CBE 20258 Computer Methods
Mid-Term Exam
March 9, 2017

You may have one page of hand written notes for this exam

Problem 1. (20 points) Error Propagation. A student needs to determine the diameter of an acrylic sphere but has lost the calipers. Thus, it is proposed that the student measure the mass of the sphere and, from the density of acrylic, calculate the diameter. The mass of the sphere is given by:

$$M = \frac{\pi}{6}\rho D^3$$

The density ρ of the acrylic is 1.180 ± 0.005. The student measures the mass M to be 0.158 ± 0.002g. Given these values, answer the following questions:

a. What is the diameter D and its standard deviation?

b. The student has a bunch of these spheres, and they are all identical (the standard deviation of the mass is due to measurement error, rather than variations among the spheres). It is proposed to improve the accuracy of the calculated diameter by weighing them one at a time and averaging the result. What is a reasonable number to use? Give a quantitative basis for your recommendation!

c. The student balks at this, and instead suggests that all the spheres be put on the scale at once and the measured mass divided by the number of spheres used. If the scale accuracy is a fixed ± 0.002 regardless of weight, is this better than measuring their weight individually and averaging? If the scale is of fixed precision (e.g., error ~ mass) does this answer change? Show your reasoning!

Problem 2. (20 points) Model Linearization. A common way to measure the viscosity (resistance to deformation of a fluid) is using a parallel-plate viscometer. Basically, you have two circular disks separated by a distance h with the fluid confined between them. You rotate one disk and measure the resulting torque on the other. In the instruments in my lab you can measure changes in the gap h very accurately, but getting the "zero" location is a problem. The solution to this is to measure the torque for a range of gap widths and use regression to calculate the true viscosity. The viscosity is given by the formula (the torque has been scaled to remove lots of constants):

$$\mu = T\left(h + \Delta h_0\right)$$

Where T is the measured torque and h is the measured gap width (thus, there will be a set of each). The unknown parameters are the viscosity μ and the gap width error Δh_0. So:

a. The error is assumed to all be in the measured torque, and there is no error in h (provided we can determine Δh_0). Using this, recast this model in a way which is linear in a new set of modeling parameters, and is suitable for **unweighted** linear regression. Set the problem up in the form Ax=b, clearly identifying A, x, and b. (Hint: your result is going to look a lot like the Lineweaver-Burke linearization of Michaelis-Menten kinetics…)

b. Show how you can calculate the matrix of covariance of the fitting parameters, and how these can be used to get the standard deviation of μ, the quantity of interest.

c. What are the key assumptions that you are making in the calculations for part b? Give me at least three important ones.

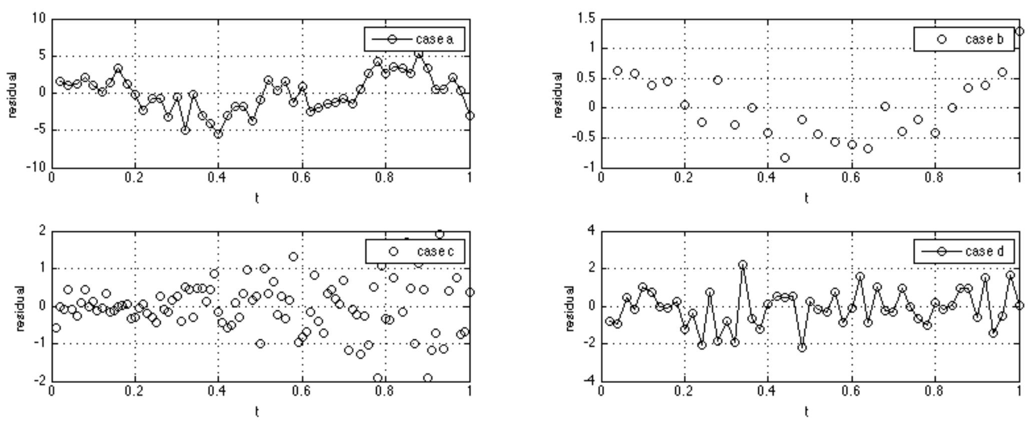
Problem 3. (20 points) Weighted Regression. In the problem above you are making very specific assumptions about the residual. Answer the following:

a. If you are using unweighted regression, what are you assuming about the standard deviation of the measured torque (e.g., how does σ_T scale with T)?

b. If we assume that the torque is measured to constant precision (e.g., $\sigma_T \sim T$) show how you can use weighted regression to improve your fitting parameters x. Clearly identify the weighting matrix and show how it is used in the solution.

c. Describe how you can use the resulting residuals r = Ax - b to calculate the matrix of covariance in x. (Hint: how can you use the residuals to figure out the precision of the measurements and matrix of covariance of T? What would it look like?)

Problem 4. (20 points) Residuals. It is always very important to plot your residuals! In four separate unweighted regression problems the following residuals were observed (e.g., r = Ax – b). Based on the material covered in class, ***briefly*** (1) describe any problems with the linear regression model that resulted in these residuals, and ***briefly*** (2) suggest how you could use the techniques described in class to either improve the analysis and/or the calculation of the matrix of covariance of the fitted parameters.



Problem 5. (20 points) Singular Value Decomposition

a. SVD is more computationally expensive than direct calculation of an inverse, but once you've got it, A^{-1} is fast to get as well ($O(n^2)$ additional operations, rather than $O(n^3)$). If $A = U \Sigma V^T$, show what A^{-1} is in terms of these matrices.

b. Using the above, prove that the 2-norm condition number of A^{-1} is the same as that for the matrix A.

c. Singular value decomposition is extremely valuable in the interpretation of the transfer problem Ax = b. Using SVD on matrix A, determine what pattern of output vector b requires the smallest input vector x (e.g., the output vector most easily produced). If b is aligned in this direction, what is the solution vector x in terms of the 2-norm of b and the decomposition matrices U, Σ, and V?