Chemistry 20262 Spring 2018
Professor J. Daniel Gezelter Due Fri. 4/13/2018

Problem Set 8

1. McQuarrie, problem 18-6. Do this problem by hand (although you may check your answers in Mathematica).
2. McQuarrie, problem 17-9.
3. McQuarrie, problem 17-11.
4. McQuarrie, problem 17-13.
5. Verify that $(AB)^T = B^T A^T$ using the matrices $A = \begin{pmatrix} 1 & 2 \\ 0 & -2 \end{pmatrix}$ and $B = \begin{pmatrix} 3 & 1 \\ -1 & -2 \end{pmatrix}$
6. The matrix
$$R_{z,\theta} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
rotates a three dimensional vector by an angle θ around the z axis.
   (a) Show that:
   $$R_{z,\pi/4} R_{z,\pi/6} = R_{z,\pi/6} R_{z,\pi/4}$$
   (b) Write down a matrix that rotates a vector by $\pi/6$ around the y xis.
   (c) Show that:
   $$R_{y,\pi/6} R_{z,\pi/6} \neq R_{z,\pi/6} R_{y,\pi/6}$$
   Does this make sense?
   You can do this problem using Mathematica, but you do not have to. You can start with the commands:
```
theta1 = Pi / 4
rzpi4 = {{ Cos[theta1], -Sin[theta1], 0},
{ Sin[theta1], Cos[theta1], 0}, {0, 0, 1}}
```
7. Find the eigenvalues and normalized eigenvectors of the following matrices:
$$A = \begin{pmatrix} 1 & 1 \\ 2 & 2 \end{pmatrix}, \quad B = \begin{pmatrix} 3 & -2 & -1 \\ 3 & -4 & -3 \\ 2 & -4 & 0 \end{pmatrix}, \text{and} \quad C = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

8. Consider the matrix $A = \begin{pmatrix} 3 & 1 & 1 \\ 1 & 0 & 2 \\ 1 & 2 & 0 \end{pmatrix}$.

   (a) What are the eigenvalues and normalized eigenvectors of A?

   (b) Show that the eigenvectors of A are orthonormal.

9. Extra Credit: Model acetylene (C_2H_2) as four masses connected by three springs.

   Use $m = 1$ for hydrogen and $m = 12$ for carbon. Use force constants $k = 1$ for the C-H bonds, and $k = 2.5$ for the C=C bond. Only consider motion in one dimension (just stretching, no bending).

   Do the following:

   (a) Write down the equations of motion in matrix form.

   (b) Show that a vector proportional to

   $$\vec{w}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

   is an eigenvector of your matrix, with an eigenvalue of 0.

   (c) Calculate the remaining three eigenvalues and the corresponding eigenvectors. You can do this by hand, but Mathematica is highly recommended.

   (d) The stretching vibrations of acetylene are usually called the symmetric C-H stretch, the asymmetric C-H stretch, and the C-C stretch. Assign an eigenvector to each. (For consideration: how much C-H motion accompanies the C-C stretch?)

   (e) The vibrational frequencies are proportional to the square roots of the eigenvalues that you obtained. The experimental frequency for the C-H symmetric stretching mode in C_2H_2 is 3374 cm^{-1}. Calculate the frequencies of the other two vibrations, as well as all three vibrations for C_2D_2 using your model. For comparison, the experimental data are:

	$\bar{\nu}$ (cm^{-1}) for C_2H_2	$\bar{\nu}$ (cm^{-1}) for C_2D_2
sym. C-H	3374	2700
asym. C-H	3278	2427
C-C	1970	1765

   (f) Explain why the frequencies go as the square root of the eigenvalues.

10. Extra credit: Steady-state solutions to Zombie Outbreaks

(Fictional) zombie outbreak scenarios can be modeled using a SZR model where humans are Susceptible (S), Zombie (Z), or Removed (R). Susceptibles can increase in population via the birth rate (b), disappear due to natural death (δ) or be converted into a zombie by an encounter (bite) from an infected individual:

$$\frac{dS}{dt} = b - \beta SZ - \delta S \tag{1}$$

Zombies, are created using the same mechanism ($+\beta SZ$) or by rising from the graves of removed individuals with some probability γ. Susceptibles can also remove zombies (usually by destroing the brain of an infected individual with efficiency α):

$$\frac{dZ}{dt} = \beta SZ + \gamma R - \alpha SZ \tag{2}$$

The removed (dead) are created via natural death of a susceptible, by removal of zombies, but the population of the dead can also decrease as they rise from the grave:

$$\frac{dR}{dt} = \delta S + \alpha SZ - \gamma R \tag{3}$$

If we assume a zombie outbreak happens over short time scales, we can set the natural birth and death rates to zero, and the differential equations become:

$$\frac{d}{dt}\begin{pmatrix} S \\ Z \\ R \end{pmatrix} = \begin{pmatrix} -\beta S(t)Z(t) \\ \beta S(t)Z(t) + \gamma R(t) - \alpha S(t)Z(t) \\ \alpha S(t)Z(t) - \gamma R(t) \end{pmatrix} \tag{4}$$

Once the outbreak has reached the steady state, the rates of change are all zero, so we have:

$$-\beta S_{ss}Z_{ss} = 0 \tag{5}$$

$$\beta S_{ss}Z_{ss} + \gamma R_{ss} - \alpha S_{ss}Z_{ss} = 0 \tag{6}$$

$$\alpha S_{ss}Z_{ss} - \gamma R_{ss} = 0 \tag{7}$$

Some questions we might have about the zombie outbreak - What are the implications of Eq. (5)? Are the two possible steady state solutions *stable*? To find out, we need to compute the eigenvalues of a matrix called the Jacobian:

$$J = \begin{bmatrix} \frac{d}{dS}\left(\frac{dS}{dt}\right) & \frac{d}{dZ}\left(\frac{dS}{dt}\right) & \frac{d}{dR}\left(\frac{dS}{dt}\right) \\ \frac{d}{dS}\left(\frac{dZ}{dt}\right) & \frac{d}{dZ}\left(\frac{dZ}{dt}\right) & \frac{d}{dR}\left(\frac{dZ}{dt}\right) \\ \frac{d}{dS}\left(\frac{dR}{dt}\right) & \frac{d}{dZ}\left(\frac{dR}{dt}\right) & \frac{d}{dR}\left(\frac{dR}{dt}\right) \end{bmatrix} \tag{8}$$

If the eigenvalues of this matrix are negative for one of the steady state solutions, that solution is asymptotically stable.

(a) Solve the eigenvalues of the Jacobian matrix, and show that the doomsday scenario, $S_{ss} = 0$ is the stable equilibrium.

(b) Are there better kinetic equations to model your favorite fictional version of the zombie outbreak scenario? What changes would you make to equations (1)-(4) to improve the quality of your model?

(c) What places on campus would be the best to set up your headquarters should this scenario arise?

Note that this problem is related to the SIR model, a *real* epidemiological model, with S = susceptible, I = infected, R = removed. The zombie version was published recently as "You can run, you can hide: The epidemiology and statistical mechanics of zombies," by Alexander A. Alemi, Matthew Bierbaum, Christopher R. Myers, and James P. Sethna, *Phys. Rev. E* **92**, 052801 (2015). `https://doi.org/10.1103/PhysRevE.92.052801`