Freie Universität Berlin
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3. Assignment
Complex Systems for Bioinformaticians
SS 2024

Deadline: May 7, 12:00 (**before** the lecture)

The homework should be worked out individually, or in groups of 2 students. Pen & paper exercises should be handed at the designated deadline. Each solution sheet must contain the names and 'Matrikulationnummer' of all group members and the name of the group. The name of the group must include the last names of the group members, in alphabetic order, e.g. "AlbertRamakrishnanRastapopoulos", for group members Mandy Albert, Mike Ramakrishnan, and Marcus Rastapopoulos. Please staple all sheets.
Programming exercises must be submitted via Whiteboard.

Homework 1 (Convergence (pen & paper), 2 points)
You have sampled a Poisson process $\left\{X^{(1)}, X^{(2)}, \ldots, X^{(p)}\right\}$ all taken at a fixed time point t using the stochastic simulation algorithm with $p = 1000$ times. Let's assume that this Poisson process has an inherent variance $\sigma^2 = 2.5$. Subsequently, you computed the sample mean $\bar{X}^{(p)}$ and you observed that the standard deviation of the sample mean $\sigma_p = \left(\mathbb{E}\left[|\bar{X}^{(p)} - \mu|^2\right]\right)^{\frac{1}{2}} = 0.05$, where μ is the true mean the Poisson process also at the time-point t. How often would you have had to sample to achieve half the precision, $\sigma_p = 0.1$?

Homework 2 (Fixed point analysis (pen & paper), 4 points (+2))
You are given the following reaction network model from (see Assignment 1, Homework 4): Stoichiometric matrix S:

	r_1	r_2	r_3
x_1	1	0	-1
x_2	0	1	-1

and reaction rate functions $r_1 \ldots r_3$.

$$
\begin{aligned}
r_1 &= k_1 \\
r_2 &= k_2 \\
r_3 &= k_3 \cdot x_1 \cdot x_2
\end{aligned}
$$

with parameters $k_1 = 1$, $k_2 = 1$, $k_3 = 0.01$ and initial state

$$
\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 10 \\ 10 \end{pmatrix}.
$$

a) (**pen & paper**) Determine <u>one</u> fixed point of the model and classify it. **hint:** This model has infinitely many fixed points. Just choose one.
b) (**Bonus: to be printed**) Write a program to draw you a vector field around the fixed point.
matplotlib.pyplot.quiver(X, Y, U, V, **kw)

Homework 3 (Implementation (to be uploaded via Whiteboard), 2+2 points)
a) (**to be uploaded via KVV**) Write a program implementing this model from Task2 and generate trajectories using the stochastic simulation algorithm. The program reads the input

file ("Input.txt") provided in the KVV. The first number in the input file is the 'seed' of the random number generator, the second is the number of trajectories N to be computed. Using this input, compute the trajectories for N simulations up to time $t_{final} = 30$. Store the population of x_1 and x_2 every 1 time unit until you reach $t_{final} = 30$ and write them into the file "Task3bTrajYTimed.txt", where 'Y' $= 1 \ldots N$ is the current simulation (e.g. "Task3aTraj3.txt" contains the jump-times and the trajectory of x_2 from the third simulation). The output text-file should be in the comma-separated text format using two digits after the comma (format '%1.2f'), e.g.

$$0.00, 1.00, 2.00, 3.00, ... \tag{1}$$
$$5.00, 6.00, 5.00, 6.00, 7.00, ... \tag{2}$$
$$7.00, 12.00, 4.00, 13.00, 9.00, ... \tag{3}$$

where the first row are the storage times (i.e. every 1 time units), second- and third correspond to the states of x_1, x_2 respectively at these time points. Call this program "Ex3_3.py" and submit it via the Whiteboard system.
b) (**to be printed and discussed**) Using a 'seed' of your choice, generate $N = 300$ trajectories to compute the sample mean and its standard deviation for x_1 every 1 time units until $t_{final} = 100$. Plot the sample mean and standard deviation for x_1 and x_2, similar to Fig. 1. Why is the standard deviation increasing?

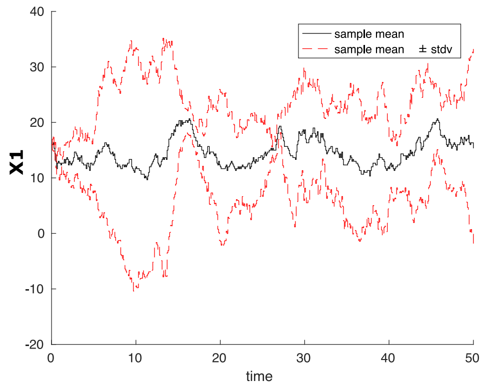

Figure 1: How to plot x_1 in Ex.3b. The black line indicates the sample mean $\bar{x}(t)$ and the red dotted lines mark the sample mean $\pm$ one standard deviation.

Good luck!

hint: compare simulations all in the same time value so check the last available time in the times store