ChE/MSE 505
Advanced Mathematic for Engineers
Final Exam
Fall Semester, 2006
Instructor: David Keffer
Administered: 8:00-10:00 am, Monday December 11, 2004

Problem 1.
We want to use the following equation to fit some vapor pressure data.

$$P^{vap} = \exp\left(\frac{A}{B+T}\right) \tag{4}$$

where T is temperature and A and B are fitting constants. We have two pieces of data: the vapor pressure at 600 K is 8 atm and the vapor pressure at 620 K is 10 atm. Given this experimental data find the best values of A and B.

Solution:

We have two unknowns A and B. Our life would be much simpler if we can rearrange the problem so that it is linear in A and B. Let's try.

$$(B+T)\ln\left(P^{vap}\right) - A = 0$$

There we have it. The equation is linear in A and B. We have a system of two linear equations and two unknowns.

$$f_1(A,B) = (B+T_1)\ln\left(P_1^{vap}\right) - A$$
$$f_2(A,B) = (B+T_2)\ln\left(P_2^{vap}\right) - A$$

We can write this in matrix notation as

$$\underline{\underline{\mathbf{J}}}\,\underline{\mathbf{x}} = \underline{\mathbf{R}}$$

where

$$\underline{\underline{\mathbf{J}}} = \begin{bmatrix} -1 & \ln\left(P_1^{vap}\right) \\ -1 & \ln\left(P_2^{vap}\right) \end{bmatrix},\ \underline{\mathbf{x}} = \begin{bmatrix} A \\ B \end{bmatrix}, \text{ and } \underline{\mathbf{R}} = \begin{bmatrix} -T_1\ln\left(P_1^{vap}\right) \\ -T_2\ln\left(P_2^{vap}\right) \end{bmatrix}$$

We need the determinant and inverse

$$\det(\underline{\underline{\mathbf{J}}}) = -\ln\left(P_2^{vap}\right) + \ln\left(P_1^{vap}\right) = \ln\left(\frac{P_1^{vap}}{P_2^{vap}}\right)$$

$$\underline{\underline{\mathbf{J}}}^{-1} = \frac{1}{\det(\underline{\underline{\mathbf{J}}})}\begin{bmatrix} j_{22} & -j_{12} \\ -j_{21} & j_{11} \end{bmatrix} = \frac{1}{\ln\left(\frac{P_1^{vap}}{P_2^{vap}}\right)}\begin{bmatrix} \ln\left(P_2^{vap}\right) & -\ln\left(P_1^{vap}\right) \\ 1 & -1 \end{bmatrix}$$

The solution is given by

$$\underline{\mathbf{x}} = \underline{\underline{\mathbf{J}}}^{-1}\underline{\mathbf{R}} = \frac{1}{\ln\left(\frac{P_1^{vap}}{P_2^{vap}}\right)}\begin{bmatrix} \ln\left(P_2^{vap}\right) & -\ln\left(P_1^{vap}\right) \\ 1 & -1 \end{bmatrix}\begin{bmatrix} -T_1\ln\left(P_1^{vap}\right) \\ -T_2\ln\left(P_2^{vap}\right) \end{bmatrix} = \frac{1}{\ln\left(\frac{P_1^{vap}}{P_2^{vap}}\right)}\begin{bmatrix} (T_2 - T_1)\ln\left(P_1^{vap}\right)\ln\left(P_2^{vap}\right) \\ -T_1\ln\left(P_1^{vap}\right) + T_2\ln\left(P_2^{vap}\right) \end{bmatrix}$$

We have two pieces of data: the vapor pressure at 600 K is 8 atm and the vapor pressure at 620 K is 10 atm.

$$\underline{\mathbf{x}} = \frac{1}{\ln\left(\frac{8}{10}\right)}\begin{bmatrix} 20\ln(8)\ln(10) \\ -600\ln(8) + 620\ln(10) \end{bmatrix} \approx -4.4814\begin{bmatrix} 95.7618 \\ 179.9378 \end{bmatrix} = \begin{bmatrix} -429.15 \\ -806.37 \end{bmatrix}$$

Problem 2. Consider the integral equation

$$\phi(x) = f(x) + \lambda\left[\int_{x_o}^{x} N(x,y)\phi(y)dy\right]$$

where

$$\begin{aligned} f(x) &= x \\ N(x,y) &= x(y+1) \\ \lambda &= 1 \\ x_o &= 2 \end{aligned}$$

(a) Is this integral equation linear or nonlinear?
(b) Is this integral equation Volterra or Fredholm?
(c) Is this integral equation of the first or second kind?
(d) Use a numerical method to find an approximate solution to $\phi(x)$ from x_o to x_f.=4. Use a discretization step of $\Delta x = 1$. You are free to solve this as you choose, as long as you state your assumptions. However, I suggest you use the trapezoidal rule to approximate the integral, although that is not mandatory. I would like to see numerical values for the solution. There is no use for calculators in this problem.

Solution:
Since the range of interest is 4-2=2 and the step size is 1, we will have n=2 intervals and n+1=3 points where the function is to be evaluated.

We write out the integral equation for each value of x=2, 4, and 6.

$$x = 2: \qquad \phi_1 = 2 + \left[\int_2^2 2(y+1)\phi(y)dy \right]$$

$$x = 3: \qquad \phi_2 = 3 + \left[\int_2^3 3(y+1)\phi(y)dy \right]$$

$$x = 4: \qquad \phi_3 = 4 + \left[\int_2^4 4(y+1)\phi(y)dy \right]$$

We use the Trapezoidal rule to evaluate the integral

$$\int_{x_o}^{x_f} f(y)dy = \frac{\Delta x}{2}\left[f(x_o) + f(x_f) + 2\sum_{j=2}^{n} f(x_j) \right]$$

In the first equation, the integral is zero because the upper and lower limits of integration are the same. The equations become.

$$x = 2: \qquad \phi_1 = 2$$

$$x = 3: \qquad \phi_2 = 3 + \frac{1}{2}\left[3(2+1)\phi_1 + 3(3+1)\phi_2\right] = 3 + \frac{9}{2}\phi_1 + 6\phi_2$$

$$x = 4: \qquad \phi_3 = 4 + 2\left[(2+1)\phi_1 + (4+1)\phi_3 + 2(3+1)\phi_2\right] = 4 + 6\phi_1 + 10\phi_3 + 16\phi_2$$

This is a set of two linear algebraic equations. There are only two unknowns because equation (1) provides the value of ϕ_1. Now we rewrite the equations:

$$x = 3: \qquad 0 = 3 + \frac{9}{2}\phi_1 + 5\phi_2$$

$$x = 4: \qquad 0 = 4 + 6\phi_1 + 9\phi_3 + 16\phi_2$$

Simplify a little more for the sake of convenience

$$x = 3: \qquad \phi_2 = -\frac{12}{5}$$

Solving the last equation for ϕ_3 yields

$$x = 4: \qquad 0 = 4 + 12 + 9\phi_3 - \frac{192}{5}$$

$$x = 4: \qquad \phi_3 = \frac{112}{45}$$

So the solution is approximated by:

$$x = 2: \qquad \phi_1 = 2$$

$$x = 3: \qquad \phi_2 = -\frac{12}{5}$$

$$x = 4: \qquad \phi_3 = \frac{112}{45}$$

This is probably a very bad approximation. We would require a much finer discretization to get a more accurate picture of the solution.