MS554 Lecture Notes: Numerical Calculations
Lecture 3; Sept. 4, 2003

Class business:

- Time/Place: Classroom C; 10:00 - 11:20 Tuesday, Thursday.
- Class lectures on blackboard.
- Homework 1 due today; in my mailbox on the 2nd floor of Franklin by close-of-business.
- Next Thursday: hand in a few sentances and tentative title describing your idea for your research project.

Materials used:

- Hornberger and Wiberg Notes, Chapter 3.
- Gerald and Wheatley; Appendix A, Chapter 5.
- Forsythe, et al. Chapter 5

Objectives:

- Taylor series expansions approximate functions at any point, and allow us to quantify the error in an approximation.
- You can numerically estimate a function's derivatives or integrals using polynomial approximations to the function.
- Error in numerical calculus decreases as step size decreases, and as the order of the approximation increases.

Taylor Series Expansion

A Taylor series expansion can be used to estimate a function at any point:

$$f(x+\Delta x) = f(x) + \Delta x f'(x) + f''(x)\frac{\Delta x^2}{2!} + f'''(x)\frac{\Delta x^3}{3!} + \cdots + f^{(n)}(x)\frac{\Delta x^n}{n!} + R_n; \quad (1)$$

$$R_n = \int_{x+\Delta x}^{x} \frac{(x-t)^n}{n!} f^{(n+1)}(t)dt \quad (2)$$

It is an infinite sum. When the up to $f^{(n)}$ terms are applied, the truncation error can be approximated by the next term in the series, $f^{(n+1)}(x)\Delta x^{n+1}/(n+1)!$. This term will generally decrease as Δx decreases, and as n increases. The error term would be said to be *of order n+1*, or in shorthand: $O(\Delta x^{n+1})$.

Numerical Differentiation

A common need in numerical calculations is to estimate derivatives of a function. This may be required when there is no analytical form for the derivative, or when it is simply more convenient than finding the analytical form of the derivative. The first derivative would be f'(x) = df(x)/dx; equal to the slope of the line of f(x) evaluated for some x. The second derivative would be $f''(x) = d^2f(x)/dx^2$, etc. Suppose you can evaluate $f(x_0)$ and $f(x_1) = f(x_0 + \Delta x)$; a Taylor series expansion can be used to estimate f'(x):

$$f(x_2) = f(x_1 + \Delta x) = f(x_1) + \Delta x f'(x_1) + f''(x_1)\frac{\Delta x^2}{2} + O(\Delta x^3). \quad (3)$$

this can be rewritten:

$$f'(x_1) = \frac{f(x_1 + \Delta x) - f(x_1)}{\Delta x} - f''(x_1)\frac{\Delta x}{2} - \cdots \quad (4)$$

So the first derivative of f(x) can be approximated by the values of f(x) and $f(x + \Delta x)$, to $O(\Delta x)$. This is the *forward difference*, the *backward difference* is found in a similar way by evaluating $f(x - \Delta x)$.

A more accurate difference method can be found evaluating both $f(x - \Delta x)$ and $f(x + \Delta x)$.

$$\begin{aligned} f(x_2) &= f(x_1 + \Delta x) \quad (5) \\ &= f(x_1) + \Delta x f'(x_1) + f''(x_1)\frac{\Delta x^2}{2} + f'''(x_1)\frac{\Delta x^3}{3!} + O(\Delta x^4) \end{aligned}$$

$$\begin{aligned} f(x_0) &= f(x_1 - \Delta x) \quad (6) \\ &= f(x_1) - \Delta x f'(x_1) + f''(x_1)\Delta x^2/2 - f'''(x_1)\frac{\Delta x^3}{3!} + O(\Delta x^4) \end{aligned}$$

Now subtract these two equations together and rearrange to get the *centered difference* approximation:

$$f'(x_1) = \frac{(f(x_2) - f(x_0))}{2\Delta x} + O((\Delta x)^2) \quad (7)$$

Add equations 5 and 6 together and rearrange to get an approximation for the second derivative:

$$f''(x_1) = \frac{(f(x_2) - 2f(x_1) + f(x_0))}{\Delta x^2} + O((\Delta x)^2) \quad (8)$$

More accurate estimates can be made using more than three points, but these become awkward to apply near a boundary. Usually, the required accuracy is achieved by decreasing the step size (Δx).

Numerical Integration

Numerical integration is often necessary. It is usually done by breaking the interval over which the integration is needed (say from x = a to b) into a series of "sub-panels", and summing the area of all sub-panels. To get the area of each sub-panel, the function is approximated locally as a constant (the rectangle rule), a trapezoid (the trapezoid rule), a cubic (Simpson's rule), or a general polynomial (Newton-Cotes). Mathematicians use the phrase *quadrature* to represent numerical integration, to differentiate it from the solution of differential equations.

Trapezoid and Rectangle Rules

To use the rectangle rule, the integral for a subpanel between x_0 and x_1 is approximated using

$$\int_{x_0}^{x_1} f(x)dx \approx (x_1 - x_0) f\left(\frac{x_0 + x_1}{2}\right); \tag{9}$$

$$L.E. = \frac{1}{24}(\Delta x)^3 f''(x). \tag{10}$$

L.E. represents the *local error*; or error within that subpanel. The trapezoid rule uses information about f(x) at each boundary and approximates the integral as the area of a trapezoid:

$$\int_{x_0}^{x_1} f(x)dx \approx (x_1 - x_0)\left(f(x_0) + f(x_1)\right)/2; \tag{11}$$

$$L.E. = \frac{-1}{12}(\Delta x)^3 f''(x). \tag{12}$$

Interestingly, both the rectangle and trapezoid rule have similar error bounds.

Both the trapezoid and rectangle rules can be applied as *composites*. That is, the region to be integrated can be divided into a series of panels, and the areas under the trapezoidal or rectangular regions for each panel estimated. The sum of these areas is then an estimate of the total integral. If you take Δx_i for each sub-panel to be equal (they don't have to be) the resulting composite trapezoidal rule is

$$\int_{a}^{b} f(x)dx \approx \sum \left[\frac{\Delta x}{2}\left(f(x_i) + f(x_{i+1})\right)\right]; \tag{13}$$

$$G.E. = N\left(\frac{-1}{12}\Delta x^3 f''(x)\right) \sim \Delta x^2. \tag{14}$$

Simpson's Rules

Simpson's rules rely on fitting piece-wise quadratics and cubics to the function f(x), and then integrating the area under these polynomials. They give more accurate results than the rectangle and trapezoid rules, and are just as easy to use. Because they fit higher-order polynomials, each fitted polynomial needs to be applied over more than one sub-panel. For example, a quadratic needs to be fit to three points. So Simpson's 3/2 rule is applied only to data sets that lend themselves to having and even number of sub-panels. The equation for integration using Simpson's 3/2 rule is

$$\int_a^b f(x)dx \approx \frac{\Delta x}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)]; \tag{15}$$

With

$$GE = \frac{b-a}{180} f^{(iv)}(x)\Delta x^4, \tag{16}$$

where n is an even number (2, 4, ...).

The general Newton-Cotes rule approximates f(x) with piece-wise polynomials and integrates each polynomial. The rectangle and trapezoid rules are special cases of this- being polynomials of order 0 and 1 (constant and linear, respectively). Simpson's rule uses a quadratic polynomial and achieves a higher degree of accuracy.