Freie Universität Berlin
Zuse Institute Berlin (ZIB)
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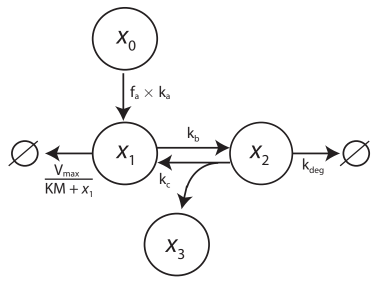
1. Homework
Numerics for Bioinformaticians
WS 2014/15

Deadline: November 02, 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 'Matrikulationnummer' of all group members and the exercise group (Wednesday/Friday). Please staple all sheets.

Homework 1 (Modelling, 2 points)
You saw the following depiction of a reaction network model in your favourite research magazine and you would like to use this model in a research project of your own. Decompose it into its



stoichiometric matrix and propensity function vector (= vector of reaction rate functions). x_0, x_1, x_2, x_3 are the systems variables. $\varnothing$ symbols denotes the elimination of molecules of type x_1 or x_2. Stoichiometric coefficients can only be -1, 0 or 1.

Homework 2 (Modelling, 2 points)
You are given the following stoichiometric matrix S:

	r_1	r_2	r_3
x_1	1	-1	0
x_2	-1	0	-1
x_3	0	1	0
x_4	0	1	1
x_5	-1	0	1

and the following propensity functions (= reaction rate functions) $r_1 \ldots r_3$.

$$\begin{aligned} r_1 &= \frac{\mathrm{k_a}}{\mathrm{K_D}\left(1+\frac{x_5}{\mathrm{K_I}}\right)} \cdot x_2 \cdot x_5 \\ r_2 &= \mathrm{k_b} \cdot x_1 \\ r_3 &= \mathrm{k_c} \cdot x_2. \end{aligned}$$

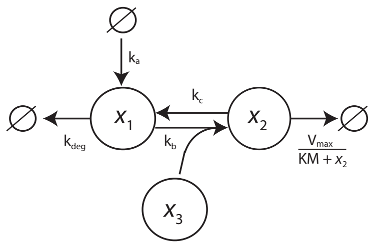
Write down the corresponding system of ordinary differential equations (ODEs).

Homework 3 (Modelling, 2 points)
You have used the following ODE-system in your research:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}x_1 &= x_2 \cdot \mathrm{k_a} - x_1\left(\mathrm{k_{cat}} \cdot x_3 + \mathrm{k_b}\right)\\
\frac{\mathrm{d}}{\mathrm{d}t}x_2 &= x_1 \cdot \mathrm{k_b} - x_2\left(\mathrm{k_{deg}} + \mathrm{k_c}\right)\\
\frac{\mathrm{d}}{\mathrm{d}t}x_3 &= \lambda.
\end{aligned}$$

Depict the corresponding reaction network network (analogous to the graphic in **Homework 1**).

Homework 4 (Implementation, 2+2 points)
a) You are given the following reaction network model: Write a small program to generate the



stoichiometric matrix and propensity function vector.
b) Compute the value of the ODEs for parameters $\mathrm{k}_a = 5$, $\mathrm{k}_b = 3$, $\mathrm{k}_c = 12$, $\mathrm{k_{deg}} = 7$, $\mathrm{V_{max}} = 5$ and $\mathrm{KM} = 0.1$, time step $\triangle t = 1$ and the current system's state:

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 5 \\ 25 \\ 15 \end{pmatrix}$$

Good luck!