ECE 520.622 Prof. John Goutsias
Principles of Complex Networked Systems

QUIZ #3

Name: ______________________________________

1. Consider a Markovian reaction network comprised of the following five species and reactions:

$$\begin{aligned} X_1 + X_2 &\rightarrow X_3 \\ X_3 &\rightarrow X_1 + X_2 \\ X_4 &\rightarrow X_3 \\ X_4 &\rightarrow X_5 \\ X_5 &\rightarrow X_4. \end{aligned}$$

The system is initialized with $X_1(0) = X_2(0) = X_3(0) = X_4(0) = 0$ and $X_5(0) = 1$. In this case, the master equation can be written as

$$\frac{d\mathbf{p}(t)}{dt} = \mathbf{P}\mathbf{p}(t),$$

where the matrix $\mathbf{P}$ is given by

$$\mathbf{P} = \begin{bmatrix} -\kappa_1 & \kappa_2 & 0 & 0 \\ \kappa_1 & -\kappa_2 & \kappa_3 & 0 \\ 0 & 0 & -(\kappa_3 + \kappa_4) & \kappa_5 \\ 0 & 0 & \kappa_4 & -\kappa_5 \end{bmatrix},$$

where κ_1 is the specific probability rate constant of the first reaction, κ_2 is the specific probability rate constant of the second reaction, etc.

(a) What is the state-space of this system?

(b) Is the network irreducible, completely reducible, or incompletely reducible?

(c) Which states are persistent and which are transient?

(d) If $\kappa_3 = 0$, what happens to the system?

(e) In the case of (d), what is the probability distribution $\overline{\mathbf{p}}$ of the population process at steady-state?

2. Let $\overline{p}(\widetilde{\mathbf{x}})$ be the steady-state distribution of the population density process in a Markovian reaction network of size Ω.

   (a) Define the potential energy function $V(\widetilde{\mathbf{x}}; \Omega) \geq 0$.

   (b) What is the form of $\overline{p}(\widetilde{\mathbf{x}})$ in terms of $V(\widetilde{\mathbf{x}}; \Omega)$?

   (c) If $V_0(\widetilde{\mathbf{x}}) = \lim_{\Omega \to \infty} V(\widetilde{\mathbf{x}}; \Omega)$, what is the relationship between the minima of $V_0(\widetilde{\mathbf{x}})$ and the stable macroscopic states of the Markovian reaction network at steady-state?

   (d) What is *Keizer's paradox*?

   (e) What is a noise-induced mode and how these modes may be generated in a complex network?

3. In a Markovian reaction network, two thermodynamic balance equations are given by

$$\frac{dS(t)}{dt} = \sigma(t) - h(t) \quad \text{and} \quad \frac{dF(t)}{dt} = f(t) - \sigma(t),$$

where $S(t)$ is the entropy of the system at time t and $F(t)$ is the Helmholtz free energy at time t.

(a) Define $S(t)$.

(b) Define $F(t)$.

(c) What are the thermodynamic roles of $\sigma(t)$, $h(t)$ and $f(t)$?

(d) How are these quantities related at steady-state?

(e) How are these quantities related if the system reaches thermodynamic equilibrium at steady-state? What happens to the system in this case?

4. The neural network model discussed in class is comprised of L neurons and is characterized by the reactions:

$$X_{2l-1} + \sum_{l' \neq l} \nu_{l'l} X_{2l'} \;\rightarrow\; X_{2l} + \sum_{l' \neq l} \nu_{l'l} X_{2l'}$$
$$X_{2l} \;\rightarrow\; X_{2l-1}.$$

(a) What do X_{2l-1}, X_{2l} denote? What does ν_{ij} measure and what is the meaning of its values?

(b) What do these reactions model?

(c) The propensity function of the previous reactions are given by

$$x_{2l-1}[\phi_l(\mathbf{x}) > 0] \tanh(\phi_l(\mathbf{x})) \quad \text{and} \quad \gamma_l x_{2l},$$

where [ ] is the Iverson bracket. What is the form and meaning of $\phi_l(\mathbf{x})$ and γ_l?

(d) The pressure $\overline{P}(\Omega)$ and bulk modulus $\overline{B}(\Omega)$ in a neural network with size parameter Ω at steady-state are given by

$$\overline{P}(\Omega) = -\frac{\partial \overline{H}(\Omega)}{\partial \Omega} \quad \text{and} \quad \overline{B}(\Omega) = -\Omega \frac{\partial \overline{P}(\Omega)}{\partial \Omega},$$

where $\overline{H}(\Omega)$ is the Helmholtz free energy. How can these quantities be used in order to quantify robustness and critical behavior in the network? What does "robustness" mean in this case?