Queens College, CUNY, Department of Computer Science

Numerical Methods

CSCI 361 / 761

Spring 2018

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March 8, 2018

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

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

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

  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

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

- 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 $O(h)$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2!}\,f''(x) + \cdots \tag{5.2.2}$$

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

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}\,. \tag{5.2.3}$$

  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" $h \to 0$.

- **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 domimated 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 roundof 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

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

- 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

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

- 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

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

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

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

- 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

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

- *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):

$$f''(x) = \frac{f(x+h)+f(x-h)-2f(x)}{h^2} - \frac{h^2}{4!}\, f''''(x) + \cdots \tag{5.5.2}$$

- 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':

$$f''(x) \simeq \frac{1}{h}\biggl[\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}\biggr]. \tag{5.5.3}$$

  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

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

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

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

- 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:
$$f_x = \frac{\partial f}{\partial x}\,, \quad f_y = \frac{\partial f}{\partial y}\,, \quad f_{xx} = \frac{\partial^2 f}{\partial x^2}\,, \quad f_{yy} = \frac{\partial^2 f}{\partial y^2}\,, \quad f_{xy} = \frac{\partial^2 f}{\partial x \partial y}\,. \tag{5.8.1}$$
The notation for the higher partial derivatives is obvious.
- We require multiple Taylor series. The first four Taylor series are
$$f(x+h, y) = f(x, y) + hf_x + \frac{h^2}{2!}\,f_{xx} + \cdots \tag{5.8.2a}$$
$$f(x-h, y) = f(x, y) - hf_x + \frac{h^2}{2!}\,f_{xx} + \cdots \tag{5.8.2b}$$
$$f(x, y+k) = f(x, y) + kf_y + \frac{k^2}{2!}\,f_{yy} + \cdots \tag{5.8.2c}$$
$$f(x, y-k) = f(x, y) - kf_y + \frac{k^2}{2!}\,f_{yy} + \cdots \tag{5.8.2d}$$
- These are essentially Taylor series in only one variable. We obtain the obvious formulas
$$\frac{\partial f}{\partial x} \simeq \frac{f(x+h, y) - f(x-h, y)}{2h}\,, \tag{5.8.3a}$$
$$\frac{\partial f}{\partial y} \simeq \frac{f(x, y+k) - f(x, y-k)}{2k}\,, \tag{5.8.3b}$$
$$\frac{\partial^2 f}{\partial x^2} \simeq \frac{f(x+h, y) + f(x-h, y) - 2f(x, y)}{h^2}\,, \tag{5.8.3c}$$
$$\frac{\partial^2 f}{\partial y^2} \simeq \frac{f(x, y+k) + f(x, y-k) - 2f(x, y)}{k^2}\,. \tag{5.8.3d}$$
- 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
$$\begin{aligned} f(x+h, y+k) = f(x, y) &+ hf_x + kf_y \\ &+ \frac{h^2}{2!}\,f_{xx} + hk\,f_{xy} + \frac{k^2}{2!}\,f_{yy} \\ &+ \frac{h^3}{3!}\,f_{xxx} + \frac{3h^2k}{3!}\,f_{xxy} + \frac{3hk^2}{3!}\,f_{xyy} + \frac{k^3}{3!}\,f_{yyy} + \cdots \end{aligned} \tag{5.8.4}$$
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

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

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

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

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

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

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

  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

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

  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 $f(x-h,y-k)$.

5.9 Unequal step sizes (homework exercises, but not for examination)

- Let us return to ordinary derivatives and a function of one variable $f(x)$.
- The forward and backward step sizes h_1 and h_2 need not be equal.

$$f(x+h_1) = f(x) + h_1 f'(x) + \frac{h_1^2}{2!} f''(x) + \frac{h_1^3}{3!} f'''(x) + \cdots \tag{5.9.1a}$$

$$f(x-h_2) = f(x) - h_2 f'(x) + \frac{h_2^2}{2!} f''(x) - \frac{h_2^3}{3!} f'''(x) + \cdots \tag{5.9.1b}$$

- For the first derivative df/dx, we can form forward and backward finite differences as usual.

$$f'_{\rm fwd}(x) \simeq \frac{f(x+h_1) - f(x)}{h_1}\,, \qquad f'_{\rm back}(x) \simeq \frac{f(x) - f(x-h_2)}{h_2}\,. \tag{5.9.2}$$

- These are obviously of first order in accuracy.
- The leading error term is $O(h_1 f''(x))$ or $O(h_2 f''(x))$.
- If $h_1 \neq h_2$, the following finite difference also contains an error term in $f''(x)$:

$$f(x+h_1) - f(x-h_2) = (h_1+h_2) f'(x) + \frac{h_1^2 - h_2^2}{2!} f''(x) + \frac{h_1^3 + h_2^3}{3!} f'''(x) + \cdots \tag{5.9.3}$$

$$f'(x) = \frac{f(x+h_1) - f(x-h_2)}{h_1+h_2} - \boldsymbol{\frac{h_1 - h_2}{2!} f''(x)} - \frac{h_1^2 - h_1 h_2 + h_2^2}{6} f'''(x) + \cdots \tag{5.9.4}$$

- Admittedly the term in $f''(x)$ is multiplied by a factor $h_1 - h_2$, which equals zero if $h_1 = h_2$, so it is not exactly a "first order" error term. Nevertheless, it is formally proportional to $f''(x)$ not $f'''(x)$.
- We require a differently weighted finite difference to cancel the term in $f''(x)$.
- That will be the subject of a homework exercise.

