Parameter estimation – Homework 6

Deadline: 30th April, 11:59:59 pm

Submission via Moodle

Task 1

rekeszes

We consider a compartmental pharmacokinetics model. The system involves two compartments representing the plasma and the extravascular fluid of the organs. $x_1(t)$ denotes the concentration of an enzyme in the plasma, $x_2(t)$ is its concentration in the other compartment. $x_3(t)$ characterizes the time evolution of a polymer concentration in the plasma, while $x_4(t)$ is its concentration in the other compartment.

$$\begin{aligned}
\dot{x}_1 &= \alpha_1(x_2 - x_1) - \frac{k_a v_m x_1}{k_c k_a + k_c x_3 + k_a x_1} \\
\dot{x}_2 &= \alpha_2(x_1 - x_2) \\
\dot{x}_3 &= \beta_1(x_4 - x_3) - \frac{k_c v_m x_3}{k_c k_a + k_c x_3 + k_a x_1} \\
\dot{x}_4 &= \beta_2(x_3 - x_4),
\end{aligned}$$

conc of enzyme in plasma

conc of enzyme in other comp

time evoulution of a polymer conc in plasma

-II- polymer conc in other comp

where $v_m = 10$, $x_1(0) = 0.27$, $x_2(0) = 0.2$, $x_3(0) = 0.2$, $x_4(0) = 0.2$ and $t_s = 0.1$.

Recorded data from such a system can be found in the *pharmacokinetics.xlsx* file. According to thermodynamic domain knowledge each feasible parametrization of the above model must satisfy $k_a + k_c \simeq 4.5$.

Using the differential equations characterizing the dynamical behavior of x_1, x_2, x_3 and x_4 implement a constrained least square estimation algorithm in order to determine the parameter values k_a, k_c, α_1, α_2, β_1 and β_2. Quantify your estimates by means of the squared loss function.

Note: while numerous ways exist for implementing LSQ estimation, the aim of these homeworks is to promote the understanding of the methods discussed during the lectures. Other solutions like iterative / numeric nonlinear optimization methods achieve the same result in some cases, but each have their own benefits and drawbacks compared to the analytic solution, which should be well understood before using one instead of the other. Hence, from now on - unless indicated otherwise - we will only accept solutions based on the lectures (which means no built-in `fmincon`, `lsqnonlin`, etc for LSQ estimations!).