CBE 20258 Numerical and Statistical Analysis

Algorithm Problem Set 6

due in the box in the CBE office Friday, 4/28/17

Problem 1. Optimal Quadrature: A sphere of dimensionless radius of unity is first heated to a uniform temperature (dimensionless value of unity as well), and then the surface is quenched to a fixed temperature T = 0 (e.g., reference value). You are assigned the task of measuring the total energy content of the sphere as a function of time, but you are only given one temperature probe to do it with.

a. It is proposed to simply put the probe in the center of the sphere and assume that the entire sphere is at that constant temperature. What would be the quadrature rule consistent with that assumption?

b. You respond with "wait a minute – we know that the temperature at the surface is zero, and that the temperature is also an even function of r from symmetry! Using this, and leaving the probe in the center, what is a better quadrature rule that takes advantage of this observation?

c. Your buddy argues that even this isn't optimal: you can instead put the probe at a location different from the center. What is the optimal location to put it, and how do you calculate the energy content from this measurement (e.g., your best quadrature rule)?

The dimensionless energy integral is given by:

$$E = \int_0^1 T\, 4\pi r^{*2} dr^*$$

d. The exact temperature and energy can be calculated from the infinite series solution:

$$T = \sum_{n=1}^{\infty} \frac{2(-1)^{n-1}}{n\pi} e^{-n^2\pi^2 t^*} \frac{\sin(n\pi r^*)}{r^*} \qquad \text{and} \qquad E^* = \sum_{n=1}^{\infty} \frac{8}{n^2\pi} e^{-n^2\pi^2 t^*}$$

Using this, plot up the results of the three quadrature rules for the total energy as well as the exact solution for t* from zero to 0.5. On a separate graph, plot up the deviation of the quadrature rules from the exact value for the same range in time. Turn the grid on so that the result is much clearer. Note that the series for the temperature converges -very- slowly for r = 0 at short times (it requires n>>1/r* at t* = 0 to converge). Thus, just evaluate the temperature for r* = 0.001 for those cases, and keep a lot of terms in the series! This can be done via an anonymous function using "sum" and taking n as a vector.

e. There is an experimental measurement error of the probe of ±0.01. What is the random experimental error of each of the quadrature rules above? Is there any point where this dominates the overall error, and which rule would be optimal in this case?

Problem 2. Quadrature and Error:

a. Any quadrature rule basically boils down to a weighted linear combination of function evaluations. Sometimes we are integrating functions of data. If we have the rule:

$$I \approx \sum_{i=1}^{n} w_i\, f(b_i)$$

where the b_i are data measurements at node locations x_i and the w_i are the quadrature weights, what is the random error in the integral in terms of the matrix of covariance of the data?

b. Often we want to integrate data, meaning that our function evaluations are done at fixed, evenly spaced node locations where the data has been measured. This is usually done via either Simpson's Rule, or the Trapezoidal Rule. Suppose we have a large number of panels (e.g., a large number of points where we have done the evaluation). Discounting the first and last point (remember that for both SR and TR the weight on these is different from interior nodes), calculate the ratio of the random error of the integral of evenly spaced data points using these two rules, assuming that the data points are independent.

Problem 3. Systems of Equations:

The velocity profile due to a heated wire (this is one of the experiments in senior lab) is governed by the pair of coupled non-linear ODE's given below.

$$f''' = -g + \frac{1}{Pr}\left[\frac{1}{5}(f')^2 - \frac{3}{5} f f''\right]$$

and

$$g' = \frac{-3}{5} f g$$

For those of you who are interested, f ' is the dimensionless vertical velocity (f is the streamfunction) and g is the dimensionless temperature. Pr is the Prandtl number, a constant determined by the fluid used in the experiment.

a. For this problem, write down the equivalent set of first order coupled ODE's, identifying all the dependent variables.

b. Show how you can calculate the stability characteristics of this set of equations (e.g., explicitly get the Jacobian).

Problem 4. Integration Error: You are integrating the non-linear ODE:

$$\frac{dy}{dt} = -3y^2 \quad ; \; y(0) = 1$$

This actually has the simple solution:

$$y = \frac{1}{1+3t}$$

a. Using a step size of ½, integrate this ODE from 0 to 1 using the Euler Method.

b. Using the same step size, integrate it using the Backward Euler Method.

c. Which integration procedure is more accurate and why? What are the stability intervals (maximum step size) for each method?

Problem 5. Quadrature and Integration in Matlab:

The following are pretty quick little programs using the matlab canned routines discussed in class, and most easily addressed using anonymous functions:

a. Integrate y/x over the triangular domain x=[0,1], y=[0,x], e.g., $Q = \int_0^1 \int_0^x \left(\frac{y}{x}\right) dy\, dx$ (using the appropriate integrator, this program is actually only three lines long…)

b. The species A undergoes a dimerization reaction 2A -> B with rate $k_1 C_A^2$. The reaction continues, however, with the further reaction B+A -> C with rate $k_2 C_A C_B$. We would like to maximize the product B, so we need to stop the reaction when this is at a maximum. If we take $k_1 = 2$ and $k_2 = 4$, and the initial concentration of C_A is 1, use an integrator such as ode23 to determine the concentrations as a function of time. Plot these up for the range times from 0 to 3, and using the "max" command estimate what the maximum concentration of B is and when it occurs. Mark this point on your plot.

Note that this point will be a little off using the "max" command: this is because there is a pretty big space between where the concentrations are evaluated. You could get a much better value via interpolation: fitting a parabola to the maximum and the points on either side of it!

c. An iron cannonball of mass 1kg is fired upwards at a velocity of 200m/s. In addition to gravity, there is a drag due to air resistance given by $F_D = -0.00292\, U|U|$ where U is dh/dt (all units SI). Note that we have to use $U|U|$ rather than U^2 because we have to keep track of the sign. Using Newton's law, set the problem up as a pair of coupled first order equations and solve it using matlab. Plot up the height and velocity as a function of time and (again using the max command) determine the maximum elevation of the cannonball and mark it on the graph.