x-h, y-k)$.

- An alternative approximation for $\partial^2 f / \partial x \partial y$ is

$$\begin{aligned} \frac{\partial^2 f}{\partial x \partial y} \simeq \frac{1}{2hk} \Big[& f(x+h, y+k) + 2f(x, y) + f(x-h, y-k) \\ & - f(x+h, y) - f(x, y+k) - f(x-h, y) - f(x, y-k) \Big]. \end{aligned} \quad (5.8.7)$$

This uses expressions that were previously computed to approximate f_x , f_y , f_{xx} , and f_{yy} . The only new computations required are $f(x+h, y+k)$ and $f(x-h, y-k)$.