

### 3. Homework Numerics for Bioinformaticians WS 2016/17

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Deadline: November 16, 10:00 (**before** the lecture)

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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 3) must be submitted to [BioInfNumerik@hotmail.com](mailto:BioInfNumerik@hotmail.com) by email. Before sending it, please 'zip' it.

#### Homework 1 (Modelling, 2 points)

You have used the following ODE-system in your research (predator-predator-prey model):

$$\begin{aligned}\frac{d}{dt}x_1 &= \lambda_b \left( x_1 + \frac{\lambda_0}{\lambda_b} \right) - x_1 (x_2 \cdot k_2 + \delta_1) \\ \frac{d}{dt}x_2 &= x_2 (k_1 \cdot x_1 - \delta_2 - x_3 \cdot k_3) \\ \frac{d}{dt}x_3 &= x_3 (x_2 \cdot k_3 - \delta_3)\end{aligned}$$

Decompose the system into stoichiometric matrix and reaction rate vector (propensity vector) and depict the corresponding reaction network.

#### Homework 2 (Stochastics, 3 points)

Let the state space  $\Omega = \mathbb{R}$ . Let  $X$  be distributed according to a Gaussian distribution with parameters  $\mu \in \mathbb{R}$  and  $\sigma > 0$ . Show that

$$\mathbb{E}[X] = \mu.$$

Hint: You can use that fact that,

$$\int_{-\infty}^{\infty} x \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}} dx = 0.$$

#### Homework 3 (Implementation, 2+1+1+1 points)

You are given the following epidemiologic model of a virulent outbreak (also called susceptible-infected-recovered (SIR) model). Stoichiometric matrix  $S$ :

	$r_1$	$r_2$	$r_3$	$r_4$	$r_5$	$r_6$
$x_1$	1	-1	-1	0	0	0
$x_2$	0	0	1	-1	-1	0
$x_3$	0	0	0	0	1	-1
$x_4$	0	0	0	1	0	0

and propensities (reaction rates):  $r_1 \dots r_6$ .

$$r_1 = \lambda \tag{1}$$

$$r_2 = x_1 \cdot \delta \tag{2}$$

$$r_3 = x_1 \cdot x_2 \cdot \beta \tag{3}$$

$$r_4 = x_2 \cdot 3 \cdot 10^7 \cdot \delta \tag{4}$$

$$r_5 = x_2 \cdot k_r \tag{5}$$

$$r_6 = x_3 \cdot \delta \tag{6}$$

where  $x_1$  denotes the number of susceptible individuals,  $x_2$  are the number of infected individuals,  $x_3$  are the number of individuals that recovered and are subsequently resistant to infection and  $x_4$  are the number of individuals that died from the infection. Parameter values are  $\lambda = 1 \cdot 10^{-4}$ ,  $\delta = 1 \cdot 10^{-8}$ ,  $\beta = 5 \cdot 10^{-5}$ ,  $k_r = 0.3$  and the initial state is  $x_1(t_0) = \frac{\lambda}{\delta}$ ,  $x_2(t_0) = 5$ ,  $x_3(t_0) = 0$ ,  $x_4(t_0) = 0$

- a) Write a program implementing this model and generate trajectories using the stochastic simulation algorithm (also called Gillespie's algorithm).
- b) Plots the trajectories for  $N = 3$  simulations up to time  $T = 10$ .
- c) Perform  $N = 1000$  simulations, generate a histogram of the number of  $x_2$  at time  $T = 10$  and depict the probability that  $0, \dots, 20$  individuals are infected by  $T = 10$ . What is the probability that the infection is still ongoing at  $T = 10$ ?
- d) From the  $N = 1000$  simulations, generate a histogram of the number of  $x_4$  at time  $T = 10$  (number of casualties), depicting the probability that  $0, \dots, 35$  individuals died by  $T = 10$ . How many individuals died on average ( $\pm$  standard deviation)?