Roll - 2020113002

Mathematical Models In Biology

Asignment-5

S24-SC 3.316

Question 1

Given, $\exists$ a deficiency zero Network & it's positive equilibrium
P.T. it is quasi - thermodynamic.

Hence, let $f(c) = \sum_{y \to y' \in R} k_{y \to y'} c^y (y' - y)$

$\Rightarrow g(c) = \sum_{y \to y' \in R} k_{y \to y'} c^y (w_{y'} - w_y)$, [where $Y w_y = y$] (1)

$\Rightarrow f(c) = Y g(c)$. [such that $f(c) = Y A_k \Psi$]

Now, let the (+) ve equilibrium that exists be c^*

$\Rightarrow f(c^*) = 0$.

$\Rightarrow Y \cdot g(c^*) = 0$

$\Rightarrow g(c^*) \in \text{Kernel}(Y)$ (2)

Now, we have: $\Delta = \{ w_{y'} - w_y : \text{s.t. } y' \sim y \}$

From (1), we can say: $g(c^*) \in \text{span}(\Delta)$ (3)
(ie, it is a linear combination of $w_{y'} - w_y$, considering $k_{y \to y'} c^y$ as a scalar constant)

From (2) & (3) $g(c^*) \in \text{span}(\Delta) \cap \text{Kernel}(Y)$ (4)

Now, let $Y : \mathbb{R}^C \to \mathbb{R}^S$ (C denotes complexes; S denotes species)
$\bar{Y} : \text{span}(\Delta) \to \mathbb{R}^S$ &

Then, here, $Y w_y = y$ [as $w_y \in \mathbb{R}^C$, $y \in \mathbb{R}^S$].

& $\bar{Y}(w_y - w_{y'}) = y - y'$ [as $w_y - w_{y'} \in \text{span}(\Delta)$]

From Rank - Nullity Theorem

$$\dim(\text{span}(\Delta)) = \dim(\text{Kernel } \bar{Y}) + \dim(\text{Image } \bar{Y})$$

$\Rightarrow \delta = \dim : \text{Kernel}(\bar{Y}) = (n - \ell) - s$ [as, $\dim(\text{span}(\Delta)) = n - \ell$, $\dim(\text{Im}(\bar{Y})) = s$]

and, $\text{Kernel } \bar{Y} = \text{Kernel } Y \cap \text{span}(\Delta)$

$\Rightarrow \dim(\text{Kernel}(\bar{Y})) = \dim(\text{Ker}(Y) \cap \text{span}(\Delta))$

$= \delta$

P-4

P-2

When $\delta = 0 \Rightarrow \dim(\text{Kernel}(Y) \cap \text{span}(\Delta)) = 0$

$\Rightarrow \text{Ker } Y \cap \text{span}(\Delta)$ contains 0 vector. (5)

From (4), $g(c^*) \in \text{Kernel}(Y) \cap \text{span}(\Delta)$

$\Rightarrow g(c^*) = 0$. (6)

$\Rightarrow$ complex balancing occurs at c^* if $g(c^*) = 0$ as

$$g(c) = \sum_{y \to y'} K_{y \to y'} c^y (w_{y'} - w_y)$$

$$\Rightarrow g(c) = \sum_{y \in C} \Big[\overset{\text{+ sum of complex balan}}{\sum_{R \to y} K_{y' \to y} c^{y'}} - \sum_{y \to R} K_{y \to y'} c^y \Big] w_y$$

$$\Rightarrow g(c^*) = 0 \Rightarrow \sum_{R \to y} K_{y' \to y} c^{*y'} = \sum_{y \to R} K_{y \to y'} c^{*y} \quad \forall \text{ complex } y \in C.$$

So it is complex balanced at given positive equilibrium

[8] Complex balancing gives a (+)ve equilibrium whose underlying Reaction Network has deficiency 0.

The reaction network is complex balanced at c^* $\Rightarrow$ the system is quasithermodynamic.

ROLL-2020113002

AS-MMB

Question 2

Given: $\dot{x} = f(x)$ is a M.A.S. ; Consider y^* be a virtual source where reversibility hold.

