School of Electronics and Computer Science
University of Southampton

COMP3212(2023/24): Computational Biology Lab Four

Issue	11 March 2024
Deadline	22 March 2024

Part 1

Write down the differential equation describing the system of chemical equations (assuming a volume of 1). You can use latex to enter the equation and have it displayed nicely in jupyter notebook if you put it between two sets of dollar signs, e.g. $$ \frac{dx}{dt} = ... \frac{dy}{dt} = ...$$ is

$$\frac{dx}{dt} = ... \quad \frac{dy}{dt} = ...$$

- $\emptyset \to X$ at a rate $k_1 = 1$
- $X \to Y$ at rate $k_2 = 2$
- $2X + Y \to 3X$ at rate $k_3 = 0.02$
- $X \to \emptyset$ at rate $k_4 = 0.04$

Part 2

Use a package to solve the differential equation for 500 time units starting from X(0)=Y(0)=0 (`from scipy.integrate import odeint`)

- plot $[X]$ and $[Y]$ against time
- Plot the trajectory, $[X]$ vs $[Y]$
- Use the `plt.quiver` function to plot a direction field on the trajectory
- Explain the pattern you see

Part 3

Write a Gillespie algorithm to simulate the same four chemical equation and plot the results for 500 time units

- Plot numbers of X and Y in different colours on the same graph and label them. *
- Plot numbers of $[X]$ vs $[Y]$
- Describe how these plots compare with the ODE model

*note that this is a lot of data to plot and you might want to save and plot the data only after X or Y have changed in number by at least 5.

Report and marking

You can ask a demonstrator or myself to mark your work in the lab, or you can submit a pdf output from your work.

Jo Grundy January 2024