Deficiency

- The *deficiency* of a chemical reaction network $\{\mathcal{S}, \mathcal{C}, \mathcal{R}\}$ is $\delta = |\mathcal{C}| - l - s$, where $\mathcal{C}$ is the number of complexes, l is the number of linkage classes of the network graph and s is the dimension of the stoichiometric subspace of the network.

David F. Anderson, Gheorghe Craciun and Thomas G. Kurtz, Bull. Math. Biol. 72 ,1947 (2010)

The Deficiency zero theorem

Theorem

If a CRN is weakly reversible and has deficiency 0 and the rate constants are positive then, for mass action kinetics and any choice of rate constants, the rate equations will have precisely one fixed point in each positive stoichiometric compatibility class. This solution is complex balanced. Any sufficiently nearby solution that starts in the same stoichiometric compatibility class will approach this equilibrium as $t \to \infty$. Furthermore, there are no other positive periodic solutions.

If the network has deficiency zero and is not weakly reversible and the rate constants are positive, then for any choice of rate constants, the rate equation does not have a positive solution or a positive periodic solution. .

Horn and Jackson *1972*; Feinberg*1987*

(10)

Examples

(1) $S_1 + S_2 \rightleftharpoons S_3$; $c = 2,\ l = 1,\ s = 1 \Rightarrow \delta = 0$

(2) $S_1 \rightleftharpoons 2S_2$; $c = 2,\ l = 1,\ s = 1 \Rightarrow \delta = 0$

(3) $S_1 + S_2 \rightleftharpoons S_3$

$S_3 \rightarrow S_4 + S_5 \rightarrow S_1 + S_2$; $c = 3,\ l = 1,\ s = 2 \Rightarrow \delta = 0$

(4) $S_1 \rightarrow S_2 \rightarrow S_3 \cdots \rightarrow S_L \rightarrow S_1$ $\quad c = L,\ l = 1,\ s = L-1$

(5) $\phi \rightarrow S_1 \rightarrow S_2 \rightarrow S_3 \cdots \rightarrow S_L \rightarrow \phi$ $\quad c = L+1,\ l = 1,\ s = L$

(6) $S_1 \rightleftharpoons 2S_1 \rightleftharpoons 3S_1$ $\quad c = 3,\ l = 1,\ s = 1 \Rightarrow \delta = 1$!

How is δ related to fixed points?

$$\frac{d\vec{x}}{dt} = AY\psi$$

There's a way to write ψ as x^{Y} !

$$[x_E, x_S, x_{ES}, x_P]^{\begin{bmatrix} 0&1&0&1&0&1 \\ 0&0&1&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \end{bmatrix}}$$

$$= [1, x_E, x_S, x_E x_S, x_{ES}, x_E x_P]$$

$$\boxed{\ln\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \ln a \\ \ln b \end{pmatrix}}$$

$$\ln \psi = Y^T \ln x$$

$$\ln\begin{bmatrix} 1 \\ x_E \\ x_S \\ x_E x_S \\ x_{ES} \\ x_E x_P \end{bmatrix} = \begin{bmatrix} 0&1&0&1&0&1 \\ 0&0&1&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \end{bmatrix} \begin{bmatrix} \ln x_E \\ \ln x_S \\ \ln x_{ES} \\ \ln x_P \end{bmatrix}$$

Coming back to the rate eqn.

$$\frac{d\vec{x}}{dt} = YA\psi = YAx^{Y}$$

$$\frac{d\vec{x}}{dt} = 0 \Rightarrow YA\psi = 0$$

$$\Rightarrow A\psi = 0 \quad \text{or} \quad A\psi \neq 0 \text{ but } YA\psi = 0$$

(1) $\Rightarrow$ ψ lies in the kernel of A

(2) $\Rightarrow$ ψ lies in $Im(A) \cap ker(Y)$

Another definition of deficiency is

$$\delta = \dim\left(Im(A) \cap ker(Y)\right)$$

$$\delta = 0 \Rightarrow \dim(Im(A) \cap ker(Y)) = 0$$

$\Rightarrow$ ψ lies in the kernel of A!

But how does this fit with the other definition?

To see this:

$\dim(A) =$ # of columns $= c$

rank-nullity theorem $\Rightarrow$ (for finite-dimensional vector spaces)

$$\text{Nullity}(A) + \text{rank}(A) = c$$

$\text{Nullity}(A) = \dim ker(A)$

$\text{rank}(A) = \dim Im(A)$ $\rightarrow$ dim of vector space spanned by columns

Eg. $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$ rank $= 2$

Nullity $= 1$ $\rightarrow \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$

$\Rightarrow \dim(\ker A) + \dim(\mathrm{Im}\, A) = c$

$\Rightarrow \quad \ell + \dim(\mathrm{Im}\, YA) + \dim(\mathrm{Im}\, A \cap \ker Y) = c$

$\Rightarrow \quad c = \ell + s + \delta$

or

$\delta = c - \ell - s$

So $\delta = 0 \Rightarrow$ that looking at $\ker A$ is enough to find the fixed pt.

[all changes in complexes $\Rightarrow$ changes in species]

But how do we know we can always find a $\ker(A)_k$ with +ve eigenvector? & how many are there?

$\boxed{\text{Perron-Frobenius theorem}}$

- So from this theorem, we know that there are as many (independent) vectors in the null space of A as there are linkage classes & these have non-zero positive elements.

So we are guaranteed to find Ψ s.t. $A\Psi = 0$

But how can we know that $\Psi \leftrightarrow x^Y$?

Eg. $P \underset{\bar{k}_1}{\overset{k_1}{\rightleftharpoons}} 2P \underset{k_2}{\overset{\bar{k}_2}{\rightleftharpoons}} 3P$; $\frac{d x_p}{dt} = [1, 2, 3] \begin{bmatrix} -k_1 & \bar{k}_2 & 0 \\ k_1 & -\bar{k}_1 - \bar{k}_2 & k_2 \\ 0 & \bar{k}_2 & -k_2 \end{bmatrix} \begin{bmatrix} x_p \\ x_p^2 \\ x_p^3 \end{bmatrix}$

$A\Psi = 0 \Rightarrow \psi \rightarrow \begin{bmatrix} a \\ k_1/\bar{k}_1\, a \\ \frac{\bar{k}_2}{k_2} \cdot \frac{k_1}{\bar{k}_1}\, a \end{bmatrix} \neq \begin{bmatrix} x_p \\ x_p^2 \\ x_p^3 \end{bmatrix}$

might work for fine-tuned rates but works in general only for $\delta = 0$