Scientific Computing, Courant Institute, Fall 2018

http://www.math.nyu.edu/faculty/goodman/teaching/ScientificComputing2018/ScientificComputing.html Always check the classes message board before doing any work on the assignment.

Assignment 2, due September 27

Corrections: [none yet]

1. The following situation arises in numerical simulations of fluid motion. There are uniformly spaced grid points $x_k = k\Delta x$ with grid spacing Δx . There is a smooth function f(x) whose values we do not know. We know the cell averages

$$\overline{f}_k = \frac{1}{\Delta x} \int_{|x-x_k| \le \frac{1}{2} \Delta x} f(x) \, dx \; .$$

The *cell* C_k about x_k is an interval of length Δx whose center is x_k , which means

$$C_k = \left\lfloor x_k - \frac{1}{2}\Delta x, x_k + \frac{1}{2}\Delta x \right\rfloor \;.$$

The cell average is

$$\overline{f}_k = \frac{1}{\Delta x} \int_{C_k} f(x) \, dx$$

- (a) Show that $\overline{f}_k = f_k + O(\Delta x^2)$.
- (b) Show that there is an asymptotic expansion of the form

$$f_k = \overline{f}_k + g_{2,k}\Delta x^2 + g_{4,k}\Delta x^4 + \cdots$$

Find a formula for $g_{2,k}$ in terms of f and its derivatives at x_k .

(c) Find a and b so that

$$f_k = a\overline{f}_{k-1} + b\overline{f}_k + a\overline{f}_{k+1} + O(\Delta x^4)$$

Hint: it suffices to find an second order accurate approximation to $g_{2,k}$. For second order accurate formulas, you can use $f_k = \overline{f}_k + O(\Delta x^2)$. Once you have the formula, verify that you have achieved the desired order of accuracy.

(d) Write a simple Python script to verify the orders claimed using $f(x) = e^x$, and $\overline{f}_k = \frac{1}{\Delta x} \left(e^{\frac{\Delta x}{2}} - e^{-\frac{\Delta x}{2}} \right) f_k$. Do a convergence study with a sequence of Δx values to verify that your formula from part (c) is fourth order accurate. Choose a sequence of Δt values that differ by a factor of 2 and continues until roundoff error is larger than truncation error.

2. Suppose we want to estimate the value of a function f(x, y) known at three places $f(hx_1, hy_1)$, $f(hx_2, hy_2)$, and $f(hx_3, hy_3)$. For the analysis, imagine that the (x_1, y_1) , etc., are fixed as $h \to 0$. We want an estimate of the form

$$\widehat{f}(0,0) = \sum_{k=1}^{3} a_k f(hx_k, hy_k)$$

Find the optimal order of accuracy $\hat{f}(0,0) - f(0,0) = h^p A_p + \cdots$ that holds for general functions f with enough derivatives. Find the corresponding weights a_k . Under what conditions are the weights all positive.?

3. Write a Python module that does panel method integration using n equal size panels over an interval [a, b]. The integration function should be something like

Write it flexibly enough so that you can easily try several of the panel integration methods including the lowest order one and one of the higher order ones. Try it on this example, which you know the answer to.

$$\int_0^2 \sin(x) \, dx = 1 - \cos(2) \; .$$

Verify using a convergence study that the methods have the claimed order of accuracy.

4. Write an adaptive integrator that calls the fixed integrator from problem 3 with a sequence of step sizes, estimates the errors, and stops when the estimated error is below a specified tolerance. Apply this to some harder problems such as

$$\int_0^2 e^{-\frac{x^2}{r^2}} \cos(kx) \, dx$$

The problem becomes more challenging when k is large and when r is large. Experiment with your code and report how well it does on the harder problems. Does work get the desired accuracy with less work using a higher order integrator?