1 Exercise 7

Using Gillespie's algoirthm, simulate and plot a single trajectory of

$$S_1 + S_2 \underset{1}{\overset{0.1}{\leftrightharpoons}} S_3,$$

up to time $T = 2$ under the assumption that $S_1(0) = 15$, $S_2(0) = 20$, and $S_3(0) = 0$. Find a 95% confidence interval for $E[X_3(2)]$ using 1,000 independent simulations of the process.

1.1 Setup

With this reaction network we have the intensity functions:

$$\begin{aligned} \lambda_1(x) &= x_1 x_2 \quad \text{for } S_1 + S_2 \xrightarrow{1} S_3, \\ \lambda_2(x) &= 0.1 x_3 \quad \text{for } \qquad S_3 \xrightarrow{0.1} S_1 + S_2, \end{aligned}$$

and the reaction vectors

$$\xi_1 = (-1, -1, 1), \quad \xi_2 = (1, 1, -1).$$

2 Exercise 8

Using the next reaction method, simulate and plot a single trajectory of the model in Example 6.3 with $\kappa_1 = 200$, $\kappa_2 = 10$, $d_M = 25$, $d_p = 1$, an initial condition of 1 gene, 10 mRNA, and 50 protein molecules, and a terminal time of $T = 8$.

This model yields the four reaction vectors:

$$\xi_1 = (0, 1, 0),\ \xi_2 = (0, 0, 1),\ \xi_3 = (0, -1, 0),\ \xi_4 = (0, 0, -1).$$

3 Exercise 11

Let

$$\xi_1 = (-1, 1, 0) \text{ and } \xi_2 = (0, -1, 1),$$

and let X_n^θ be a discrete time Markov chain on $\mathbb{Z}^3_{\geq 0}$ with the following transition probabilities:

$$p_{\vec{x},\vec{x}+\xi_1} = \frac{\theta xy}{\theta xy + y} \tag{1}$$

$$p_{\vec{x},\vec{x}+\xi_2} = 1 - p_1(x, y, z), \tag{2}$$

Assume that $X_0^\theta = (100, 5, 0)$ and $\theta = 0.05$. Let $f(X^\theta) = \left(X_1^\theta\right)_{100}$; that is the first component of the process after 100 steps. We estimate $\frac{d}{d\theta}E\left[f(X^\theta)\right]$ using a number of different techniques.

3.1 Finite Difference Method (Common Random Variables)

In this problem, we employ a centered finite difference method using the estimator

$$\Delta_k^{\theta,h} = \frac{f(X_k^{\theta+h/2}) - f(X_k^{\theta-h/2})}{h}.$$

After taking a number of simulation, we will take the sample average

$$\mu^{\theta,h} = \frac{1}{N-1}\sum_{k=0}^{N}\Delta_k^{\theta,h}.$$

In an attempt to reduce the variance, we employ the common random variables technique; in which we will use the same sequence of uniform random variables when generating relizations $X_k^{\theta+h/2}$ and $X_k^{\theta-h/2}$. We took $n = 10,000$ samples and obtained the following results for various h.

h	$\mu^{\theta,h}$	σ^2	Confidence
0.01	-306.59	18,230.86	2.56
0.005	-304.76	36,782.56	3.76
0.001	-296.61	215,947.83	9.11
0.0005	-298.46	507,757.71	13.97

3.2 Finite Difference Method (Independent Random Variables)

Out of curiosity, I also tried employing the algorithm without using a common sequence of uniform random variables for constructing relaizations of $X_k^{\theta+h/2}$ and $X_k^{\theta-h/2}$. The results were astonishing; the variance increased by upto a factor of 10. The following results were taking from $n = 10,000$

simulations.

h	$\mu^{\theta,h}$	σ^2	Confidence
0.01	-312.09	246,520	9.73
0.005	-314.66	991,336	19.51
0.001	-339.00	24,931,389	97.87
0.0005	-417.40	99,077,950	195.09

3.3 Likelihood Ratio Method

For likelihood ratio method, we took $n = 100,000$ samples.

$\hat{Y}^\theta$	σ^2	Confidence
-331.29	564,0541.81	46.55

While emplying a control variate with the weight function obtained using the Likelihood Ratio method, we had a dramatic reduction in variance.

$\hat{Y}^\theta$	σ^2	Confidence
-302.56	190,379.28	8.55