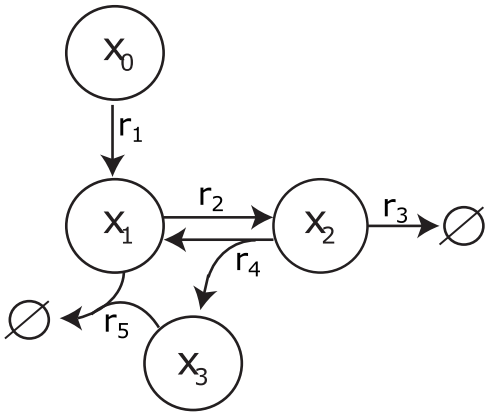
Freie Universität Berlin
Prof. Dr. Max von Kleist

1. Homework (Complex Systems block)
Introduction to Focus Areas
WS 2024/25

Deadline: November 25, 10:00 (**before** the lecture)

The homework should be worked out in groups and programming excercises must be submitted via whiteboard. Please hand in pen & paper excercises before the lecture (print-out or hand written, with the names and 'Matrikulationnummer' of all group members stated). Pen & paper exercises will be discussed on the board.

Homework 1 (Modelling (pen & paper), 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 S and a vector of **reaction rate** functions $r_1, \ldots, r_5$. x_1, x_2, x_3 are the systems variables. $\varnothing$ symbols denote the elimination of molecules. Stoichiometric coefficients can only be -1, 0 or 1; **Reaction constants** are: $k_1 = k_a$; $k_2 = \pi \cdot c_2$; $k_3 = \pi \cdot \ k_{\text{deg}}$; $k_4 = k_4$; $k_5 = \text{CL}$. Reaction rates $r_1, \ldots, r_4$ are of first order, while r_5 is a second order reaction rate.

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

	r_1	r_2	r_3	r_4
x_1	1	-1	0	0
x_2	-1	0	-1	0
x_3	0	1	0	1
x_4	-1	1	1	0

and the following propensity functions (= reaction rate functions) $r_1 \ldots r_4$.

$$\begin{aligned} r_1 &= \frac{\text{k}_\text{a}}{\text{K}_\text{D}\left(1 + \frac{x_4}{\text{K}_\text{I}}\right)} \cdot x_2 \cdot x_4 \\ r_2 &= \text{k}_\text{b} \cdot x_1 \\ r_3 &= \text{k}_\text{c} \cdot x_2 \\ r_4 &= \text{k}_\text{d} \end{aligned} \tag{1}$$

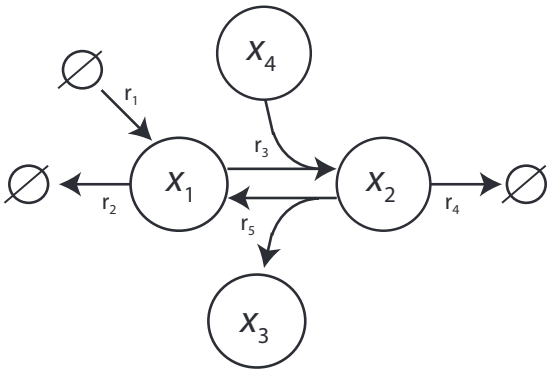
Write down the corresponding system of ordinary differential equations (ODEs).

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

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

Write down the rate functions $r_1, \ldots$ akin to **Homework 2**. Then, depict the corresponding reaction network (analogous to the graphic in **Homework 4**, where you just write the rate that corresponds to the 'arrow', i.e. r_1).

Homework 4 (Implementation (upload via Whiteboard), 2+2 points)
a) You are given the following reaction network model: All reactions are mass-action, reaction



r_1 is of zero order, reactions r_2, r_4 and r_5 are first order and reaction r_3 is of second order, with respective reaction constants $k_1, \ldots, k_5$. Write a small program to generate the stoichiometric matrix and propensity function vector. Regrading the former, only use stoichiometric coefficients -1, 0 or 1.
Your program must write the stoichiometric matrix into a text file named "SMatrix.txt", columns should be comma-delimited. *E.g., in Python the numpy function 'savetxt' using a comma-delimiters (',')*. Write numbers as signed integers, e.g. '-1' instead of '-1.00'.
b) Compute the value of the ODEs for parameters $\mathrm{k_1} = 5$, $\mathrm{k_2} = 3$, $\mathrm{k_3} = 12$, $\mathrm{k_4} = 7$, $\mathrm{k_5} = 3$ and time step $\triangle t = 1$ and the current system's state, which is given in the "Input.txt" file:

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 5 \\ 25 \\ 15 \\ 5 \end{pmatrix}$$

Your program must write an output into a text file named "ODEValue.txt" using the above described format. Round the output to the first two digits after the comma, e.g. '1.20' or '0.34'. Name your program "Exc1_4.py" and submit via Whiteboard.
Tipp: There is a code scaffold provided for you in whiteboard which you can adapt.

Good luck!