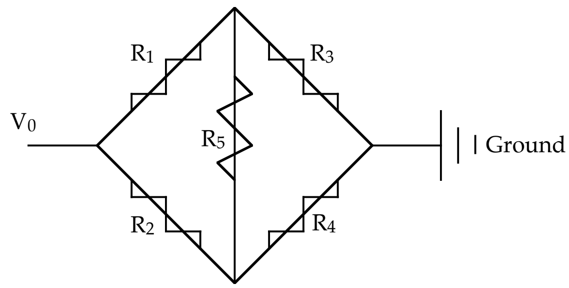
CBE 20258 Algorithm Problem Set 2

Due in class 2/9/17

Problem 1). A Wheatstone Bridge is an electrical circuit that is used in many chemical engineering sensor applications. As just one example, it forms the basis for solute detection in a gas chromatograph. It is depicted below:



A voltage V_0 is applied across the bridge, and the voltage differential between the two nodes in the middle is measured.

a. Using Ohm's Law V = I R, set up the system of five equations which the current through each of the five resistors must satisfy. Remember that current is conserved, and that voltage is a single value at any position. (e.g., voltage drop along any paths connecting the same two nodes must be identical)

b. Recast these equations in matrix form (e.g., Ax = b), clearly identifying A, b, and x.

Problem 2). Protein Assay: In your laboratory you are doing protein separations, and are using UV absorbance to measure protein concentrations. For dilute solutions, the protein absorbance is proportional to the concentration, and the total absorbance is just the sum of that resulting from each species independently. Suppose you have calibrated the absorbance at three different wavelengths for the three protein species:

Absorbance measurements (units = 1/(g/liter))

Species \ λ	200*nm*	300*nm*	400*nm*
BSA	0.1	0.2	0.1
BHb	0.1	0.2	0.3
Insulin	0.1	0.3	0.2

If you measure the absorbance at 200nm, 300nm, and 400nm to be 0.05, 0.13, and 0.08, respectively (dimensionless values):

a. Set up the problem for the concentration of each of the species in matrix form and

b. Solve for the concentrations.

Problem 3). Singular Value Decomposition. A non-square (nxm where n≠m) matrix $\underset{\approx}{A}$ undergoes SVD such that:

$$\underset{\approx}{A} = \underset{\approx}{U}\,\underset{\approx}{\Sigma}\,\underset{\approx}{V}^T$$

a. What are the dimensions of:

1) $\underset{\approx}{U}$

2) $\underset{\approx}{\Sigma}$

3) $\underset{\approx}{V}$

b. What is the inner product of the first and second columns of $\underset{\approx}{U}$ (e.g., U(: , 1)'*U(: , 2) in matlab)

c. What does matlab yield for the inner product of the first column of $\underset{\approx}{U}$ with the first column of $\underset{\approx}{V}$?

Problem 4) Singular Value Decompostion. A **square** matrix $\underset{\approx}{A} = \underset{\approx}{U}\,\underset{\approx}{\Sigma}\,\underset{\approx}{V}^T$ is decomposed as depicted below. All norms in this problem are taken to be **2-norms**.

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{bmatrix} = \begin{bmatrix} -0.2093 & 0.9644 & 0.1617 \\ -0.5038 & 0.0353 & -0.8631 \\ -0.8380 & -0.2621 & 0.4785 \end{bmatrix} \begin{bmatrix} 17.4125 & 0 & 0 \\ 0 & 0.8752 & 0 \\ 0 & 0 & 0.1969 \end{bmatrix} \begin{bmatrix} -0.4647 & -0.5538 & -0.6910 \\ -0.8333 & 0.0095 & 0.5528 \\ 0.2995 & -0.8326 & 0.4659 \end{bmatrix}$$

We are using this to solve the problem $\underset{\approx}{A}\,\underset{\sim}{x} = \underset{\sim}{b}$

a. Suppose $\underset{\sim}{b} = \begin{bmatrix} 1.9288 \\ 0.0706 \\ -0.5243 \end{bmatrix}$ (e.g., twice the second column of $\underset{\approx}{U}$). Using SVD (rather than the matrix $\underset{\approx}{A}$ - show how you do this via orthogonality with pencil & paper!) what is the solution vector $\underset{\sim}{x}$?

b. If, for an arbitrary $\underset{\sim}{b}$ (not necessarily that in part a!), we have an error given by $\Delta\underset{\sim}{b}$, this will yield some error in $\underset{\sim}{x}$ given by $\Delta\underset{\sim}{x}$. What is the maximum of $\|\Delta\underset{\sim}{x}\| / \|\Delta\underset{\sim}{b}\|$?

c. In control, we often go the other way – there is some error in the output $\Delta\underset{\sim}{b}$ due to error in the input $\Delta\underset{\sim}{x}$. What is the maximum value of $\|\Delta\underset{\sim}{b}\| / \|\Delta\underset{\sim}{x}\|$?

What you should get from these questions:

These questions all are exam questions, actually, so it really shouldn't take you more than an hour to complete the problem set – and if it takes longer, that means that you need to study the relevant material until you understand it better and can solve them quickly without book or notes!

1. The Wheatstone Bridge is a classic example of how to set up a system of linear equations based on a circuit diagram, and is very similar to last week's project. On a gas chromatograph, such a bridge is used in a thermal conductivity detector. The idea is that R_5 is very large, and that there is electrical dissipation from R_3 and R_4 (e.g., they are little heaters). A reference gas stream is passed over one of these, and the carrier gas containing the sample is passed over the other. The thermal conductivity of the gas stream with the sample changes with solute concentration, leading to a change in the temperature of the resistor, and hence its resistance. By measuring the voltage across the bridge, you can get a measure of the concentration of gases in the sample stream (related to the change in conductivity) with suitable calibration. It's a pretty robust technique for high sample concentrations, but not nearly as sensitive as other types of detectors.

2. This is another system of equations problem, pretty much identical to the paint can problem you did on the first assignment. Now, however, you are working with absorbances and figuring out concentrations from UV spectra. It's the same approach, though, as (for a dilute system) the absorbances at each frequency add up. While the numbers in this problem are "made up", we actually did use precisely this approach as a quick and easy way of determining protein concentrations using Brennecke's UV-Vis spectrometer when we were developing a novel prep-scale protein separation system.

3 & 4. These are problems dealing with the matrices produced by SVD. Note that actually -doing- SVD is something we leave to the computer, but it is important to know how to use it: what the properties of the various matrices are and what they tell you about the system of equations corresponding to the matrix A.