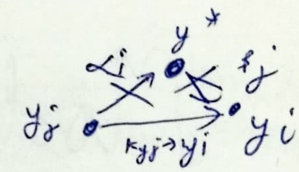
This means,

$y^* \to y_i \in G, \forall i \in C$ | $y_i \to y^* \in G \; \forall i \in C$

$\Rightarrow \alpha_i = K_{y^* \to y_i}$ | $\Rightarrow \beta_i = K_{y_i \to y^*}$

Consider G' which is reversible reaction network such that

$$K'_{y_j \to y^*} = K'_{y^* \to y_i} = 0$$



$$K'_{y_j \to y_i} = K_{y_j \to y_i} + \frac{\beta_j (\alpha_i)}{\sum \alpha_i}$$

Where y^* is the virtual source which is such that

$$\sum_i \alpha_i y_i = \sum_i \alpha_i y^*$$

$$\Rightarrow \sum (y_i - y^*) \alpha_i = 0$$

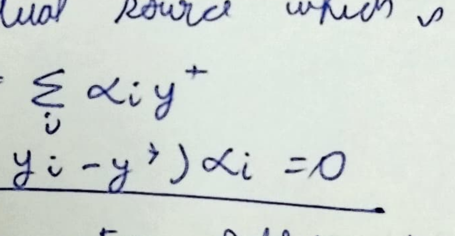
Let z_j be an arbitrary vector. Difference due to the reaction $z_j \to y_i^*$ is given as:

$$= \sum_{i=1}^{N} (K'_{z_j \to y_i^*} - K_{z_j - y_i})(y_i - z_j)$$

$$= \sum_{i=1}^{N} \frac{\beta_j \alpha_i}{\sum \alpha_i}(y_i - z_j) = \frac{\beta_j}{\sum \alpha_i}\left[\sum_{i=1}^{N} \alpha_i y^* - \sum_{i=1}^{N} \alpha_i z_i\right]$$

$$= \frac{\beta_j}{\sum \alpha_i}(\sum \alpha_i)(y^* - z_j) = \beta_j (y^* - z_i)$$

Which is the contribution from $z_j \to y^*$!! It is dynamically equivalent to Z_j s.t.



$\therefore \exists$ dynamical equivalence at arbit vertex z_j: giving dynamical equivalence to exist at every vector. G' obtained from G by replacing $z_j \to y^* \to y_i$ with $z_j \to y_i$. Now repeat same procedure for $y_i \leftrightarrows z_j$; we will get dynamical equilibrium by using $z_j \in y^* \in y$. as dynamic equivalance happens in both direction $y_i \to z_j$ & $z_j \in y_i$ we can say that G' is reversible. The value of K' should be chosen to ensure dynamical equivalence condition. The vertices of weakly reversible M.A.S. are exactly exponents of monomials of $f(x)$. Reversible reaction are weakly reversible as well & all vertices of M.A.S are exact exponents of monomials of $f(x)$.

$\therefore$ proved.

P4

Roll - 2020113002

Question 3]

(i) All cycles in the Species - Reaction (S-R) graph are odd cycles or are 1-cycles.
(ii) No two even cycles have S-R interactions
Here, odd cycle is such that in SR graph, ∃ odd no. of c-pairs
1-cycle is a cycle in SR graph having coefficients $=1 \; \forall$ edges.
The above two are the conditions on SR graph for Reaction networks not processing multiple non-degenerative equilibrium within same stoichiometric class.

Question 4]

Given a detailed balanced linear mass action system, find a Lyapunov function that is infinite at the boundary of the positive orthant.

Let $\vec{x}$ s.t. $\vec{x} = [x_1, x_2 \ldots x_n]$; in n-dimensional hyperspace, where x_i = conc. of ith component / species.

Given, the M.A.S. is detailed balanced; & is thus quasithermodynamic

Let us consider $h'(c) = \sum_{s \in S} c_s(\ln c_s - \ln c_s^* - 1) + c_s^*$

Now, $h'(c) > 0 \; \forall \; \vec{c} \in$, also note $f(c) \times h'(c) \leq 0$ where $\mu(c) = \nabla h'(c)$

consider

$\Rightarrow h(c) = \sum_{s \in S} c_s(\ln c_s - \ln c_s^*) + \frac{1}{c_s} + c_s^*$

Now, $\nabla h(c) \cdot f(y) = \sum_{s \in S} \left(\ln c_s - \ln c_s^* - \frac{1}{c_s^2}\right)$ for

$\Rightarrow \nabla h(c) \cdot f(y) = \nabla h'(c) \times f(c) - \sum_{S} \frac{1}{c_s^2} f(c)$

Detailed balance $\Rightarrow$ Quasithermodynamic

$\Rightarrow \nabla h(c) \cdot f(c) \leq 0$, so $h(c) = \sum_{s \in S} c_s(\ln c_s - \ln(c_s^*)) + \frac{1}{c_s} + c_s^*$ is a Lyapunov function

Now $c_s \to 0$ then

$\lim_{c_s \to 0} h(c) = \lim_{c_s \to 0} \sum_{s \in S} \underset{\downarrow 0}{\ln(c_s)} - \sum_{s \in S} \underset{\downarrow 0}{\ln c_s^*} + \sum_{s \in S} \frac{1}{c_s} + \sum c_s^*$

