Solution to the Midterm

1 Q1

A. b)

B. c)

C. c)

D. d)

E. b)

F. c)

G. c)

H. a)

I. c)

J. b)

2 Q2

A. Refer to Figure 1.

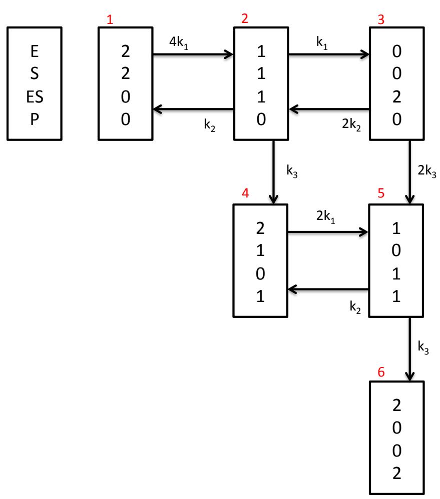

Fig. 1: Reachability graph of the CRN given in the exam

B. This refers to the transition from state 3 to state 5. There are two exit transitions from state 3 : 1) Dissociation of ES into E and S and 2) Conformational change of bound S into P and resulting in E and P. The total exit transition rate is $2k_2 + 2k_3$ and the probability that the transition is to the state in which there is one ES and one P is $\dfrac{2k_2}{2k_2 + 2k_3} = 1/2$.

C. The expected dwell time is the inverse of exit transition rate. For the state where there is one E, one ES and one S (state 2), the sum of exit transition rates is $k_1 + k_2 + k_3$. Thus the expected dwell time is $(k_1 + k_2 + k_3)^{-1} = 1/3$.

D. Notice that state 6 is a sink state with no exit transition. Therefore, at steady-state, the probability distribution of state 6 is 1, while all the other states will have distribution of 0. Then, the expected number of P is 2 with variance 0. More formal derivation of this is,

$$\begin{aligned} <P> &= \sum_i n p_n && (1) \\ &= p_4 + p_5 + 2p_6 && (2) \\ &= 2 && (3) \\ <P^2> - <P>^2 &= \sum_i n^2 p_n - 2^2 && (4) \\ &= 2^2 - 2^2 && (5) \\ &= 0 && (6) \end{aligned}$$

3 Q3

A. Solve the first equation for equilibrium:

$$\begin{aligned} k_1 A^2 &= k_2 B && (7) \\ B &= \frac{k_1}{k_2}(A^2) && (8) \\ &= \frac{k_1}{k_2}(A_{tot} - 2B)^2 \quad \text{(conservation of mass : } A_{tot} = A + 2B \text{)} && (9) \\ &= \frac{k_1}{k_2}\left(A_{tot}^2 - 4A_{tot}B + 4B^2\right) && (10) \\ 0 &= \frac{4k_1}{k_2}B^2 - \left(\frac{4k_1}{k_2}A_{tot} + 1\right)B + \frac{k_1}{k_2}A_{tot}^2 && (11) \\ B &= \frac{k_2}{8k_1}\left[\frac{4k_1}{k_2}A_{tot} + 1 \pm \sqrt{\left(\frac{4k_1}{k_2}A_{tot} + 1\right)^2 - \left(\frac{4k_1}{k_2}A_{tot}\right)^2}\right] && (12) \end{aligned}$$

Solve the second equation for equilibrium:

$$\begin{aligned} k_3 g_{off} B &= k_4 g_{on} && (13) \\ g_{off} &= \frac{k_4 g_{on}}{k_3 B} && (14) \end{aligned}$$

Then, the fraction of g_{on} is

$$\begin{aligned} \frac{g_{on}}{g_{off} + g_{on}} &= \frac{1}{1 + \frac{k_4}{k_3 B}} && (15) \\ &= \frac{k_3 B}{k_3 B + k_4} && (16) \\ f(A_{tot}) &= \frac{k_3 \frac{k_2}{8k_1}\left[\frac{4k_1}{k_2}A_{tot} + 1 \pm \sqrt{\left(\frac{4k_1}{k_2}A_{tot} + 1\right)^2 - \left(\frac{4k_1}{k_2}A_{tot}\right)^2}\right]}{k_3 \frac{k_2}{8k_1}\left[\frac{4k_1}{k_2}A_{tot} + 1 \pm \sqrt{\left(\frac{4k_1}{k_2}A_{tot} + 1\right)^2 - \left(\frac{4k_1}{k_2}A_{tot}\right)^2}\right] + k_4} && (17) \end{aligned}$$

B.

$$\begin{aligned} \lim_{A_{tot} \to 0} f(A_{tot}) &= 0 && (18) \\ \lim_{A_{tot} \to \infty} f(A_{tot}) &= 1 && (19) \end{aligned}$$

4 Q4

$$\begin{aligned}
\frac{d}{dt}\langle X\rangle &= \langle k_1(\langle X+2\rangle - \langle X\rangle) + k_2X(\langle X-1\rangle - \langle X\rangle)\rangle && (20)\\
&= 2k_1 - k_2\langle X\rangle && (21)\\
\langle X\rangle^* &= \frac{2k_1}{k_2} && (22)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dt}\langle X^2\rangle &= \left\langle k_1\left(\langle X^2+4X+4\rangle - \langle X^2\rangle\right) + k_2X\left(\langle X^2-2X+1\rangle - \langle X^2\rangle\right)\right\rangle && (23)\\
&= \langle k_1(4\langle X\rangle + 4) + k_2X(-2\langle X\rangle + 1)\rangle && (24)\\
&= (4k_1+k_2)\langle X\rangle - 2k_2\langle X^2\rangle + 4k_1 && (25)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dt}Var(X) &= \frac{d}{dt}\langle X^2\rangle - 2\langle X\rangle\frac{d}{dt}\langle X\rangle && (26)\\
&= k_2\langle X\rangle - 2k_2Var(X) + 4k_1 && (27)\\
Var(X)^* &= \frac{k_2\langle X\rangle^* + 4k_1}{2k_2} && (28)\\
&= \frac{k_1}{k_2} + \frac{2k_1}{k_2} && (29)\\
&= \frac{3k_1}{k_2} && (30)
\end{aligned}$$

5 Grade Distribution

1. (20pts)
   - 2 pts each
2. (10pts)
   - 2.5 pts each
3. (10pts)
   - 7 pts
   - 3 pts
4. (10pts)
   - 5 pts each : correct set up of extended generator, correct answer.