MATH 6397 Homework 2

Mark Jayson Cortez

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1. Consider the reaction network
$$\begin{cases} Y_1 \xrightarrow{c1} 2Y_1 \\ Y_1 + Y_2 \xrightarrow{c2} 2Y_2 \\ Y_2 \xrightarrow{c3} \emptyset \end{cases}.$$

Here, Y_1 is the prey and Y_2 is the predator. The prey reproduces with propensity $c_1[Y_1]$ through the reaction $Y_1 \xrightarrow{c1} 2Y_1$. When the predator catches a prey, another unit of Y_2 is produced with propensity $c_2[Y_1][Y_2]$ as seen in the reaction $Y_1 + Y_2 \xrightarrow{c2} 2Y_2$. The death of the predator is represented by $Y_2 \xrightarrow{c3} \emptyset$, which occurs with propensity $c_3[Y_2]$. Taking these together, we can form the system of ODEs,

$$\begin{cases} \dfrac{d[Y_1]}{dt} = c_1[Y_1] - c_2[Y_1][Y_2] \\ \dfrac{d[Y_2]}{dt} = c_2[Y_1][Y_2] - c_3[Y_2] \end{cases}$$

Clearly, we see that the prey, Y_1, can exist in isolation. Without intervention by the predator, the prey population will grow exponentially through a pure-birth process.

With parameters $c_1 = 1$, $c_2 = 0.005$, and $c_3 = 0.6$, a stochastic simulation of the system is found in Figure 1 below, where we observe a cyclic system.
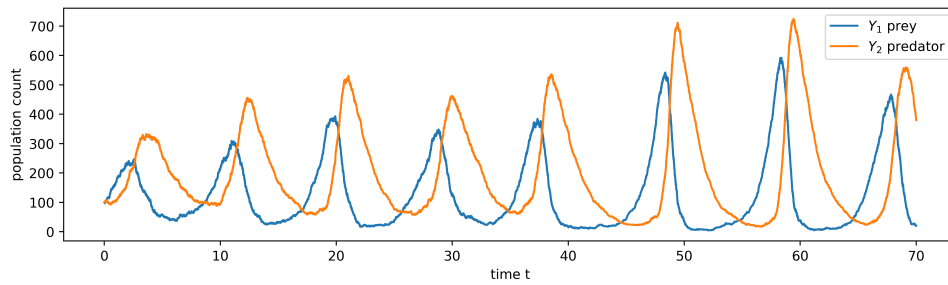

Figure 1: Stochastic simulation of the predator-prey system.

An increase in predation will most likely lead to the extinction of the prey population. A simulation, seen in Figure 2 where the predation rate c_2 is slightly increased to 0.01 shows an extinction event for both populations, where the prey population dies out first and was naturally followed by the predator which exclusively feeds on it.
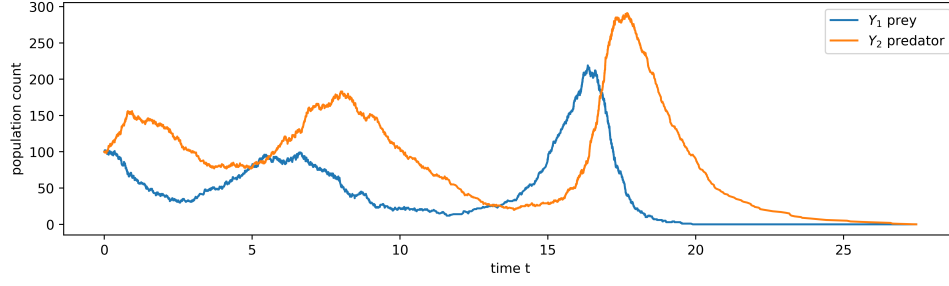
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Figure 2: Stochastic simulation of the predator-prey system which results to extinction of the prey, and eventually of the predator.

Decreasing the population of the prey will very likely lead to the extinction of the predator. Since Y_2 solely relies on Y_1, a decrease in prey poluation will lead to less chances of interaction between the two species thereby limiting the reproduction of Y_2. Figure 3 shows a simulation where c_1 is decreased to 0.2. Here we see that after a certain point when the prey population is very low, the predator population started declining that lead to the species extinction.
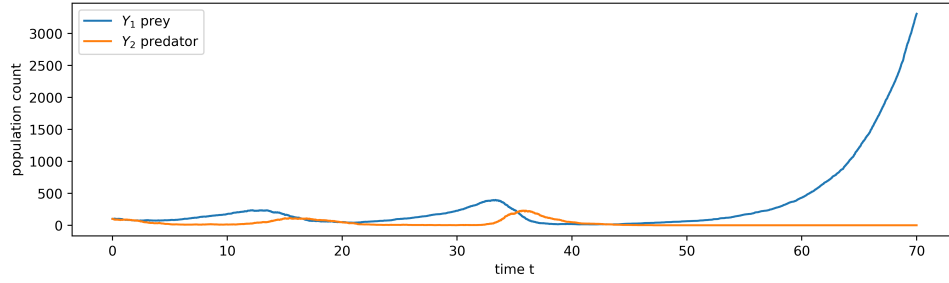

Figure 3: Stochastic simulation of the predator-prey system which results to extinction of the predator and thriving of the prey.

