Topics in Applied Algebraic Geometry

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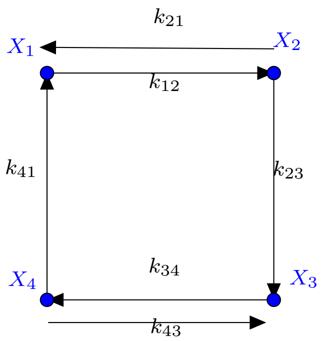
Homework # 3, due April 18

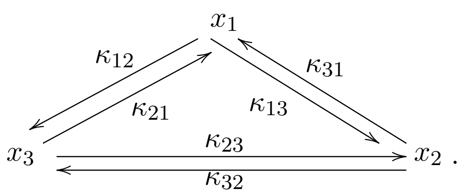
Exercise 1. Consider the linear chemical reaction network associated with the following labeled digraph G:



- Find all the steady states x which satisfy $\sum_{i=1}^{4} x_i = 0$.
- Find all the positive steady states x which verify $\sum_{i=1}^{4} x_i = 1$.
- Find all choices of positive rate constants k_{ij} for which the vector $x = (1/4, 1/4, 1/4, 1/4)$ is a steady state.

Assume that the edge from node 4 to node 1 is deleted and let x be a steady state. Is the resulting digraph G' connected? Is G' strongly conected? Prove that $x_1 = x_2 = 0$.

Exercise 2. Consider the labeled digraph



Assume that all rate constants equal 1. Prove that the corresponding Laplacian matrix is the following matrix A:

$$A = \begin{bmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{bmatrix}, \ J = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & -3 \end{bmatrix}, \ Q = \begin{bmatrix} \frac{1}{3} & -\frac{1}{3} & -1 \\ \frac{1}{3} & -\frac{1}{3} & 0 \\ \frac{1}{3} & \frac{2}{3} & 1 \end{bmatrix}, \ Q^{-1} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -2 & 1 \\ -1 & 1 & 0 \end{bmatrix}.$$

Check that J is a Jordan normal form matrix for A and that $A = QJQ^{-1}$. Find the matrix $exp(At)$ and prove that for any initial value $V = (v_1, v_2, v_3)$, the trajectory x of the associated dynamical system starting at any point V (that is, $x(0) = V$), converges to the steady state $1/3(v_1 + v_2 + v_3, v_1 + v_2 + v_3, v_1 + v_2 + v_3)$ when t tends to $+\infty$.

Exercise 3. Consider a linear system associated to a digraph G with vertices labeled $X_1, \dots X_n$ (that is, there are n complexes consisting of each one of the species). Prove that the stoichiometric subspace S has dimension $n - \ell$, where ℓ is the number of connected components of G. Moreover, let $G_1, \dots, G_\ell$ denote the connected components of G. Prove that a basis of the orthogonal $S^\perp$ is given by the $(0,1)$-vectors $v_i = \sum_{X_j \text{ node in } G_i} e_j$ (thus, the linear equation it defines is $\sum_{X_j \text{ node in } G_i} x_j = 0$), for all $i = 1, \dots, \ell$.

Exercise 4. Let $s = 2$, $m = 3$, and consider be the following network, with the same underlying graph as in the previous exercise, but now nonlinear:

$$\begin{tikzcd}
& x_1^2 \arrow[dl, shift right, "\kappa_{12}"'] \arrow[dr, shift left, "\kappa_{13}"'] & \\
x_2^2 \arrow[ur, shift right, "\kappa_{21}"'] \arrow[rr, shift left, "\kappa_{23}"] & & x_1x_2 \arrow[ul, shift left, "\kappa_{31}"'] \arrow[ll, shift left, "\kappa_{32}"]
\end{tikzcd}$$

(i) Write down the resulting mass-action kinetics system

$$\frac{dx}{dt} = (f_1, (x), f_2(x)).$$

(ii) Describe all rate constants for which the steady state ideal $I = \langle f_1, f_2 \rangle$ is binomial.

(iii) Describe all rate constants for which the system is *detailed balanced.*

(iv) Set $k_{31} = k_{23} = 2, k_{13} = k_{32} = k_{12} = 1, k_{21} = 4$, and check that the system is detailed balanced in this case but I is not binomial. Find its "positive real radical" $J := \{g \in \mathbb{R}[x_1, x_2] : g(c) = 0 \text{ for all } c \in V_{\mathbb{R}_{>0}}(I)\}$. Is J binomial?

Exercise 5. The *deficiency* δ of a chemical reaction network with digraph G is defined as:

$$\delta = m - \ell - \dim(S),$$

where m is the number of complexes, ℓ is the number of connected components of G and S is the stoichiometric subspace. It is known that when G is weakly reversible, δ equals the codimension of the variety of positive rate constants for which the system is complex balanced.

Consider the following mass-action kinetics chemical reaction network:

$$S_0 + E \underset{k_2}{\overset{k_1}{\rightleftarrows}} ES_0 \underset{k_4}{\overset{k_3}{\rightleftarrows}} S_1 + E \tag{1}$$

$$S_1 + F \underset{\ell_2}{\overset{\ell_1}{\rightleftarrows}} FS_1 \underset{\ell_4}{\overset{\ell_3}{\rightleftarrows}} S_0 + F \ .$$

and the following reaction network, in which the substrate S_1 in the first set of reactions acts as an enzyme in the second set of reactions:

$$S_0 + E \underset{k_2}{\overset{k_1}{\rightleftarrows}} ES_0 \underset{k_4}{\overset{k_3}{\rightleftarrows}} S_1 + E \tag{2}$$

$$T_0 + S_1 \underset{\ell_2}{\overset{\ell_1}{\rightleftarrows}} T_0S_1 \underset{\ell_4}{\overset{\ell_3}{\rightleftarrows}} T_1 + S_1 \ .$$

In both cases, compute the deficiency of the network and describe the varieties (in the positive orthant of rate constant space) of those vectors of rate constants for which (a) the system is detailed balanced, (b) the system is complex balanced.

Exercise 6. One of the known results about injectivity close to the one we mentioned in class, is the following:

Assume $C \in \mathbb{R}^{n\times r}, A \in \mathbb{Z}^{n\times r}$ with columns $a_1, \ldots, a_r$, $k = (k_1, \ldots, k_r) \in \mathbb{R}^r_{>0}$ and denote $x = (x_1, \ldots, x_n)$. The function σ assigns to any x the vector of signs of the coordinates of x. Consider the family of Laurent polyomials $f_{k,i} = \sum_{j=1}^r c_{ij} k_j x^{a_j}, i = 1, \ldots, n$. Then, the following assertions are equivalent:

- *The map $f_k : \mathbb{R}^n_{>0} \to \mathbb{R}^n$ is injective for all k.*
- $\sigma(\ker(C)) \cap \sigma(\mathrm{im}(A^t)) = \{0\}$.

Your task:

(i) Translate the previous result in case the system is linear (thus, A is the identity matrix) and relate it to known results in linear algebra.

(ii) Translate the previous result in case $n = 1$ and relate it to the following statement: A nonzero polynomial $f = c_0 + c_1 x + \ldots, c_s x^s$ with $c_1, \ldots, c_s \geq 0$ has at most one positive real root.

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