Molecular and Neural Computation (CSE 590)
Homework 3 Solution

1 Mass Action Kinetics

Part a (3 points)

$$\emptyset \xrightarrow{k_1} A$$
$$A \xrightarrow{k_2} \emptyset$$

The mass action kinetics for this reaction network are,

$$\frac{d}{dt}[A] = k_1 - k_2[A].$$

Part b (3 points)

$$\text{Rabbit} \xrightarrow{\alpha} 2 \text{ Rabbit}$$
$$\text{Rabbit} + \text{Fox} \xrightarrow{\beta} 2 \text{ Fox}$$
$$\text{Fox} \xrightarrow{\gamma} \emptyset$$

The mass action kinetics for Rabbits are,

$$\begin{aligned} \frac{d}{dt}[\text{Rabbit}] = \alpha[\text{Rabbit}](2-1) & \qquad \text{(from the first reaction)} \\ - \beta[\text{Rabbit}][\text{Fox}] & \qquad \text{(from the second reaction).} \end{aligned}$$

The mass action kinetics for Foxes are,

$$\begin{aligned} \frac{d}{dt}[\text{Fox}] = \beta[\text{Rabbit}][\text{Fox}](2-1) & \qquad \text{(from the second reaction)} \\ - \gamma[\text{Fox}] & \qquad \text{(from the third reaction).} \end{aligned}$$

All together,

$$\frac{d}{dt}[\text{Rabbit}] = \alpha[\text{Rabbit}] - \beta[\text{Rabbit}][\text{Fox}]$$
$$\frac{d}{dt}[\text{Fox}] = \beta[\text{Rabbit}][\text{Fox}] - \gamma[\text{Fox}].$$

Part c (5 points)

The equations are,

$$\frac{d}{dt}[X] = k_5 - [X](k_1[Y] + k_4)$$
$$\frac{d}{dt}[Y] = -[Y](k_1[X] + k_2[Z])$$
$$\frac{d}{dt}[Z] = k_1[X][Y] - k_3[Z]^2.$$

Rewritten, these exquations are,

$$\begin{aligned}\frac{d}{dt}[X] &= -k_1[X][Y] - k_4[X] + k_5\\ \frac{d}{dt}[Y] &= -k_1[X][Y] - k_2[Y][Z]\\ \frac{d}{dt}[Z] &= k_1[X][Y] - k_3[Z]^2\\ &= k_1[X][Y] + k_2[Y][Z](1-1) + k_3[Z]^2(2-1).\end{aligned}$$

These equations are the mass action kinetics for the following chemical reaction network,

$$\begin{aligned}X + Y &\xrightarrow{k_1} Z\\ Y + Z &\xrightarrow{k_2} Z\\ Z + Z &\xrightarrow{k_3} Z\\ X &\xrightarrow{k_4} \emptyset\\ \emptyset &\xrightarrow{k_5} X.\end{aligned}$$

2 Visual DSD

Part a (5 points)

The following VisualDSD code encodes the reaction network from the class slides.

```
directive duration 10000.0 points 1000
directive scale 10.0
def Input() = <t^ 1 t^>
def Gate1() = {t^*}[1 t^]<2 t^>
def Gate2() = {t^*}[2 t^]<3 t^>
( 5 * Input()
| 10 * Gate1()
| 10 * Gate2()
)
```

Note that the code above specifies the initial conditions where there are $10 * 5 = 50$ copies of **Input** and $10 * 10 = 100$ copies of **Gate1** and **Gate2**. A stochastic simulation of this code generated the trajectory in Figure 1. Changing the **scale** directive to 100 encodes the initial conditions where there are 500 copies of **Input** and 1000 copies of **Gate1** and **Gate2**. A trajectory using these initial conditions is shown in Figure 2.

