## Exercise to MATLAB Course lecture 3

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## 1 Problem formulation

A chemical isothermal reactor (Van de Vusse) is studied in this example. The relationship from the feed flow rate u into the reactor to the concentration of the product y at the outlet of the reactor is modeled by the following non-linear state space model.

$$\dot{x_1} = -k_1 x_1 - k_3 x_1^2 + (v - x_1) u, \qquad (1)$$

$$\dot{x}_2 = k_1 x_1 - k_2 x_2 - x_2 u, \tag{2}$$

$$y = x_2, \tag{3}$$

where the reaction rate coefficients are given by  $k_1 = 50$ ,  $k_2 = 100$ ,  $k_3 = 10$ . The concentration of the by-product into the reactor, v, is treated as an unknown constant or slowly varying disturbance with nominal value  $v^s = 10$ .

The following steady state nominal (equilibrium) values are given:

$$v^s = 10, (4)$$

$$u^s = 25, (5)$$

$$x_1^s = 2.5,$$
 (6)

$$y^s = x_2^s = 1.$$
 (7)

The above model may be written as a vector Ordinary Differential Equation (ODE) model of the form

$$\dot{x} = f(x, u, v), \tag{8}$$

$$y = g(x), \tag{9}$$

where

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \ f(x, u, v) = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix},$$
(10)

where

$$f_1 = -k_1 x_1 - k_3 x_1^2 + (v - x_1)u, (11)$$

$$f_2 = k_1 x_1 - k_2 x_2 - x_2 u. (12)$$

Furthermore the output equation is linear in this example due to  $y = x_2$  in the model.

## 2 Exercise Tasks

Use MATLAB in all tasks below. Write an m-file script for the solutions. Write with advantage separate m-file scripts for Tasks 3 and 4 below.

- 1. Show that the given steady state nominal values,  $v^s, u^s, x_1^s, x_2^s$ , actually is equilibrium values so that  $\dot{x_1^s} = 0$  and  $\dot{x_2^s} = 0$ .
- 2. We want to define the time interval

$$0 \le t \le t_f \tag{13}$$

and with a step length parameter, h = 0.001, and final time instant  $t_f = 0.3$ . Define a vector

$$t = \begin{bmatrix} 0 & h & 2h & \cdots & t_f \end{bmatrix}$$
(14)

in MATLAB using the : (column) operator. Find the number of discrete time instants, N, in the discrete time vector, t.

- 3. Simulate (solve) the differential equation  $\dot{x} = f(x, u)$ , y = g(x) by using the explicit Euler method for integration. Implement the simulation in a for-loop. Store the solutions in data matrices X for the states  $x^T$ , Y for the output y = y(t). Plot the results. Assume that the initial values for the states are  $x_1(t=0) = x_1^s$  and  $x_2(t=0) = x_2^s$ . Specify a step in the input feed flow rate from u = 25 to u = 30 at time  $t = \frac{t_f}{2}$ .
- 4. Simulate (solve) the differential equation  $\dot{x} = f(x, u)$ , y = g(x) by using the built in ODE solver, **ode15s** for the integration. Plot the results and compare with the Euler simulation results from the previous task. Assume that the initial values for the states are  $x_1(t = 0) = 0$  and  $x_2(t = 0) = 0$ . Specify a step in the input feed flow rate from u = 25 to u = 30 at time  $t = \frac{t_f}{2}$ .
- 5. In the response from the input u to the output  $y = x_2$  there is a so called "inverse response". Use the zoom MATLAB figure function to display this better. Plot the response from u to  $y = x_2$  in one figure.

6. Assume that the model,  $\dot{x} = f(x, u, v)$  is linearized around the nominal values  $x^s$ ,  $u^s$  and  $v^s$ . Find the time constants of the system (around nominal values).

Find the Jacobian system matrix

$$A_c = \frac{\partial f(x, u, v)}{\partial x^T}|_0 \tag{15}$$

where  $|_0$  means nominal values used in the arguments.

- Find  $A_c$  and the time constants analytically. remember that the relationship between the eigenvalues,  $\lambda_1$  and  $\lambda_2$ , and the time constants is,  $T_1 = -\frac{1}{\lambda_1}$  and  $T_2 = -\frac{1}{\lambda_2}$
- Find matrix  $A_c$  numerically by using the function jacobi.m.

## Solutions

Some background and solution of topics regarding this exercise is presented in the following.

A linearized model around steady state is given by

$$\Delta \dot{x} = A_c \Delta x + B_c \Delta u, \tag{16}$$

where  $\Delta x = x - x^s$  and  $\Delta u = u - u^s$  and

$$A_c = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{x^s, u^s} = \begin{bmatrix} -k_1 - 2k_3x_1^s - u^s & 0 \\ k_1 & -k_2 - u \end{bmatrix} = \begin{bmatrix} -125 & 0 \\ 50 & -125 \end{bmatrix}, (17)$$

$$B_c = \begin{bmatrix} \frac{\partial f_1}{\partial u} \\ \frac{\partial f_2}{\partial u} \end{bmatrix}_{x^s, u^s} = \begin{bmatrix} v^s - x_1^s \\ -x_2^s \end{bmatrix} = \begin{bmatrix} 7.5 \\ -1 \end{bmatrix}.$$
(18)

A discrete time model is obtained by using a zero order hold on the input and a sampling interval h = 0.002, i.e.,

$$x_{k+1} = Ax_k + Bu_k + v, \tag{19}$$

$$y_k = Dx_k, (20)$$

where

$$A = e^{Ach} = \begin{bmatrix} 0.7788 & 0\\ 0.0779 & 0.7788 \end{bmatrix},$$
 (21)

$$B = A_c^{-1} (e^{A_c h} - I) B_c = \begin{bmatrix} 0.0133\\ -0.0011 \end{bmatrix},$$
(22)

$$D = \begin{bmatrix} 0 & 1 \end{bmatrix}, v = x^{s} - Ax^{s} - Bu^{s} + C(v - v^{s}).$$
(23)

Choosing an LQ criterion

$$J_{i} = \frac{1}{2} \sum_{k=i}^{\infty} (Q(y_{k} - r)^{2} + P\Delta u_{k}^{2}), \qquad (24)$$

with

$$P = 1, Q = 500, \tag{25}$$

gives the LQ-optimal control

$$u_k = u_{k-1} + G_1 \Delta x_k + G_2 (y_{k-1} - r), \qquad (26)$$

where

$$G_1 = \begin{bmatrix} -23.4261 & -84.5791 \end{bmatrix}, G_2 = -20.0581.$$
 (27)

Simulation results after changes in the reference signal r are illustrated in Figure 1.



Figure 1: Simulation of the chemical reactor in Example **??** with LQ-optimal control. This figure is generated by the MATLAB file **dlq\_ex3\_du.m**.