Mathematics 371 – Numerical Analysis
Discussion 3 – Numerical Differentiation and Extrapolation
October 24-26, 2001

Background

On Monday, we introduced some basic techniques for numerical approximation of derivatives and derived the following error terms:

$$f'(x_0) = \begin{cases} \frac{f(x_0+h)-f(x_0)}{h} - \frac{f''(\xi_f)}{2}h & \text{(2 point forward difference)} \\ \frac{-3f(x_0+2h)+4f(x_0+h)-f(x_0)}{2h} + \frac{f'''(\xi_f)}{3}h^2 & \text{(3 point forward difference)} \\ \frac{f(x_0+h)-f(x_0-h)}{2h} - \frac{f'''(\xi_c)}{6}h^2 & \text{(3 point centered difference)} \end{cases}$$

where $\xi_f \in [x_0, x_0 + h]$ for the 2-point formula, $\xi_f \in [x_0, x_0 + 2h]$ for the 3-point forward difference formula, and $\xi_b \in [x_0 - h, x_0]$, and $\xi_c \in [x_0 - h, x_0 + h]$. Because the error term for the centered difference approximation goes to zero faster as $h \to 0$, to get a desired accuracy, we will not need to take h as small, and round-off problems will be correspondingly smaller!

Today, we want to think about a way to get more accurate approximations, without causing roundoff error problems by trying to use very small h values. The error for both the 2 point forward difference approximation above is $O(h)$. The errors for 3 point forward difference and centered difference approximations are $O(h^2)$.

There is a general way to combine several approximations derived from a particular method with a known error term that yields an *improved error term*. The name for the method in general is *Richardson extrapolation*. The idea is reminiscent of Aitken acceleration in some ways, but it is different. Here is the basic idea, in general terms. Suppose we have some way to produce approximations $N(h)$ to some quantity M using different values of h, and suppose, for instance, that the error is $O(h)$. Suppose we can expand the error in a *power series* in h as follows:

$$M = N(h) + c_1h + c_2h^2 + c_3h^3 + \cdots$$

Then if we combine the two approximations:

$$M = \begin{cases} N(h) + c_1h + c_2h^2 + \cdots \\ N(\frac{h}{2}) + c_1\frac{h}{2} + c_2\left(\frac{h}{2}\right)^2 + \cdots \end{cases}$$

by taking

$$\begin{aligned} M &= 2M - M \\ &= 2\left(N\left(\frac{h}{2}\right) + c_1\frac{h}{2} + c_2\left(\frac{h}{2}\right)^2 + \cdots\right) - (N(h) + c_1h + c_2h^2 + \cdots) \\ &= \left(2N\left(\frac{h}{2}\right) - N(h)\right) + c_2'h^2 + \cdots \end{aligned}$$

then the h terms *cancel*! That is, using $M \doteq \left(2N\left(\frac{h}{2}\right) - N(h)\right)$, we get an error term that is $O(h^2)$ rather than $O(h)$!

Discussion Questions

A) Suppose the error term for the "N-method" was $O(h^2)$ instead of $O(h)$. How could you combine $N(h)$ and $N(h/2)$ to get an error term that is $O(h^3)$ or better? Apply this to the three-point forward difference formula to derive an approximation to $f'(x_0)$ with error $O(h^3)$ or better.

B) Apply your method from part A to the 3-point *centered difference formula* to produce an approximation method for $f'(x_0)$ with error $O(h^3)$ or better. It can be shown, using Taylor series, that the error term for the centered difference approximation actually has the form $c_2h^2 + c_4h^4 + \cdots$ (only even powers of h). What does that say about the actual order of the error?

C) Generalizing part A, suppose the error term for the "N-method" was $O(h^k)$ instead of $O(h)$. How could you combine $N(h)$ and $N(h/2)$ to get an error term that is $O(h^{k+1})$ or better?

D) Use a degree 2 interpolating polynomial for f to derive a forward difference approximation to $f''(x_0)$. What is the error of your approximation? For which k is the error $O(h^k)$?

E) Use your answer from C and Richardson extrapolation to derive an approximation method for $f''(x_0)$ with error $O(h^2)$ or better.

F) There's nothing magic about h and $h/2$ in Richardson Extrapolation. Do Exercise 9 from Section 4.2 in the text to see how the same sort of improvement of the order of the error could be done with h, $h/3$, $h/9$, etc.

Assignment

Write-ups due in class Wednesday, October 31.