SC3.316: Mathematical Methods in Biology
Midterm 2 solutions

1. (15 points) Find the reduced echelon form of the following matrix:

$$A = \begin{pmatrix} 1 & 2 & 1 & 9 \\ 2 & 4 & 1 & 18 \\ 3 & 5 & 1 & 24 \end{pmatrix}$$

Solution:

1. $R_2 = R_2 - 2R_1$: (2 marks)
$$\begin{pmatrix} 1 & 2 & 1 & 9 \\ 0 & 0 & -1 & 0 \\ 3 & 5 & 1 & 24 \end{pmatrix}$$
2. $R_3 = R_3 - 3R_1$: (2 marks)
$$\begin{pmatrix} 1 & 2 & 1 & 9 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & -2 & -3 \end{pmatrix}$$
3. Swap the second and third rows: (2 marks)
$$\begin{pmatrix} 1 & 2 & 1 & 9 \\ 0 & -1 & -2 & -3 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$
4. $R_2 = -R_2$ (2 marks)
$$\begin{pmatrix} 1 & 2 & 1 & 9 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$
5. $R_1 = R_1 - 2R_2$ (2 marks)
$$\begin{pmatrix} 1 & 0 & -3 & 3 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$
6. $R_3 = -R_3$ (2 marks)
$$\begin{pmatrix} 1 & 0 & -3 & 3 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$
7. $R_1 = R_1 + 3R_3$ (2 marks)
$$\begin{pmatrix} 1 & 0 & 0 & 3 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$
8. $R_2 = R_2 - 2R_3$ (1 mark)
$$\begin{pmatrix} 1 & 0 & 0 & 3 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

2. (10 points) State the Deficiency Zero Theorem.

Solution:

Let (S, C, R) be a reaction network of deficiency zero.

1. If the network is not weakly reversible, then for any arbitrary choice of kinetics, the differential equations for the kinetic system (S, C, R, K) cannot admit a positive equilibrium. (4 marks)
2. If the network is weakly reversible, then assuming mass-action kinetics, the following holds: (2 marks)
   (a) Within each positive stoichiometric compatibility class, there exists exactly one positive equilibrium. (2 marks)
   (b) The equilibrium is asymptotically stable. (2 marks)

3. (15 points) Consider a reaction network with l linkage classes. Let δ_i denote the deficiency of the i^{th} linkage class and let δ denote the deficiency of the whole network. If $\delta = 0$, then $\delta_i = 0$ for every linkage class.

   Solution:

   Note that $\sum_{i=1}^{l} \delta_i = \sum_{i=1}^{l} (n_i - 1 - s_i) = n - l - \sum_{i=1}^{l} s_i$. (7 marks)

   In addition, $\delta = n - l - s$. Since $\sum_{i=1}^{l} s_i \geq s$, we get $\delta \geq \sum_{i=1}^{l} \delta_i$. (5 marks)

   This implies that if $\delta = 0$, then $\delta_i = 0$ for every linkage class. (3 marks)

4. (15 points) A reaction network is "forest-like" if every direct link connecting two complexes in a linkage class is a cut-link. Show that every forest-like weakly reversible reaction network is reversible.

   Solution:

   For contradiction, assume that the forest-like weakly reversible reaction network is not reversible. (3 marks)

   Then there exists complexes y_0, y_0' such that there is a reaction from y_0 to y_0', no reaction from y_0' to y_0 (5 marks)

   and a reaction pathway from y_0' to y_0 (due to weak reversibility). (5marks)

   Then the link from y_0 to y_0' is not a cut-link, contradicting the fact that the reaction network is "forest-like". (2 marks)

5. (15 points) A reaction network is consistent if there exists positive real numbers $c_{y \to y'}$ such that

   $$\sum_{y \to y'} c_{y \to y'} (y' - y) = 0. \tag{1}$$

   Show that a weakly reversible reaction network is consistent.

   Solution:

   Consider a weakly reversible consisting of a single cycle. (3 marks)

   In this case, we can choose $c_{y \to y'} = 1$ for each reaction $y \to y' \in E$ so that the network is consistent. (7 marks)

   Repeating this argument for multiple cycles, we get that a weakly reversible reaction network is consistent. (5 marks)

6. (15 points) Show that a reversible star-like network (as in Figure 1) is quasi-thermodynamic.

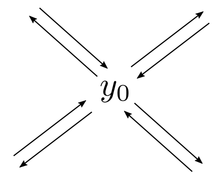

Figure 1: Star-like network.

