CBE 20258 Numerical & Statistical Analysis
Final Exam
May 4, 2015

You may have one hand-written sheet of notes for this exam

Problem 1. (15 points) Singular Value Decompostion. A **square** matrix can be decomposed via singular value decomposition as: $\underset{\approx}{A} = \underset{\approx}{U}\underset{\approx}{\Sigma}\underset{\approx}{V}^T$.

a. Once SVD has been done (computationally expensive, alas), it can be used to calculate the inverse of $\underset{\approx}{A}$. Using the properties of orthogonal and diagonal matrices, derive the relationship between $\underset{\approx}{A}^{-1}$ and the decomposition of $\underset{\approx}{A}$.

b. From the results of part a, show why a matrix with any singular value of zero must be singular.

c. In the problem $\underset{\approx}{A}\underset{\sim}{x} = \underset{\sim}{b}$, if the units of $\underset{\sim}{x}$ are time, and the units of $\underset{\sim}{b}$ are length, what are the units of the elements of $\underset{\approx}{U}$, $\underset{\approx}{\Sigma}$ and $\underset{\approx}{V}$?

d. In class we have interpreted the problem $\underset{\approx}{A}\underset{\sim}{x} = \underset{\sim}{b}$ as the transfer function between inputs ($\underset{\sim}{x}$) and outputs ($\underset{\sim}{b}$). Based on this, explain how you can determine from SVD what pattern in $\underset{\sim}{b}$ is most difficult to produce (requires the largest input $\underset{\sim}{x}$).

Problem 2. (15 points) Quadrature: Often we want to integrate data, meaning that our function evaluations is 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. Here we study this.

a. 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.

b. 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?

c. Simpson's Rule is based on fitting the function to a parabola over a pair of panels and then integrating the parabola. Thus, it should be of polynomial degree 2. Yet it is observed to be of degree 3. By comparison with the basis of Gaussian Quadrature rules, briefly explain why you get the extra degree.

Problem 3. (15 points) Quadrature again: You are assigned to measure the heat content of a sphere (e.g., the integral of the temperature over the volume of the sphere). The integral is thus:

$$E = \int_0^a \rho \hat{C}_p T \, 4\pi r^2 dr$$

where the sphere radius is a. The problem is that you only have two thermocouples: one at the center which measures a value T_c and one located at the surface with value T_s.

a. Based on symmetry arguments, it is expected that the actual temperature in the interior is an even function of r (no odd powers of r). Using this information, develop a method for determining the heat content.

b. What is the random error in the calculated heat content based on this rule?

c. Suppose you have one additional thermocouple which can be placed somewhere in the interior. Qualitatively (briefly!) explain how you might modify your algorithm if the error is dominated by random error in temperature measurements.

d. Qualitatively, how would you modify your algorithm if the temperature probes were very accurate (negligible random error)?

Problem 4. (15 points) 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. (10 points) Systems of Equations and Scaling: The solubility of CO_2 in water is a strong function of the pH, due to the conversion of dissolved CO_2 to carbonic acid (H_2CO_3) and dissociation into HCO_3^- and CO_3^{2-}. We are tasked with determining the equilibrium concentration of all dissolved species in a 0.001 M NaOH solution. Assuming that the NaOH completely dissociates (it is a very strong base), we want to calculate the pH and species concentrations for a solution in equilibrium with a 0.5 atm CO_2 gas (e.g., $pCO_2 = 0.5$ atm).

a. We have the following equilibrium relationships:

$$\frac{[CO_2]}{pCO_2} = K_{abs} = 3.36x10^{-2}\ M/atm \qquad \frac{[H_2CO_3]}{[CO_2]} = K_{eq} = 1.7x10^{-3}$$

$$\frac{[HCO_3^-][H^+]}{[H_2CO_3]} = Ka_1 = 2.5x10^{-4}\ M \qquad \frac{[CO_3^{2-}][H^+]}{[HCO_3^-]} = Ka_2 = 4.8x10^{-11}\ M$$

Using this, write out the relevant equations which must be solved to obtain the concentrations, defining all variables. Don't forget the electroneutrality condition! The net charge of any aqueous solution must be zero – all charges must balance.

b. How should you recast these equations to get a set of equations that can be easily solved in Matlab? (Hint: in addition to the tricks used in the project earlier this term, two of the variables can be eliminated right off analytically.)

c. In optimization problems with inequality constraints, it is important to normalize the constraint and variables -before- introducing the slack variable. Why?

Problem 6. (10 points) Systems of Equations: A projectile launcher is set up in the front of the classroom. It is desired to hit a target $y_t = 7$m in elevation and a distance of $x_t = 12$m from the launcher. The initial velocity of the launcher is fixed at U_0, but the angle of elevation is an adjustable parameter θ_0. The differential equations governing the projectile are:

$$M\frac{d^2x}{dt^2} = -\tfrac{1}{2}AC_D\rho\frac{dx}{dt}\left[\left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2\right]^{1/2} \qquad \left.\frac{dx}{dt}\right|_{t=0} = U_0\cos(\theta_0)$$

$$M\frac{d^2y}{dt^2} = -\tfrac{1}{2}AC_D\rho\frac{dy}{dt}\left[\left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2\right]^{1/2} - Mg \qquad \left.\frac{dy}{dt}\right|_{t=0} = U_0\sin(\theta_0)$$

a. Convert these equations into a system of first order equations.

b. Describe how you could use Matlab to solve for the desired angle of elevation.