Assignment 2

Deadline = Tuesday of Week 3

To start with, I've got a warm up revision question on linear algebra as you need to be familiar with matrices. As last week, download the Maple file 'assignment2.mw' from VITAL in the Homework folder under sessions/resources, and save it as 'assignment2<name>.mw', where you should write your name instead of <name>. ASK FOR HELP IF YOU HAVE PROBLEMS!! Please submit written solutions in lectures, and email me your Maple file by Tuesday of Week 3.

Q1. (Math 103) Consider the following system of linear equations:

$$\begin{aligned} 3x_1 + 2x_2 &= 4, \\ x_1 + 4x_2 &= 3. \end{aligned}$$

Write the equations in the form $A\mathbf{x} = \mathbf{b}$, where A is a matrix and $\mathbf{b}$ is a vector. Solve the equations using (i) elimination, and (ii) by computing A^{-1}. Check your results with Maple.

Q2. Consider the system of two simultaneous nonlinear equations in x_1, x_2

$$\begin{cases} x_1^2 + x_2^2 - 1 = 0, \\ 5x_1^2 + 21x_2^2 - 9 = 0, \end{cases}$$

Sketch the 2 curves, and show that an initial guess of $x_1^{(0)} = x_2^{(0)} = 0.6$ is reasonable if we are looking for a solution with $x_1, x_2 > 0$. Solve the equations using 2 steps of the 2D Newton-Raphson method keeping at least 4 digits in all calculations. Perform additional iterations with Maple until you have a solution correct to 2 decimal places.

Q3. As an example application of the 2D Newton-Raphson method, consider the coupled pair of reversible chemical reations:

$$\begin{aligned} 2A + B &\rightleftharpoons C \\ A + D &\rightleftharpoons C \end{aligned}$$

where A, B, C and D represent certain chemical compounds. If 20 moles of chemical A and 10 moles each of chemical B and D are injected into a reaction chamber, at equilibrium the first reaction produces c_1 moles of C and the second reaction produces c_2 moles of C, where c_1 and c_2 satisfy the following equations:

$$\begin{aligned} c_1 + c_2 - k_1(20 - 2c_1 - c_2)^2(10 - c_1) &= 0, \\ c_1 + c_2 - k_2(20 - 2c_1 - c_2)(10 - c_2) &= 0. \end{aligned}$$

If you've not already done so, open the Maple file. Taking the equilibrium constants as $k_1 = 1.64 \times 10^{-4}$ and $k_2 = 3.27 \times 10^{-3}$, use Maple to implement the 2D Newton-Raphson method to compute c_1 and c_2 to 2 decimal places, starting from an initial guess of $c_1 = c_2 = 0.5$.

Q4. Solve the linear system $Ax = b$ using exact arithmetic (i.e. fractions), where

$$A = \begin{pmatrix} 2 & 4 & 2 \\ 1 & 0 & 3 \\ 3 & 1 & 2 \end{pmatrix}, \quad b = \begin{pmatrix} -4 \\ 4 \\ 3 \end{pmatrix}$$

by Gaussian elimination. Hence identify the $A = LDM$ decomposition. Check your factorization by multiplying the matrices L, D & M together.