2. Consider the chemical reaction system $\begin{cases} A \xrightarrow{k} X \xrightarrow{\alpha 1} \emptyset \\ B \xrightarrow{k} Y \xrightarrow{\alpha 2} \emptyset \\ X+Y \xrightarrow{k_\alpha} C \end{cases}$, whose corresponding deterministic ODE sys-

tem is $\begin{cases} \dfrac{d[X]}{dt} = k - \alpha_1[X] - k_\alpha[X][Y] \\ \dfrac{d[Y]}{dt} = k - \alpha_2[Y] - k_\alpha[X][Y] \end{cases}$.

The fixed points of the deterministic system is determined by solving

$$\frac{d[X]}{dt} = 0 \tag{1}$$

$$\frac{d[Y]}{dt} = 0 \tag{2}$$

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From equation (1) and (2) we get $\alpha_1[X] + k_\alpha[X][Y] = \alpha[Y] + k_\alpha[X][Y] \implies [X] = \frac{\alpha_2[Y]}{\alpha_1}$. Substituting this back to equation (2) gives

$$k_\alpha \alpha_2[Y]^2 + \alpha_1 \alpha_2[Y] - \alpha_1 k = 0$$
$$\implies [Y] = \frac{-\alpha_1 \alpha_2 + \sqrt{(\alpha_1 \alpha 2)^2 + 4k_\alpha \alpha_1 \alpha_2 k}}{2k_\alpha \alpha_2},$$

considering only the positive equilibrium. So given a set of parameters, the pair

$$([X]^*, [Y]^*) = \left(\frac{\alpha_2}{\alpha_1} \cdot \frac{-\alpha_1 \alpha_2 + \sqrt{(\alpha_1 \alpha 2)^2 + 4k_\alpha \alpha_1 \alpha_2 k}}{2k_\alpha \alpha_2}, \frac{-\alpha_1 \alpha_2 + \sqrt{(\alpha_1 \alpha 2)^2 + 4k_\alpha \alpha_1 \alpha_2 k}}{2k_\alpha \alpha_2} \right)$$

is the fixed point of the deterministic system. Given two sets of paramers $[k, \alpha_1, \alpha_2, k_\alpha]$ equal to $set_1 = [10, 10^{-6}, 10^{-5}, 10^{-5}]$ and $set_2 = [10^3, 10^{-4}, 10^{-3}, 10^{-3}]$, a quick substitution to the computed fixed point above, we see that both parameter sets will give $([X]^*, [Y]^*) \approx (3161.77769969685, 316.177769969685)$.

We qualitatively analyze the behavior of the system in the two cases by looking at sample trajectories with initial condition $(0, 0)$. As seen in Figure 4, the initial segment of the trajectories are very different as molecule counts for both species grows so much slower when using parameter set 1. At time 50, we observe molecule count of around 40 for parameter set 1, while count when using parameter set 2 registers at around 1000.
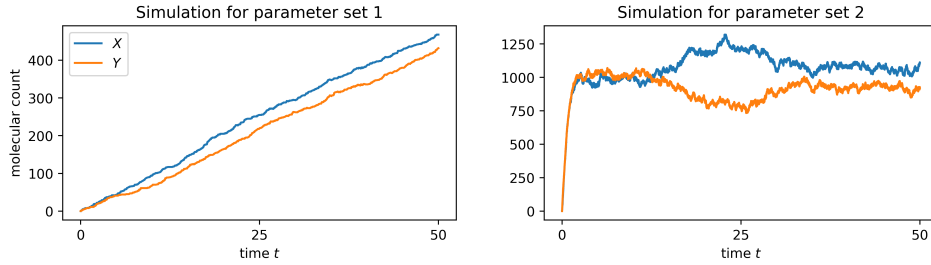

Figure 4: Stochastic simulation of the chemical reaction system with initial condition $(0, 0)$.

Also, it is worth noting that when using parameter set 2, the number of reactions occuring are so much larger than when using the other parameter set. Now, specifying as initial condition $(3000, 300)$, something very close to the computed deterministic fixed point, we see in Figure 5 that the behavior in both cases are similar.

Figure 6 shows the stationary distributions obtained in both cases. Each was obtained by running 1000 simulations of the system.