P5

Roll - 2020113002

$\because \lim_{x \to 0} x \ln x = 0 \Rightarrow \lim_{x \to 0^+} \frac{1}{\lambda} \to \infty$

Lyapunov function is at founding of (+ive) cooler

$\Rightarrow h(c) = \sum_{s \in S} c_s (\ln c_s - \ln c_s^*) + \frac{1}{c_s} + c_s^{*1}$

Question 5

let $y_1 \leftrightarrow y_2 \leftrightarrow y_3 \leftrightarrow y_4$

$y_5 \leftrightarrow y_6$

---

① Suppose that $y \leftrightarrow y'$ is an internal cut link. (such as $y_2 \leftrightarrow y_3$), i.e, in which both complex are participants in reaction other than those contained in the cut link $y \leftrightarrow y'$ sh the subnetwork obtained by removing $y \leftrightarrow y'$, there will be as many complexes as before but now there will one more linkage class

② suppose that $y \leftrightarrow y'$ is an end cut link, like $y_1 \leftrightarrow y_2$ is an end cut link in which exactly one is a participating reaction and not in cut link $y \leftrightarrow y'$. In the subnetwork obtained by removing $y \leftrightarrow y'$, the no. of linkage classes ~~remains same~~ increases but there is ~~less complex~~ same no. of complex due to removal of y.

③ Suppose $y \leftrightarrow y'$ is an isolated cut link ($y_5 \leftrightarrow y_6$) (Eg.) such that neither is (y or y') a participant in a reaction contained in cut link $y \leftrightarrow y'$. In the subnetwork obtained by removing the link $y \leftrightarrow y'$ the no of linkage classes increases by 1 & no of links remain the same

$\Rightarrow \tilde{n} = n$ (i.e)

$\Rightarrow \tilde{l} = l + 1.$ (i.e)

$\rightarrow \tilde{n} - \tilde{l} = n - l - 1$ $\therefore$ proved

 Roll 2020113002

Question 6

given $\frac{dx}{dt} = Y A_K \Psi$.

P.T. $\delta = \dim(\ker(Y) \cap \operatorname{Im}(A_K))$ $\forall$ weakly reversible reactions / networks

We know

$$f(c) = \sum_{y \to y' \in R} k_{y \to y'} c^y (y' - y)$$

& $$g(c) = \sum_{y \to y' \in R} k_{y \to y'} c^y (w_{y'} - w_y)$$

where $w \mid \neq Y$ ~~=~~ $Y w_y$

Now, $Y : R^c \longrightarrow \mathbb{R}^S$

$\Rightarrow \bar{Y} : \operatorname{span}(A) \longrightarrow \mathbb{R}^S$. where c = no. of complex, S = no. of species

From Rank - Nullity Theorem,

$\dim(\operatorname{span}(A)) = \dim(\ker(\bar{Y})) + \dim(\operatorname{Im} \bar{Y})$.

$\Rightarrow \dim(\ker \bar{Y}) = n - l - s$

$\Rightarrow \ker \bar{Y} = \ker Y \cap \operatorname{span}(A)$.

$\Rightarrow \delta = \dim(\ker(Y) \cap \operatorname{span}(A))$

Claim $\operatorname{span}(A) = \ker(A_K)$ $\forall$ weakly reversible networks

$\Rightarrow A_K(x) = \sum_{y \to y'} x_y (w_{y'} - w_y)$

Roll - 2020113002

From above solution $\Rightarrow A_K x \subseteq \text{span}(A)$

$\Rightarrow A_K(X) \subseteq \text{span}(A)$

We know,

$A_K \rightarrow R^c \rightarrow R^s$

From rank nullity theorem

$\dim(R^c) = \dim(\mathrm{Im}(A_K)) + \dim(\mathrm{kernel}(A_K))$

↳ domain.

$\Rightarrow \dim(\mathrm{Im}(A_K)) = -\dim(\mathrm{Ker}(A_K)) + n$

$= n - t$ | n. of strong terminal linkage classes

$\therefore$ the reaction network is weakly reversible

terminal strong linkage class # no of linkage cla

$\Rightarrow \dim(\mathrm{Im}(A_K)) = n - \ell$ (2)

From this we can say that image (A_K) is a subspace of span (A), but

From (2) we got $\dim(\mathrm{Im}(A_K)) = n - \ell$
$= \dim(\text{span}(A))$

So, we can say that $\mathrm{Im}(A_K) = \text{span}(A)$

$\therefore \Rightarrow \delta = \dim(\mathrm{kernel}(Y) \cap \text{span}(A))$

$= \dim(\mathrm{Ker}(Y) \cap \mathrm{Im}(A_K))$

Ans.