

MA 289: Lecture Notes of Nov 12, 2008

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Recall:

Mass Action Kinetics:

Deterministic fluid model: $\dot{c} = f(c) = Y A_{\tilde{\kappa}} \Psi(c)$

Complex balance solution: $c \in \mathbb{R}_{>0}^n$ such that $A_{\tilde{\kappa}} \Psi(c) = 0$

i.e., for each complex i ,

$$\sum_{j \neq i} \tilde{\kappa}_{j \rightarrow i} c^{y(j)} = \sum_{l \neq i} \tilde{\kappa}_{i \rightarrow l} c^{y(l)}$$

i.e., rate of flow into i = rate of flow out of i

Theorem : (see Gunawardena for proof)

Define the deficiency $\delta = \dim(\ker(Y) \cap \text{Image}(A_{\tilde{\kappa}}))$. Suppose that $\delta = 0$. Then the network has a complex balance solution if and only if the network is weakly reversible.

Remark

In fact, $0 \leq \delta \leq p - l - s$, where,

p = No. of complexes

l = No. of linkage classes: linkage classes are connected components of the complexes graph

s = dimension of space spanned by $\nu'_k - \nu_k, k = 1, \dots, K$

Examples:

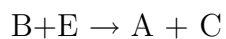
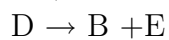
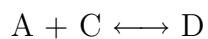
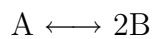
1.



$$\begin{aligned} p &= 3 \\ l &= 1 \\ s &= 2 \\ \Rightarrow p - l - s &= 0 \\ \Rightarrow \delta &= 0 \end{aligned}$$

This reaction network is not weakly reversible.

2.



$$\begin{aligned} p &= 5 \\ l &= 2 \\ s &= 3 \\ \Rightarrow p - l - s &= 0 \\ \Rightarrow \delta &= 0 \end{aligned}$$

This reaction network is weakly reversible, hence there is a complex balance equilibrium.

Note: When you have weak reversibility, $\delta = p - l - s$.

Theorem : (Horn and Jackson, '72 , Feinberg '72, Gunawardena '03)

Suppose $\exists$ a complex balance solution. Then,

- The network is weakly reversible.

- Every $c \in \mathbb{R}_{>0}^n$ such that $f(c) = 0$ is a complex balance solution.
- Let $\mathbb{Z} = \{c \in \mathbb{R}_{>0}^n : f(c) = 0\}$, then for any $c^* \in \mathbb{Z}$,
 $\mathbb{Z} = \{c \in \mathbb{R}_{>0}^n : \ln(c) - \ln(c^*) \in \mathcal{S}^\perp\}$, where
 $\mathcal{S} = \text{span}\{\nu'_k - \nu_k : k = 1, \dots, K\}$
- There is one and only one complex balance solution in each set of the form,
 $(c + \mathcal{S}) \cap \mathbb{R}_{>0}^n \neq \emptyset$, $c \in \mathbb{R}_{>0}^n$, in other words, a positive stoichiometric compatibility class that is non empty.
- Each complex balance solution in a given positive stoichiometric compatibility class is locally asymptotically stable within that class.

Connection between complex balance solutions for fluid models and product form stationary distributions for stochastic models: (Anderson, Craciun, Kurtz)

Stochastic Model:

$$\begin{aligned} X(t) &= \# \text{ of molecules of each species at time } t \\ &= X(0) + \sum_{k=1}^K N_k \left(\int_0^t \lambda_k(X(s)) ds \right) (\nu'_k - \nu_k) \end{aligned}$$

$$\text{where } \lambda_k(x) = \kappa_k \prod_{i=1}^n x_i (x_i - 1) \dots (x_i - \nu_{ik} + 1)$$

Consider the fluid model with $\dot{c} = f(c) = Y A_\kappa \Psi(c)$ (rate constants are κ_k and not $\tilde{\kappa}_k$). Assume that there is a complex balance solution c for this fluid model.

Recall:

X is a continuous time Markov chain.

X takes values in $\mathbb{Z}_+^n = \mathbb{N}^n$.

$x \leftrightarrow y$ (state x communicates with state y) iff

$P(X(t) = y \text{ for some } t \geq 0 | X(0) = x) > 0$ and

$P(X(t) = x \text{ for some } t \geq 0 | X(0) = y) > 0$.

- So, we can partition $\mathbb{Z}_+^n$ into equivalence classes of communicating states.
- All states in a given communicating class are of the same type, i.e., either all transient or all recurrent.
- A recurrent class is closed in the sense that there are no “arrows” leading out of it.

Claim: (Anderson, Craciun and Kurtz)

Assume c is a complex balance solution. Consider a closed communicating class Γ . Let

$$\begin{aligned}\pi(x) &= M \frac{c^x}{x!}, & x \in \Gamma \subset \mathbb{Z}_+^n \\ \text{where } c^x &= \prod_{i=1}^n c_i^{x_i} \\ \text{and } x! &= \prod_{i=1}^n x_i!\end{aligned}$$

M is a normalizing constant such that $\sum_{x \in \Gamma} \pi(x) = 1$. Then π is the unique stationary distribution for X on Γ .

Note:

$$\begin{aligned}\sum_{x \in \mathbb{Z}_+^n} \frac{c^x}{x!} &< \infty \\ \text{because } \sum_{j=1}^{\infty} \frac{c_i^j}{j!} &= e^{c_i} < \infty\end{aligned}$$

Proof:

We give the proof for the case when

$$\Gamma = \mathbb{Z}_+^n.$$

Since X is a continuous time Markov chain:

$$P(X(t+h) = x' | X(t) = x) = q_{xx'}h + o(h) \quad \forall x \neq x'$$

Q - matrix :

$$Q = (q_{xx'})$$

$$q_{xx} = -\sum_{x' \neq x} q_{xx'} \quad (\text{Row sums are zero})$$

Since Γ is the whole space and the MC X does not explode in finite time, it suffices to show,

$$\begin{aligned} \pi' Q &= 0 \\ \text{i.e., } \sum_{x \in \mathbb{Z}_+^n} \pi(x) q_{xx'} &= 0 \quad \forall x' \in \mathbb{Z}_+^n \\ \Leftrightarrow \sum_{x \neq x'} \pi(x) q_{xx'} &= \pi(x')(-q_{x'x'}) = \pi(x') \sum_{x \neq x'} (q_{x'x}) \quad \forall x' \in \mathbb{Z}_+^n \end{aligned}$$

$x \rightarrow x'$ can occur via the k^{th} reaction provided $x - \nu_k + \nu'_k = x'$ and $x - \nu_k$ is in the positive orthant (i.e., there are enough reactants in x to make the reaction feasible). Similarly, $x' \rightarrow x$ can occur by the k^{th} reaction provided x' has enough of each of the species to make the reaction go and $x = x' + \nu'_k - \nu_k$. So the above equation is equivalent to having the following for each x' in $\mathbb{Z}_+^n$:

$$\sum_{k=1}^K \pi(x) \lambda_k(x) 1_{\{x=x'-\nu'_k+\nu_k; x-\nu_k \in \mathbb{Z}_+^n\}} = \pi(x') \sum_{k=1}^K \lambda_k(x') 1_{\{x'-\nu_k \in \mathbb{Z}_+^n\}}$$

$$\text{where} \quad \lambda_k(x) = \kappa_k \prod_{i=1}^n x_i(x_i - 1) \dots (x_i - \nu_{ik} + 1).$$

Proof to be continued.