As seen in the initial segment of the trajectories, the behavior in the cases are very different because of the differences in the number of birth per unit time. Comparing the two, we see that using $k = 10^3$ as in case 2, will induce more birth reactions for both X and Y as compared to when $k = 10$. The two eventually behaving similarly at equilibrium, result from the consumption and degradation reaction propensities catching up with birth.
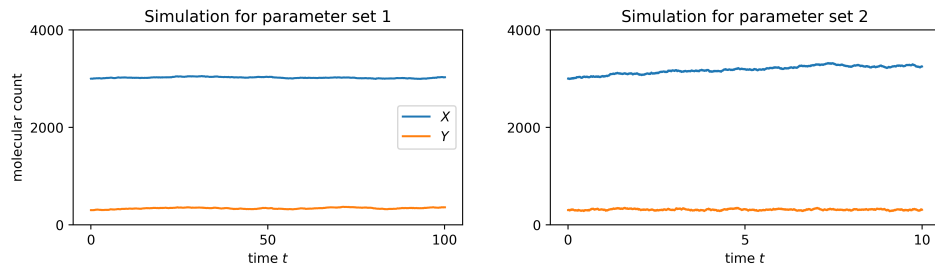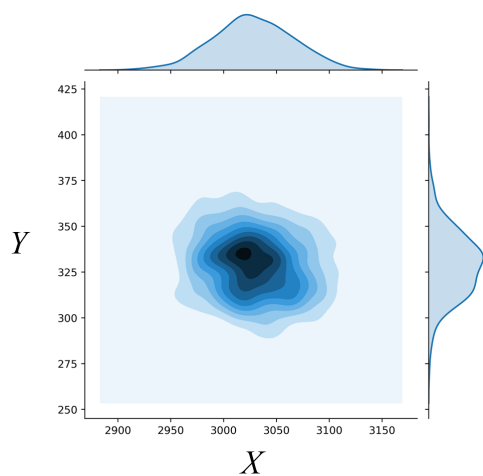
Figure 5: Stochastic simulation of the chemical reaction system with initial condition $(3000, 300)$.

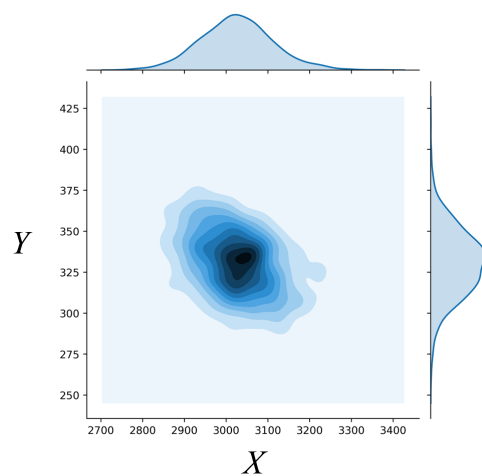(a) Parameter set 1   (b) Parameter set 2

Figure 6: Stationary distribution of the system obtained using two different parameter sets.

3. Consider the set of ODEs describing mRNA r and protein p dynamics, $\begin{cases} \dfrac{dr}{dt} = k_l + \phi\left(p\right) - \gamma_r r \\ \dfrac{dp}{dt} = r k_p - \gamma_p p \end{cases}$.

Given an infinitesimal time-step h, the transition probabilities at time t are given by

$P\left(r \to r+1; p \to p\right) = \left(k_l + \phi\left(p\right)\right) h + o\left(h\right)$

$P\left(r \to r-1; p \to p\right) = \gamma_r r h + o\left(h\right)$

$P\left(r \to r; p \to p+1\right) = k_p r h + o\left(h\right)$

$P\left(r \to r; p \to p-1\right) = \gamma_p p h + o\left(h\right)$

$P\left(r \to r; p \to p\right) = 1 - \left(k_l + \phi\left(p\right) + \gamma_r r + k_p r + \gamma_p p\right) h + o\left(h\right)$

Consider the case of positive autoregulation. We see in Figure 7 the phase portrait of the ODE system when $n = 1$. The null-clines reveal that there are two fixed points E_1 and E_2. The fixed point $E_1 = (0,0)$ is an unstable fixed point while $E_1 = (0.5, 0.5)$ is stable.
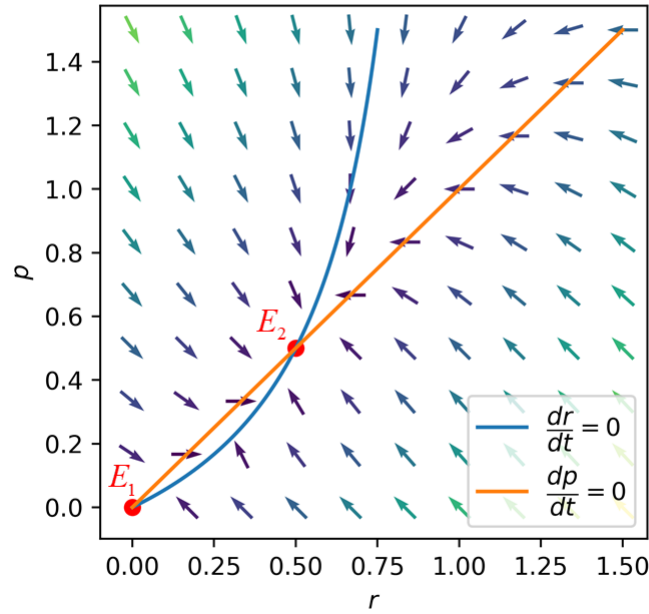

Figure 7: Phase portrait of the mRNA and protein concentrations given $n = 1$.

