

BO HU NOTES

11/10/08

Correction

$$f_k^r(\bar{x}^r(\cdot)) \leq f_k(\bar{x}^r(\cdot))$$

$$\text{but } f_k^r(c) \neq f_k(c)$$

CRNT

(Chemical Reaction Network Thm)

$$\dot{c} = f(c), \quad c \in \mathbb{R}_{\geq 0}^n$$

f given by mass-action kinetics

Complex Balance Equilibria

Refs: - Horn, F. + Jackson, R.

General mass action kinetics

Arch. Rat. Math. Anal 47 (1972), 81-116

- M. Feinberg, Lecture Notes, 1979

- J. Gunawardena, Chemical Reaction Network theory for non-biologists, 2003

- D. F. Anderson, G. Gracium + T. G. Kurtz
Product form Stationary distributions
for deficiency zero chemical reaction
networks, preprint

Mass Action:
$$f(c) = \sum_k (v_k' - v_k) \bar{K}_k c^{v_k} = S r(c)$$

S = stochastic matrix, k^{th} col. of $S' = v_k' - v_k$

$$(r(c))_k = \bar{K}_k c^{v_k}$$

$$v_k \xrightarrow{\bar{K}_k} v_k'$$

We will rewrite

$$f(c) = Y A_{\mathbb{R}} \underline{\Psi}(c)$$

$$c \in \mathbb{R}_{\geq 0}^n$$

$p = \#$ complexes

can represent complexes as elements $y \in \mathbb{Z}_{\geq 0}^n$

where; $\underline{\Psi}(c) = \left\{ \begin{pmatrix} \vdots \\ c^y \\ \vdots \end{pmatrix} \right\}_P$
 complex $y \rightarrow c^y$

$$(\underline{\Psi}(c))_i = c^{y(i)} = \prod_{j=1}^n c_j^{y_j(i)} \quad \left(\begin{array}{l} \text{mapping } c \in \mathbb{R}_{\geq 0}^n \\ \mapsto \mathbb{R}_{\geq 0}^p \end{array} \right)$$

where $y(i)$ is the vector in $\mathbb{Z}_{\geq 0}^n$ representing i^{th} complex

$\mathbb{R}^p$ is "complex space". Also think of i^{th} complex as i^{th} unit basis vector e_i in $\mathbb{R}^p$

i) Y is an $n \times p$ matrix (ie. linear mapping from $\mathbb{R}^p$ into $\mathbb{R}^n$)

The i^{th} col. of Y is the representation of the i^{th} complex in $\mathbb{Z}_{\geq 0}^n$

$$y(i) = Y e_i, \quad i = 1, \dots, p$$

iii) $A_{\mathbb{R}}: \mathbb{R}^p \rightarrow \mathbb{R}^p$ ($p \times p$ matrix)

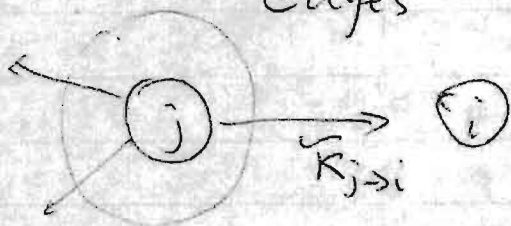
(or

$$A_{\bar{K}}^{ij} = \begin{cases} \bar{K}_{j \rightarrow i}, & \text{for } j \neq i, \text{ corresponding to reaction} \\ & \text{complex } j \xrightarrow{\bar{K}_{j \rightarrow i}} \text{complex } i \\ -\sum_{l \neq j} \bar{K}_{j \rightarrow l}, & \text{for } j = i. \end{cases}$$

Complex Graph;

Nodes - Complex

Edges - directed induced reactions



A^T is an infinitesimal generator for a cts time Markov Chain on $\{1, \dots, p\}$ finite set of complexes

