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Numerical Optimization with Differential Equations 1 - WS 2018/2019

Excercise 1

Exercise 1 Modeling of chemical systems
Let $\alpha, \beta, \gamma \in \mathbb{N}$ and $k \in \mathbb{R}$. A reaction of α units of substance A and β units of substance B into γ units of substance C can be written as

$$\alpha A + \beta B \xrightarrow{k} \gamma C.$$

The integers α, β, γ are called *stoichiometric factors* and k is the reaction rate. We model this chemical reaction with a system of ordinary differential equations that describes the temporal change of the concentrations $[A]$, $[B]$ and $[C]$ according to

$$\frac{d[A]}{dt} = -\alpha k[A]^\alpha [B]^\beta\,, \quad \frac{d[B]}{dt} = -\beta k[A]^\alpha [B]^\beta\,, \quad \frac{d[C]}{dt} = \gamma k[A]^\alpha [B]^\beta.$$

The first equation describes the relation of the reaction rate of A being proportional to the product of $[A]^\alpha$ and $[B]^\beta$, i.e., the concentrations to the power of their respective stoichiometric factors. Every (elementary) reaction consumes α units of A, which leads to the factor $-\alpha$. In general, several reactions happen simultaneously and the concentration changes must be added. Formulate a system of ordinary differential equations for the system of reactions

$$\begin{aligned} A &\xrightarrow{k_1} B, \\ B + C &\xrightarrow{k_2} A + C, \\ B + B &\xrightarrow{k_3} B + C. \end{aligned}$$

Exercise 2 On a remote and lonely island in the Neckar live populations of predators and prey with R respectively B individuals. The birth rate of the prey is proportional to B with the proportional factor α. The mortality rate of B depends on the number of encounters between the species, therefore it is proportional to R and B with the factor β. The birth rate of the predator is also proportional to R and B with the factor γ. The predator dies due to diseases, therefore the mortality rate of the predator is proportional to R with the factor δ.

a. Describe this process with a system of differential equations for the development over time of the number of R and B.

b. Animal rights activists try to limit the suffering. They rescue at a certain time moment t_w (Christmas) n prey and take them to Australia. Describe this switching point by an equation.
Notation: t_w^- *und* t_w^+ *mit* $x(t_w^-) = \lim\limits_{t \to t_w, t < t_w} x(t)$, $x(t_w^+ = \lim\limits_{t \to t_w, t > t_w} x(t)$.

c. Heinious fur traders come before the animal rights activists and kill half of the preys as soon as there exist k individuals. Formulate also this switching point t_k. What does it depend on implicitly and explicitly? The switching point from part b) is not relevant here.

d. Develop the system of equations of the two populations by neglecting the interdependence. The terms for the mortality rate of the prey and the birth rate of the predators will be dropped. According to which functions do the numbers of both species develop in time?

M1 Programming: Matlab installation

a. The URZ offers free Matlab student licenses. Obtain a license and a copy from:

`https://www.urz.uni-heidelberg.de/de/matlab`

Install the software on your computer.

You do not have to hand in these exercises, there will be a discussion in the tutorials.