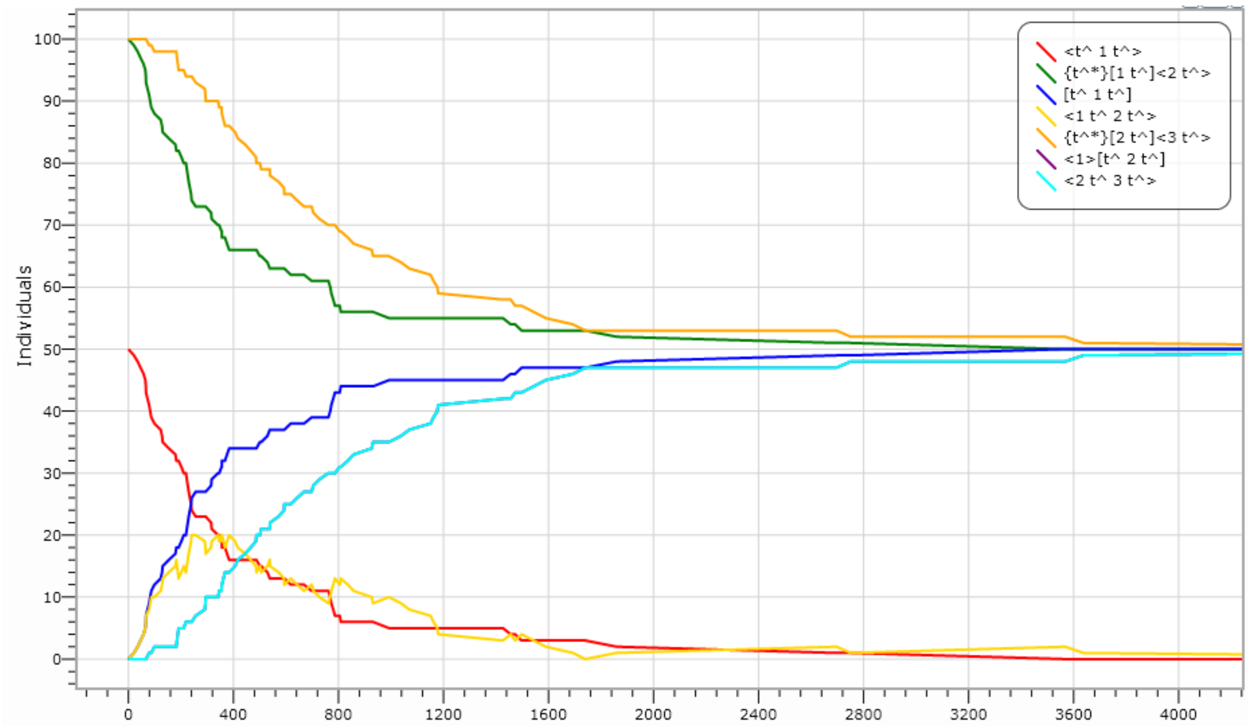

Figure 2.1: Initial species counts: Input=50, Gate=100.

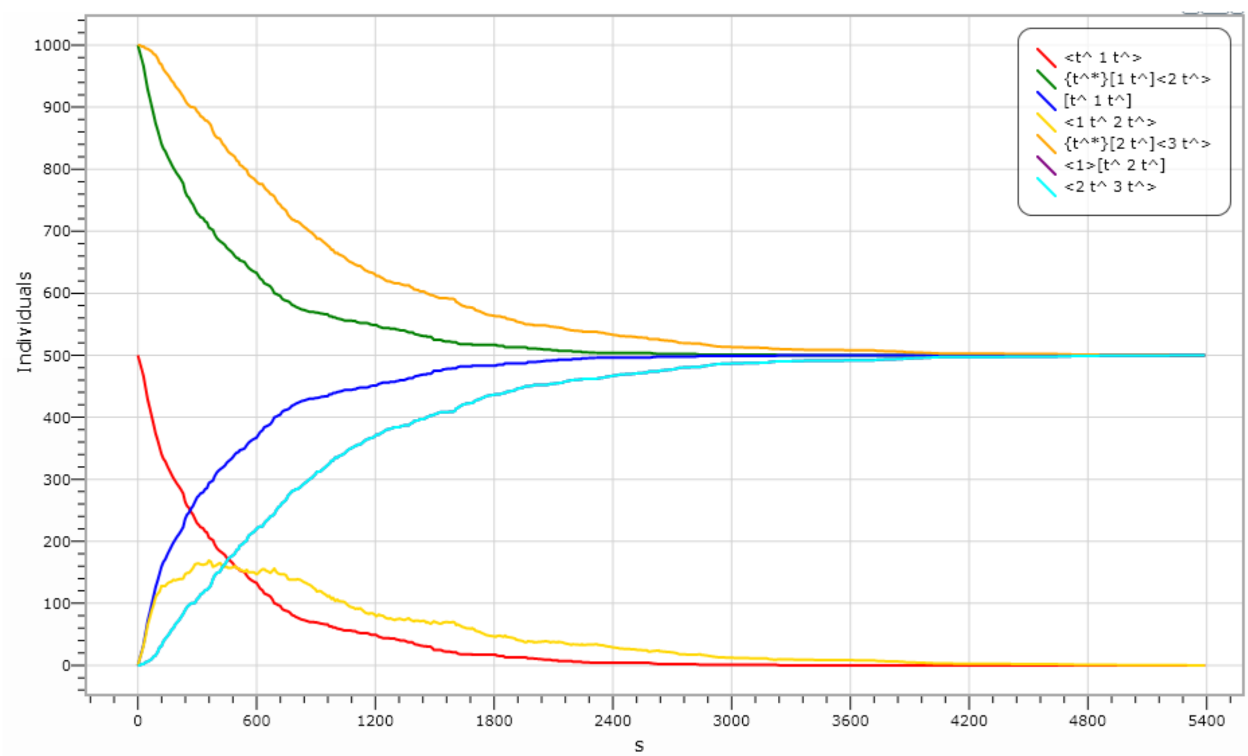

Figure 2.2: Initial species counts: Input=500, Gate=1000.

3 Nano Crafter game (4 points)

Thanks for your feedback! Your comments are being passed on to the development team.