Check: $f(c) = \gamma A_{\bar{K}} \psi(c)$

$$(A_{\bar{K}} \psi(c))_i = \sum_j A_{\bar{K}}^{ij} (\psi(c))_j$$

$$= \sum_{j \neq i} \bar{K}_{j \rightarrow i} c^{y(j)} - \sum_{l \neq i} \bar{K}_{i \rightarrow l} c^{y(i)}$$

$$\Rightarrow A_{\bar{K}} \psi(c) = \sum_i \sum_{j \neq i} \bar{K}_{j \rightarrow i} c^{y(j)} e_i - \sum_i \sum_{l \neq i} \bar{K}_{i \rightarrow l} c^{y(i)} e_i$$

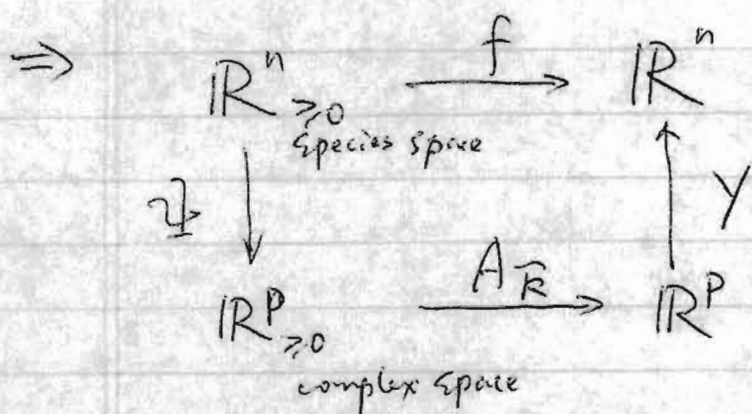
$$= \sum_i \sum_{j \neq i} \bar{K}_{j \rightarrow i} c^{y(j)} e_i - \sum_j \sum_{i \neq j} \bar{K}_{j \rightarrow i} c^{y(j)} e_j$$

$$= \sum_i \sum_{j \neq i} \bar{K}_{j \rightarrow i} c^{y(j)} e_i - \sum_j \sum_{i \neq j} \bar{K}_{j \rightarrow i} c^{y(j)} e_j$$

$$= \sum_i \sum_{j \neq i} \bar{K}_{j \rightarrow i} c^{y(j)} (e_i - e_j)$$

$$\gamma A_{\bar{K}} \psi(c) = \sum_i \sum_{j \neq i} \bar{K}_{j \rightarrow i} c^{y(j)} (y(i) - y(j))$$

$$= \sum_{\substack{k \\ \text{reactions} \\ v_k \rightarrow v'_k}} \bar{K}_k c^{v_k} (v'_k - v_k) = f(c) \quad \text{checked } \square$$



γ & $A_{\bar{K}}$ are linear mappings, while ψ is nonlinear.

(commutative diagram)

