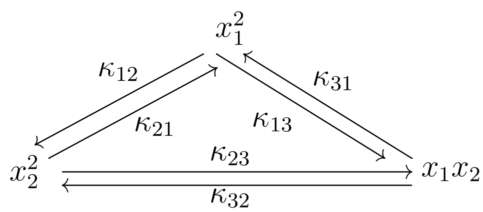
5. Exercise List. Friday Week 1

Exercise 5.1. Recall that given a *reversible* network (i.e., every edge is reversible) with mass-action kinetics, we say that a positive steady state x is *detailed balanced* if for every reaction $y_i \underset{k_{ji}}{\overset{k_{ij}}{\rightleftharpoons}} y_j$, it holds that $k_{ij}x^{y_i} - k_{ji}x^{y_j} = 0$.

Let $n = 2$, $m = 3$, and consider the the following network:



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

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

(ii) Describe the set of reaction 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 $\kappa_{31} = \kappa_{23} = 2, \kappa_{13} = \kappa_{32} = \kappa_{12} = 1, \kappa_{21} = 4$, and check that the system is detailed balanced in this case but I is not binomial. Find the "positive real radical" J of I:

$$J := \{g \in \mathbb{R}[x_1, x_2] \,:\, g(c) = 0 \text{ for all } c \in V_{\mathbb{R}_{>0}}(I)\}.$$

Is J binomial?

Exercise 5.2. Consider the one-site phosphorylation cycle:

$$S_0 + E \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES_0 \underset{k_4}{\overset{k_3}{\rightleftharpoons}} S_1 + E$$
$$S_1 + F \underset{\ell_2}{\overset{\ell_1}{\rightleftharpoons}} FS_1 \underset{\ell_4}{\overset{\ell_3}{\rightleftharpoons}} S_0 + F \ ,$$

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 creating a signaling cascade:

$$S_0 + E \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES_0 \underset{k_4}{\overset{k_3}{\rightleftharpoons}} S_1 + E$$
$$T_0 + S_1 \underset{\ell_2}{\overset{\ell_1}{\rightleftharpoons}} T_0S_1 \underset{\ell_4}{\overset{\ell_3}{\rightleftharpoons}} T_1 + S_1 \ .$$

For both networks, 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.

Note: You will need some results that we didn't have time to cover in the lectures. You could for instance use the following references available at arXiv.org: [Craciun, Dickenstein, Shiu, Sturmfels: Toric dynamical systems, Journal of Symbolic Computation 44 (2009), 1551–1565], [Pérez Millán-Dickenstein: How far is complex balancing from detailed balancing?, Bulletin of Mathematical Biology (2011), 73(4), 811–828.].