Solution:

Since the network is reversible, it is weakly reversible and hence a positive equilibrium exists. Let us call the positive equilibrium c^*. Let C^* denote the set of all complexes except y_0. Therefore, we have

$$\sum_{y\in C^*} k_{y\to y_0}(c^*)^y(y_0-y)+\sum_{y\in C^*} k_{y_0\to y}(c^*)^{y_0}(y-y_0)=0\ (2\,marks)$$

This implies that

$$\sum_{y\in C^*} k_{y\to y_0}(c^*)^y(y_0-y)=\sum_{y\in C^*} k_{y_0\to y}(c^*)^{y_0}(y_0-y)\ (2\,marks) \tag{2}$$

Define $\mu(c)=\log(c)-\log(c^*)$. (1 mark)

This means that the rate function can be written as

$$\begin{aligned} f(c) &= \sum_{y\to y'\in\mathcal{R}} k_{y\to y'}c^y(y'-y) \\ &= \sum_{y\to y'\in\mathcal{R}} k_{y\to y_0}(c^*)^y e^{y\cdot\mu(c)}(y_0-y) \\ &= \sum_{y\in C^*} k_{y\to y_0}(c^*)^y e^{y\cdot\mu(c)}(y_0-y) - e^{y_0\cdot\mu(c)}\sum_{y\in C^*} k_{y_0\to y}(c^*)^{y_0}(y_0-y)(4\,marks) \end{aligned}$$

Using Equation 2, we get that

$$f(c)=\sum_{y\in C^*} k_{y\to y_0}(c^*)^y(e^{y\cdot\mu(c)}-e^{y_0\cdot\mu(c)})(y_0-y)$$

Hence $\log(c)-\log(c^*)\cdot f(c)=\sum_{y\in C^*} k_{y\to y_0}(c^*)^y(e^{y\cdot\mu(c)}-e^{y_0\cdot\mu(c)})(y_0\cdot\mu(c)-y\cdot\mu(c))$. (2 marks)

Since the exponential function is increasing, we have $(x_2-x_1)(e^{x_1}-e^{x_2})\leq 0$. This implies that

$$\mu(c)\cdot f(c)\leq 0.$$

with equality holding iff $(y-y_0)\cdot\mu(c)$ for all $y\in C^*$. (1 mark)

We still need to show that the dynamical system is quasi-static, i.e., show that the set of equilibria is identical to the set $E=\{c\in\mathbb{R}^S_{>0}:\log(c)-\log(c^*)\in S^\perp\}$. If c is an equilibrium, then we have equality in Equation 3. This implies that $\log(c)-\log(c^*)\in S^\perp$. Conversely, if $\log(c)-\log(c^*)\in S^\perp$, then we have equality in Equation 3. Therefore, the dynamical system is quasi-thermodynamic. (3 marks)

7. (15 points) Let $A_{n\times n}$ be a square matrix and let $x \in \mathbb{R}^n$. Show that the following are equivalent

   1. For every vector $b \in \mathbb{R}^n$, the system $Ax = b$ has at least one solution.
   2. For every vector $b \in \mathbb{R}^n$, the system $Ax = b$ has exactly one solution.

   Solution:

   $(1 \Rightarrow 2)$ This is certainly true since if for every $b \in \mathbb{R}^n$, the system $Ax = b$ has a unique solution, then it has at least one solution. (2 marks)

   $(2 \Rightarrow 1)$ Take $b = e_j$, where e_j is the j^{th} column vector of the identity matrix. Then the consistency of $Ax = e_j$ yields a vector x_j such that $Ax_j = e_j$. (3 marks)

   Let B be the matrix with vectors $[x_1, x_2, ..., x_n]$. Then

$$\begin{aligned} AB &= A[x_1, x_2, ..., x_n] \\ &= [Ax_1, Ax_2, ..., Ax_n] \\ &= [e_1, e_2, ..., e_n] \end{aligned} \tag{3}$$

   This implies that $AB = I$. (5 marks)

   We now show that the matrix B is invertible. Towards this we show that $Bx = 0$ has only the trivial solution $(x_1 = x_2 = ..., = x_n = 0)$. If $Bx = 0$, then $A(Bx) = 0 = A0 = 0$, which implies $x = 0$. So B is invertible. (3 marks)

   This implies that $ABB^{-1} = IB^{-1}$ so that $A = B^{-1}$. Thus A is invertible and the system $Ax = b$ has the unique solution $x = A^{-1}b$. (2 marks)