5.10 Why use unequal steps? Answer #1: computational finance

- Depending on the problem, there may not be a choice.
- In computational finance, which has occupied a lot of my career, one has to solve the so-called **Black–Scholes equation.**
- The full equation is a partial differential equation. Simplifying somewhat, we need to solve an ordinary differential equation of the form

$$\tfrac{1}{2}\sigma^2 S^2 \frac{d^2 f}{dS^2} + rS\,\frac{df}{dS} - rf = R(S)\,. \tag{5.10.1}$$

- We must solve the above equation for $f(S)$, where S is the stock price, σ and r are constant parameters and $R(S)$ is a known right–hand side function.
- In general, eq. (5.10.1) is too difficult to solve analytically and must be solved numerically.
- One technique is to approximate the derivatives using finite differences.
- This is a widely employed technique for solving many differential equations.
- We solve eq. (5.10.1) using a set of points S_i, $i = 0, 1, 2, \dots$.
- Then the sreps are of unequal size.
- A simple–minded finite difference approximation is (see Sec. 5.9)

$$f'(S_i) \simeq \frac{f(S_{i+1}) - f(S_{i-1})}{2(S_{i+1} - S_{i-1})}\,, \qquad f''(S_i) \simeq \frac{f(S_{i+1}) - 2f(S_i) + f(S_{i-1})}{(S_{i+1} - S_{i-1})^2}\,. \tag{5.10.2}$$

- Even with a better quality weighted finite difference approximation, the steps in S are unequal.
- *Why do this?*
- **The answer is that the function $R(S)$ may not be continuous, or it may be continuous but it may have "kinks" (discontinuous changes of slope) at irregularly spaced values of S. To match the locations of those kinks, the values of S_i must be unequally spaced.**
- It is usually not possible to find a uniform set of steps $S_i = ih$, $i = 0, 1, 2, \dots$. If we do so, the kinks or discontinuities in $R(S)$ will not in general coincide with any of the values S_i.
- Hence we must compromise.
    1. We use non–uniform steps in S and place a point (a value of S_i) at every kink in $R(S)$. The numerical derivatives are more complicated but we match the function $R(S)$.
    2. We use uniform steps in S and but we do not place a point (a value of S_i) at every kink in $R(S)$. The numerical derivatives are simpler but we do not match the function $R(S)$.
- Using equal finite–difference steps is not always the best choice.
- There are consequences, in important practical applications.
- I have seen this many times in my career.

5.11 Why use unequal steps? Answer #2: particle accelerators

- We can model a particle accelerator (actually some but not all) as a closed loop of magnets.
- To keep things simple, suppose the accelerator is "circular" and define a variable θ such that $0 \le \theta \le 2\pi$ spans one full circle, i.e. the circumfreence of the accelerator.
- If the accelerator is not a closed loop we simply say the value of θ does not go up to 2π.
- We have to solve equations of motion for the particles, to calculate their trajectories in the accelerator.
- We go back to Newton's force law $\vec{F} = m\vec{a}$, where $\vec{F}$ is the force vector and $\vec{a}$ is the particle's acceleration vector (and m is the particle mass).
- We gloss over the complications of Einstein's theory of relativity.
- Let the particles be indexed by $j = 1, 2, \ldots$. The coordinate vector of each particle is $\vec{x}_j$ and the acceleration vector is $\vec{a}_j = d^2\vec{x}_j/d\theta^2$ (glossing over more technical details).
- Then we must solve equations of motion of the form

$$\frac{d^2 x_j}{d\theta^2} = \vec{F}_j \,. \tag{5.11.1}$$

- The force $\vec{F}_j$ depends on $\vec{x}_j$ and other things and is usually complicated.
- Hence eq. (5.11.1) is a set of ordinary differential equations, which in general must be solved numerically.
- **However, the magnets do not all have equal length, and they are not spaced uniformly around the circumference of the accelerator.**
- Hence if we employ uniform steps $\theta_i = ih$, $i = 0, 1, 2, \ldots, N$, where say $h = 2\pi/N$, in general the values of θ_i will not match the entrance/exit locations of the magnets.
- ***This is not acceptable.*** We will take finite difference steps where, in some cases, we begin inside a magnet and end up outside the magnet.
- Hence the numerical finite difference for $d^2\vec{x}_j/d\theta^2$ cannot in general employ equal steps in θ.
- This has also been an important part of my career.
- Hence, for essentially all of my career, it has not been possible to employ equal steps for finite difference numerical derivatives.