Math 563, Spring 2019
Last updated: 1/21/20

HOMEWORK 2
MATH 563, SPRING 2020

DUE WEDNESDAY, JAN. 29

Reading: Read the following (book sections refer to Quarteroni unless otherwise noted).

- Suggested: The section in Chapter 10 on differentiation (10.10.1)

Code to turn in:

- Your `deriv(x,y)` function from Q5 that computes the derivative of data `x,y` (no working example required, but you can turn other code for feedback if desired).

1. Problems (some with, some without code)

Q1 (heuristic for choice of h). Consider using a formula with an error of size $O(h^2)$ to approximate the fourth derivative of $f(x)$ at a point x_0, where $f(x)$ is computed to machine precision.

a) Suppose you are writing code that uses this formula (with a free choice of h) for the fourth derivative. Determine a rough order of magnitude estimate of the choice of h and associated (best possible) error to inform your choice.

b) Generalize to the k-th derivative.

Q2 (a typical derivation). Use Taylor series to derive a four point formula with the error term for $f'(0)$ using the points $0, -h, -2h$ and $-3h$. (We will use such a formula later when solving ODEs, where this is useful because it depends on data at earlier times).

You can assume the individual error terms with $f^{(n+1)}(\eta)$ merge together as if the η's were equal, as done in the notes (since we justified it there).

Q3 (Richardson extrapolation). Consider the error series for the three-point forward difference, which does not have any nice symmetry:

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + \sum_{i=2}^{\infty} c_i h^i. \tag{1}$$

Denote the approximation by $D(h)$.

a) Use Richardson extrapolation to derive a more accurate formula $D_1(h)$ for $f'(x)$ that uses (at most) the five points $0, h/2, h, 3h/2$ and $2h$; write it in terms of $D(h)$.

b) Derive a computable error estimate for $D(h)$ that uses the quantities $D(h)$ and $D(h/2)$.

c) Continue the process in (a) to get a sequence of formulas $D_k(h)$.

d) A complicated function has been supplied (`func.m`)[1]. Estimate its derivative at $x_0 = 1$ using the three point formula (1). Make an error plot (vs. h) and show that the order of convergence is correct.[2]

Tip: You don't need to do a rigorous fit to the data if there is a clear linear trend (just figure out the slope). The other way this is done is bv preparing a table of data and estimating the slope from that.

e) Suppose you are asked to estimate the derivative at $x_0 = 1$ to within an error of 10^{-9}. Use the process in (c) to do so, and justify the accuracy of your proposed answer.

Q4. Consider the function $f(x) = \sin(x + x^{3/2})$, the three-point forward difference from Q3 (that is, $D(h)$) and the two-point difference $(f(x + h) - f(x))/h$.

Compare the error as a function of h for the two formulas at $x_0 = 0$. Explain your results. *You may also want to consider* $x_0 = 1$.

Q5 (estimate with boundaries; perils of differentiating data). Modify the `deriv` code from HW 1 to provide an estimate for $f'(x)$ at the given points that is **second order** at all points.

a) Test your function against $f(x) = \sin x$ on $[0, \pi]$ with equally spaced points; show that the maximum error in $f'(x)$ has the correct order.

b) (AC) Now load the data `deriv_data.txt` (code provided). The data was created by sampling the function $f(x) = \sin x$. adding a small amount of random noise - the sort of data you might obtain from a physical experiment.

Compute the estimate of the derivative on this 'noisy data' and plot it against the true derivative without noise. What do you see?

Iterate this to compute the next order derivative and keep going. What happens as you take more and more derivatives? Discuss briefly.

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[1] This is the **Airy function** $\text{Ai}(x)$, which appears in solving differential equations and asymptotics; it is the solution to $y'' = xy$ with $y \to 0$ as $x \to \pm\infty$ and does not have a closed form

[2] The process here is the typical one for a 'convergence plot' to validate numerics - derive the predicted behavior and a computable estimate from theory, then compare the real results to the prediction.

Q6 (half-point derivative approximations) (AC)**.** Let $a(x)$ and $b(x)$ be some given (known) functions. Expressions like

$$(a(x)u')' \tag{2}$$

appear often in applications (in studying **convection-diffusion** processes) for $u(x)$, and are often used in numerical methods for PDEs.

Suppose $u(x)$ is known at points $x_0, x_1, \cdots, x_n$ (with value $u_0, u_1, \cdots$) with equal spacing h.

Define the **half-points**

$$x_{i+1/2} = x_i + h/2, \quad i = 0, \cdots, n-1$$

and associated values $u_{i+1/2}$ (which are not known!).

a) Let $\delta_h f = (f(x+h) - f(x-h))/(2h)$ be the usual centered difference. Show that the $O(h^2)$ centered difference formula can be written as $\delta_{h/2}^2 f$ (i.e. $\delta_{h/2}$ applied to $\delta_{h/2} f$).

b) Take the centered difference with $h/2$ to $f = a(x)u'$, then use it again on u' (also with $h/2$ to get a formula that involves only values of u at $x_{i\pm 1}$ and x_i (be careful with $a(x)$).

c) What is the order of accuracy for this approximation? Give a reasonable justification (from theory, not computation). (messier problem: prove your answer).