Stochastic Section (4.10) Problem 1, stated in better detail.

Consider the following reaction network:

$$0 \to X \to Y \to 0$$

with the respective kinetic constants 10, 1, 2, i.e. the propensities are:

$$\rho_1 = 10\,, \quad \rho_2 = x\,, \quad \rho_3 = 2y\,,$$

There are two species, and we have these matrices:

$$\Gamma = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}, \quad B = \Gamma \begin{pmatrix} 10 & 0 & 0 \\ 0 & \mu_x & 0 \\ 0 & 0 & 2\mu_y \end{pmatrix} \Gamma^T$$

where μ_x and μ_y (which depend on time) are the means of X and Y.

The differential equation is

$$\begin{aligned} \dot{\mu} &= f(\mu) \\ \dot{\Sigma} &= \Sigma J' + J\Sigma + B(\mu) \end{aligned}$$

where f is the deterministic dynamics. Since all the reactions have order zero or one, we know that the dynamics for the mean $\mu = (\mu_x, \mu_y)$ are given by $\dot{\mu} = \Gamma R(\mu)$, that is:

$$\begin{aligned} \dot{\mu}_x &= 10 - \mu_x \\ \dot{\mu}_y &= \mu_x - 2\mu_y\,. \end{aligned}$$

The Jacobian of f is J (or "A") as follows:

$$J = \begin{pmatrix} -1 & 0 \\ 1 & -2 \end{pmatrix}.$$

We multiply out to get B:

$$\begin{aligned} B(\mu) &= \Gamma\,\mathrm{diag}\,(\rho_1(\mu), \rho_2(\mu), \rho_3(\mu))\;\Gamma' \\ &= \begin{pmatrix} \mu_{\mathrm{x}} + 10 & -\mu_{\mathrm{x}} \\ -\mu_{\mathrm{x}} & \mu_{\mathrm{x}} + 2\,\mu_{\mathrm{y}} \end{pmatrix} \end{aligned}$$

Let us write the components of Σ explicitely:

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

(of course, $\Sigma_{12} = \Sigma_{21}$, because Σ is symmetric), and therefore, multiplying out $\Sigma J'$ and $J\Sigma$, we end up with the differential equation for Σ by equating all four terms in each side of:

$$\dot{\Sigma} = \Sigma J' + J\Sigma + B(\mu)$$

and from here we can write the separate differential equations for Σ_{11}, etc. For example, we will get:

$$\dot{\Sigma}_{12} \;=\; \Sigma_{11} - \mu_{\mathrm{x}} - 3\,\Sigma_{12}\,.$$

(a) Write out the differential equations for Σ_{11}, Σ_{12} (same as for Σ_{21}) and Σ_{22}, Then compute the steady state means of X and Y and the steady state covariances (that is, the variances of X and Y and the covariance of (X, Y), at steady state). Please use the fluctuation-dissipation approach discussed in class. If you do this right, you will find that the covariance is zero. (Which is actually very surprising, if you think of it!)

In other words solve $\dot{\mu}_x = \dot{\mu}_y = \dot{\Sigma}_{11} = \dot{\Sigma}_{12} = \dot{\Sigma}_{22} = 0$, which is a set of linear equations on these variables.

The equations are

$$\dot{\Sigma} \;= \Sigma\,J' \,+\, J\,\Sigma \,+\, B(\mu) \;=\; \begin{pmatrix} \mu_{\mathrm{x}} - 2\,\Sigma_{11} + 10 & \Sigma_{11} - \mu_{\mathrm{x}} - 3\,\Sigma_{12} \\ \Sigma_{11} - \mu_{\mathrm{x}} - 3\,\Sigma_{12} & \mu_{\mathrm{x}} + 2\,\mu_{\mathrm{y}} + 2\,\Sigma_{12} - 4\,\Sigma_{22} \end{pmatrix}$$

At steady state, one gets $\mu_x = 10$, $\mu_y = 5$, $\Sigma_{11} = 10$ (this is the variance of X), $\Sigma_{22} = 5$ (this is the variance of Y), and $\Sigma_{12} = 0$ (the covariance of X and Y.

