

10.34. Numerical Methods Applied to Chemical Engineering
Fall 2005. HW # 2. Linear algebra
Due Wednesday 9/21/2005. 9 am

Again, you are to submit your work electronically to the MIT server. Submit a MS-Word document *username_HW2.doc* with a description of your work. The names to use individual programs are found in the problem statements below. All problems are from chapter 1 of the text.

1. Solve problem 1.A.3, with your routine taking the name *username_calc_poly_coeff.m*. Test and show the results of your program by fitting $f(x) = \exp(x)$ at the points $x = 1, 1.5,$ and 2 . What happens to the accuracy of your approximation as you move outside of the range $[1, 2]$? In chapter 4, we will see how to do polynomial approximation much more efficiently.
2. Solve problem 1.A.4 and name your routine *username_Gram_Schmidt.m*. Demonstrate its use for the vector $\underline{y} = [1.3; 2.1; -0.9]$ and show that your generated set of basis vectors is indeed orthogonal.
3. Solve problem 1.B.2 to use linear regression to estimate the Michaelis-Menten rate constants of the enzymatic reaction from the data of Table 1.2. The tables are found in the back of the text. Write your routine as *username_P1B2.m*. Make a plot comparing the data of Table 1.2 with the predictions of your fitted model.
4. Solve problem 1.B.3 using finite differences to obtain a set of sparse linear algebraic equations. Write your routine as *username_P1B3.m*. While I ask for you to put the problem in dimensionless form, this is for now not strictly necessary. I am sure that by the end of 10.50, putting problems in dimensionless form will seem like second nature. Show your numerical solution for $D_A = 1, k = 1, B = 2, H_A p_A = 1$ and then redo the calculation for $D_A = 0.1$ and 0.01 . What happens to the concentration profile as the diffusivity is reduced? You should for each calculation increase the number of grid points until you obtain sufficient accuracy (for example, no longer see any significant change in the solution when you vary the number of grid points).