Homework 4
MA/CS 375, Fall 2005
Due November 11

This homework will count as part of your grade so you must work independently. It is permissible to discuss it with your instructor, the TA, fellow students, and friends. However, the programs/scripts and report must be done only by the student doing the project. Please follow the guidelines in the syllabus when preparing your solutions.

1. (25 pts.) In this problem we approximate the derivative of a function defined on a uniform grid on the interval (a,b), i.e. for the grid

$$x_k = a + k\frac{(b-a)}{n} \ , \ k = 0, 1, \cdots, n$$

   (a) Show (using Taylor series) that the formula

$$f'(x_k) - \frac{f(x_{k+1}) - f(x_{k-1})}{2h} = \frac{h^2}{6} f'''(\xi_k) \ , \ \xi_k \in (x_{k-1}, x_{k+1})$$

   is valid for all interior grid points, i.e. $k = 1, 2, \cdots, n-1$.

   (b) For the end points, use Taylor series to show that

$$\begin{aligned} f'(x_0) - \frac{-3f(x_0) + 4f(x_1) - f(x_2)}{2h} &= -\frac{h^2}{3} f'''(\xi_0) \ , \ \xi_0 \in (x_0, x_2) \\ f'(x_n) + \frac{-3f(x_n) + 4f(x_{n-1}) - f(x_{n-2})}{2h} &= +\frac{h^2}{3} f'''(\xi_n) \ , \ \xi_n \in (x_{n-2}, x_n) \end{aligned}$$

   (c) Write a code that uses the above formulas to produce a second order accurate approximation for the derivative of the function

$$f(x) = \cos(10x) - 3\sin(13\pi x)$$

   on the interval $-1 \le x \le 1$, with an error no larger than $tol = 10^{-6}$. You must estimate the third derivative of your function using a worst case senario, and choose the stepsize h based on your estimates. You must compute the exact derivative at the same grid points and produce a plot of your absolute error.

2. (25 pts.) Modify one of the programs in the text (midpointc, trapc or simpsonc) to use the composite Newton's 3/8-rule on a uniform partition to approximate an integral. On a subinterval (x_{k-1}, x_k) of width h the 3/8-rule is defined by:

$$\int_{x_{k-1}}^{x_k} f(x)dx \approx \frac{h}{8}\left(f(x_{k-1}) + 3f(x_{k-1} + h/3) + 3f(x_{k-1} + 2h/3) + f(x_k)\right).$$

Show that the rule is exact for polynomials of degree 3 or less and use this fact to predict the order of the method. Use the method with $n = [5\ 10\ 20\ 40\ 60\ 80\ 100]$ subintervals to approximate:

$$\int_0^1 \sin(\pi x) e^{2x} dx.$$

Using the fact that the exact value of the integral is $\frac{\pi}{4+\pi^2}(e^2+1)$, compute the errors in your approximations and make a loglog plot of the error versus n. Is the result approximately a straight line? Use polyfit to compute a linear approximation, $\log(\text{error}) = a\log(n) + b$ to the data. Is the slope, a, what you expect from the error analysis?

3. (25 pts.) The four point Gauss-Lobatto formula for approximating integrals takes the form:

$$\int_{x_{k-1}}^{x_k} f(x)dx \approx h\left(w_1 f(x_{k-1}) + w_2 f(x_{k-1} + c_1 h) + w_3 f(x_{k-1} + c_2 h) + w_4 f(x_k)\right), \quad h = x_k - x_{k-1}.$$

The weights w_j, $j = 1, \ldots, 4$ and constants c_1, c_2 can be chosen so that the formula is exact for polynomials of degree 5. Find them. What is the order of the resulting method?
Hint: solve the problem on the standard interval $[-1, 1]$ and then translate the results to an arbitrary interval. The weights w_j can be determined for arbitrary values of c_j using cubic interpolation and will lead to methods exact for cubic polynomials. You can then determine the two free node locations so that the formula is exact for x^4 and x^5. You will need to solve an algebraic equation - you can do this either symbolically or using fzero. Solve it accurately enough so that you can give us the w_j and c_j to 14 digits.

4. (25 pts.) The adaptive quadrature code given in the text, estimates the error in Simpson's rule by performing two integrations over the interval A. The first uses the simple Simpson rule, with the nodes $[a, (a+b)/2, b]$, i.e. with stepsize $H_1 = b - a$ to compute the approximation I_s. The second uses the composite Simpson's rule with 2 subintervals, i.e. nodes $[a, (a+b)/4, (a+b)/2; (a+b)/2, 3(a+b)/4, b]$ and stepsize $H_2 = (b-a)/2$, to compute the (more accurate) approximation I_s^c.

   The text uses the two approximations to estimate the error and, if that turns out to be less than a predefined tolerance, it uses the more accurate result of the two, i.e. I_s^c, as the actual estimate for the integral in the interval A. This problem is about improving this calculation through the judicious use of both results, I_s and I_s^c.

   It can be shown that the error in Simpson's method for integrating a function that is differentiable at least five times can be actually written as

$$I[f] - I_s^c[f; M] = c_1 * \left(\frac{b-a}{M}\right)^4 + c_2 * \left(\frac{b-a}{M}\right)^5 + \cdots$$

where c_1, c_2, etc are constants, independent of M (for functions f that have more derivatives in the interval of integration, we can add more terms to that expression, but that is not important here). The leading term in this expression is of order 4, which is the order of the method. In this problem we learn how to get a more accurate result using the work already performed. To that purpose:

(a) Find a linear combination of the two results that has leading error term of order 5; that is you must find constants A_1 and A_2 such that

$$I[f] - (A_1 I_s^c + A_2 I_s) = c_2' \left(\frac{b-a}{M}\right)^5 + \cdots$$

The idea is to combine the two results in such a way so that the leading error term is cancelled.

(b) Now alter the program simpadpt in the text, p.98, to use this improved estimate of the integral over A instead of the (less accurate) estimate I_s^c. Demonstrate your code by producing a more accurate computation of the integral in example 4.3. Your computation should employ the same tolerance ($tol = 10^{-5}$) and minimum stepsize ($hmin = 10^{-3}$) as the values in the text, and therefore end up using the same number of subintervals. Nevertheless, your result ought to be closer to the exact value

$$\int_{-1}^{1} e^{-(10)(x-1)^2} dx = 0.28024956081990 ,$$

than the one found by program simpadpt.