

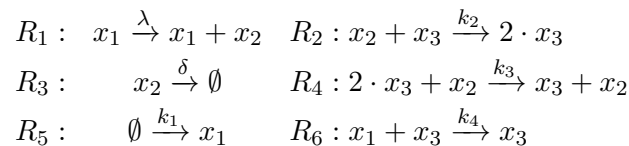
5. Homework Numerics for Bioinformaticians WS 2016/17

Deadline: November 30, 10:00 (**before** the lecture)

The homework should be worked out in groups of two or three students. Each solution sheet must contain the names and student numbers ('Matrikulationsnummer') of all group members and the exercise group (Wednesday/Friday). Solutions to homework 1&2 must be handed in in paper form, either hand written or printed out if generated electronically. Please staple all sheets. Programming tasks (homework 4) must be submitted to max.kleist2@fu-berlin.de or BioInfNumerik@hotmail.com by email. Before sending it, please 'zip' it.

Homework 1 (Modelling, 2 points)

You are given the following model:



write down the corresponding ordinary differential equations (ODE).

Homework 2 (Integration: 3 points)

Using Proposition 4 compute the $\mathcal{O}(0.1^4)$ Taylor approximation of

$$\int_0^{0.1} e^{x^2} dx.$$

Homework 3 (Implementation: Stochastics, 1 + 1 + 2 + 1 points)

Predator-Prey model. Let us consider the following model with stoichiometric matrix S :

$$\begin{array}{c|cccc} & r_1 & r_2 & r_3 & r_4 \\ \hline x_1 & 1 & -1 & -1 & 0 \\ x_2 & 0 & 0 & 1 & -1 \end{array}$$

and propensities (reaction rates): $r_1 \dots r_4$.

$$\begin{aligned} r_1 &= x_1 \cdot \lambda \\ r_2 &= x_1 \cdot x_2 \cdot k_1 \\ r_3 &= x_1 \cdot x_2 \cdot k_2 \\ r_4 &= x_2 \cdot \delta_2 \end{aligned} \tag{1}$$

where x_1, x_2 denotes the population of prey and predators (x_2 eats x_1). Parameters are 0.3, 0.01, 0.01 and 0.3 for λ, k_1, k_2 and δ_2 and initial conditions are $x_1(t_0) = 32$ and $x_2(t_0) = 16$.

a) Implement this model, and generate 3 trajectories using the stochastic simulation algorithm until $t_{final} = 50$. Generate one plot per species with the 3 trajectories in it (e.g. as in Fig. 1, left panel).

- b) Store the population of x_1 and x_2 every 0.1 time units until you reach $t_{final} = 50$ and compute the sample mean and its standard deviation for x_1 and x_2 for each time instance (every 0.1 time units) and plot them similar to Fig. 1 (right panel) where the black line indicates the sample mean $\bar{x}(t)$ and the red dotted lines mark the sample mean \pm one standard deviation.
- c) Generate 300 trajectories and plot the sample mean and standard deviation for x_1 and x_2 , similar to Fig. 1 (right panel). Why is the sample mean \bar{x}_1 increasing?
- d) From the 300 trajectories: Compute the the probability that x_2 died out by t_{final} .

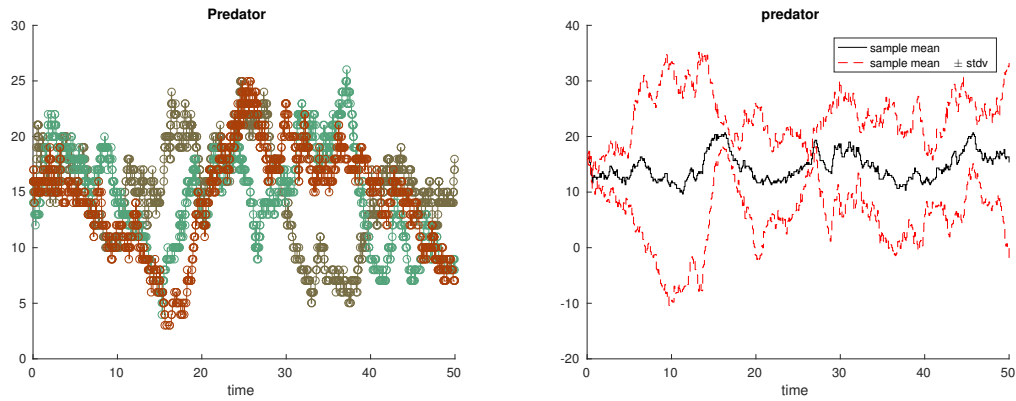


Figure 1: Left:How to plot in Ex.3a exemplified for x_2 . Right: How to plot in Ex.3b exemplified for x_2 .