Equilibrium Solution: is a $c \in \mathbb{R}_{\geq 0}^n$ such that

$$f(c) = 0 \quad \text{Since } f(c) = \gamma A_{\bar{K}} \psi(c)$$

if c is an equilibrium point, then

$$A_{\bar{K}} \psi(c) \in \ker(\gamma) = \text{null space of } \gamma$$

$$E = \text{equilibrium set} = \{c \in \mathbb{R}_{\geq 0}^n \mid f(c) = 0\}$$

Complex Balance Solution: is a $c \in \mathbb{R}_{\geq 0}^n$ such that

$$A_{\bar{K}} \psi(c) = 0 \quad (\text{Note such } c \text{ is in } E)$$

$C :=$ complex balance solutions

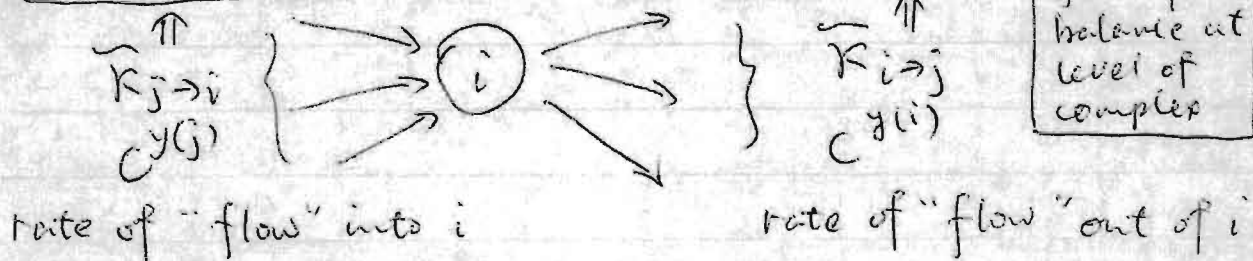
$$= \{ c \in \mathbb{R}_{>0}^n : A_{\tilde{K}} \Psi(c) = 0 \}$$

Network is complex balanced if $C = E \neq \emptyset$

Note: c is a complex balance solution iff for each complex i : $(A_{\tilde{K}} \Psi(c))_i = 0 \Rightarrow$

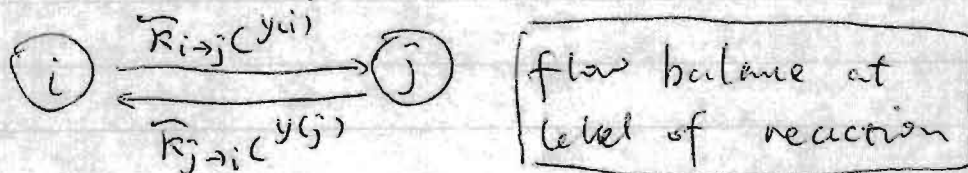
$$\sum_{j \neq i} \tilde{K}_{j \rightarrow i} c^{y(j)} - \sum_{j \neq i} \tilde{K}_{i \rightarrow j} c^{y(i)} = 0 \Rightarrow$$

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



Detailed Balance Solution: is a $c \in \mathbb{R}_{>0}^n$ s.t.

for each reaction $i \rightarrow j$, there is a reaction $j \rightarrow i$ and $\tilde{K}_{i \rightarrow j} c^{y(i)} = \tilde{K}_{j \rightarrow i} c^{y(j)}$



Every detailed balance Soln is a Complex balance Soln.

$$D := \{ c \in \mathbb{R}_{>0}^n : c \text{ is a detailed balance Soln} \}$$

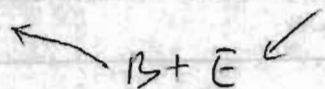
Network is detailed balanced if $D = E \neq \emptyset$

Defn: The reaction network is weakly reversible if whenever the reaction $i \rightarrow j$ occurs there is a sequence of reactions

$j \rightarrow j_1 \rightarrow j_2 \rightarrow \dots \rightarrow j_l \rightarrow i$, l is finite, leading back to i .

Example: $A \rightleftharpoons B$ reversible

$A + C \rightleftharpoons D$ weakly reversible.



Not weakly reversible $A + E \rightleftharpoons AE \rightarrow B + E$

Lemma: If there is a complex balance solution, then the reaction network is weakly reversible

Proof: Suppose $\exists c \in \mathbb{R}_{>0}^n : A_{\overline{K}} \underline{\nu}(c) = 0$

$\pi = \underline{\nu}(c)$ is a vector with strictly positive components

$\pi' A_{\overline{K}}' = 0$, π can be renormalized to be a prob. vector

then there is a stationary dist. for, cts.
time M.C. with inf. generator A_R'
on the set $\{1, \dots, P\}$.

A finite ~~state~~ cts. time M.C. has
States that are pos. recurrent or transient.
A stat. dist. does not change transient
states

Hence all of the states for the A_R' M.C.
are pos. recurrent.

Follows from this that reaction network
is weakly reversible.