In Figure 8, we see the phase portrait when $n = 10$. We observe three fixed points $E_1 = (0,0)$, $E_2 = (0.5, 0.5)$ and $E_3 \approx (0.998, 1)$. Both E_1 and E_3 are stable fixed points while E_2 is unstable.

Consider the case of negative autoregulation. We parametrize the system using $[k_l, k_p, k_0, \gamma_p, \gamma_r, n] = [0.001, 0.17, 0.01, 0.00028, 0.0083, 10]$. The stationary distributions of protein count when $K = 100$ and 1000 are given in Figure 9. It can be seen that in the case of strong regulation, i.e. $K = 100$, the mean is around 140. This value is low as compared to when $K = 10000$ where the mean is around 800. The ratio of the standard deviation to the mean is 0.22 when $K = 100$ and is lower when $K = 10000$
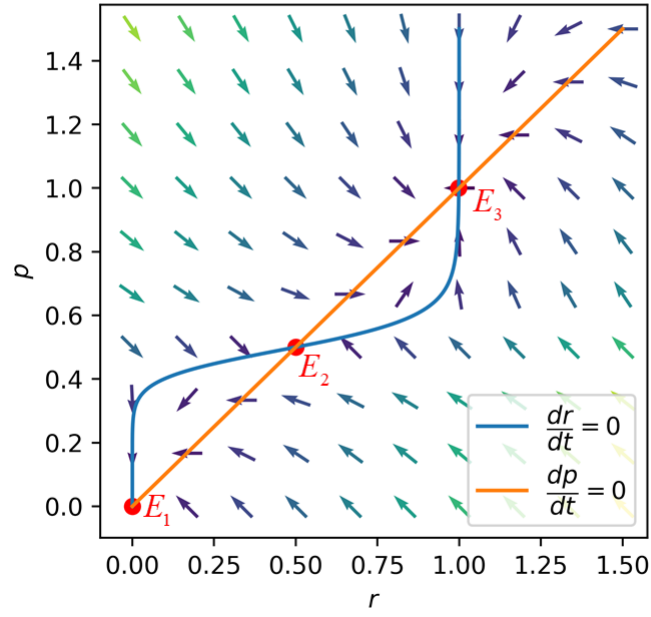
Figure 8: Phase portrait of the mRNA and protein concentrations given $n = 10$.

with value 0.16. This shows that the stationary distribution of protein count has more variation relative to its mean in the case of strong regulation.
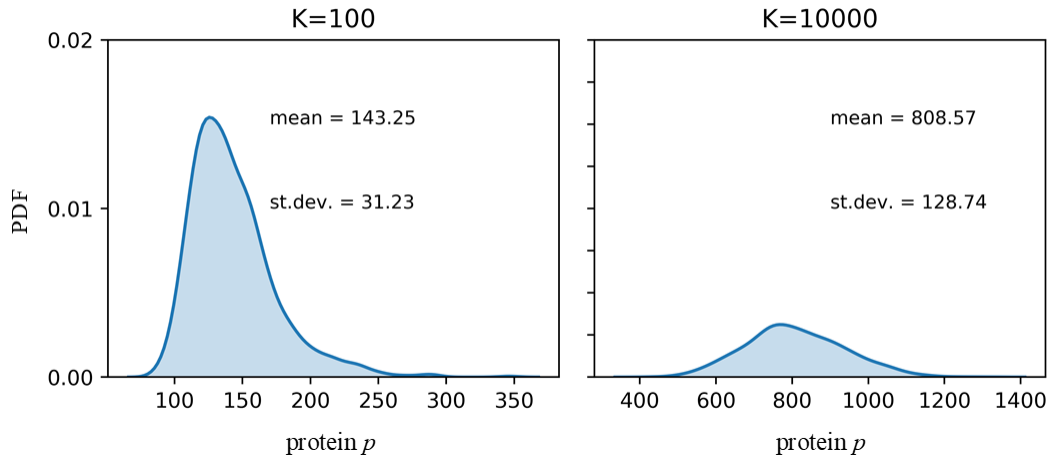

Figure 9: Stationary distribution of protein count for different regulation constants K.