(b) Run the following script:

`gillespie_XY.m`

found in this folder

for which an alternative short-URL is here: https://bit.ly/3uLvzjX

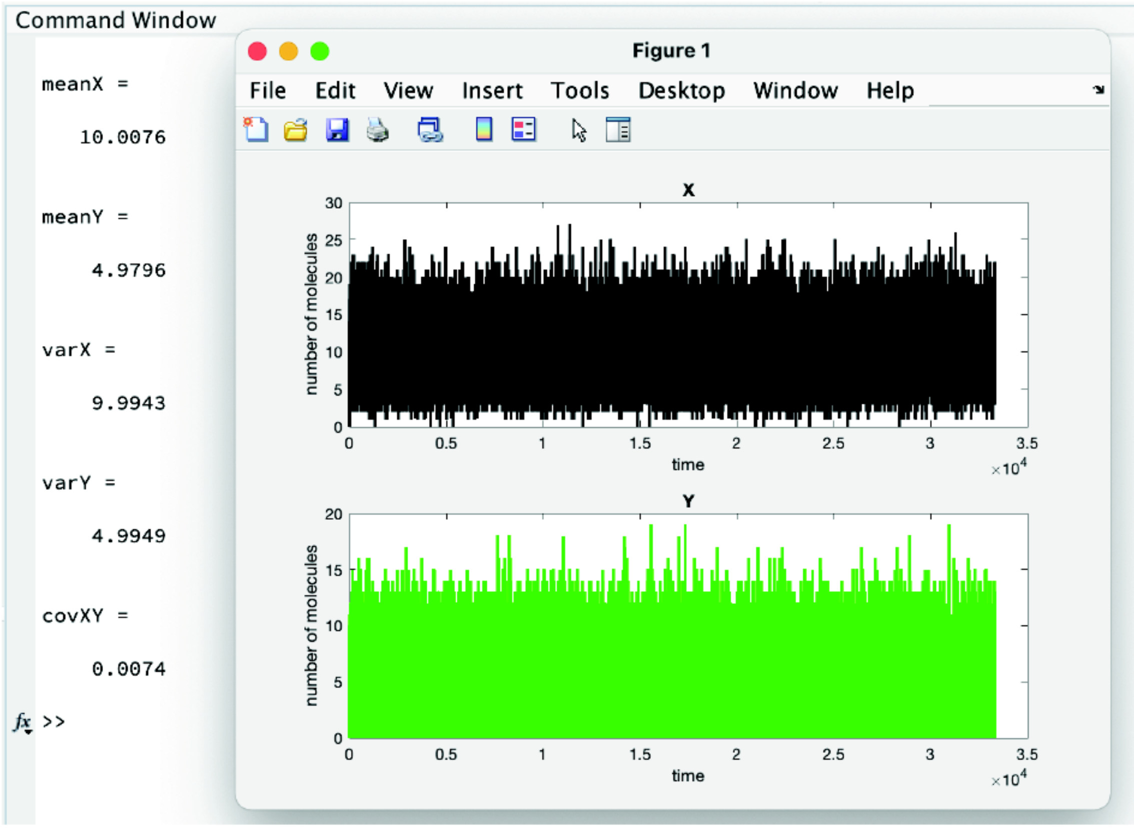
`gillespie_XY.m`

I suggest that you run these script a few times, as each time you will get a different answer.

(i) Print out a plot (from one of the runs).

(ii) Compare the results from the simulation(s) to the theoretical calculation.

(iii) Subtle question: why is “mean(X(:,1))” the wrong way to compute the mean? (Looking at how I computed the mean, in the code, will help you answer this question. You will learn a lot from answering this, actually.)



the mean X should be not calculated as “mean(X(:,1))”, because the time interval is stochastic, and one needs to take X_i weighted by its corresponding random time interval to compute the average value for X .