CHEM-E7225/2020-2021: Exercise 03

Task 1 (Optimal control). Consider the following optimal control problem

$$
\begin{aligned}
\min_{\substack{x(0\rightsquigarrow t_f)\\ u(0\rightsquigarrow t_f)}} \quad & E\left(x(t_f)\right) + \int_0^{t_f} L\left(x(t), u(t)\right) dt \\
\text{subject to} \quad & \dot{x}(t) = f\left(x(t), u(t), d(t)|\theta_x\right), && t \in [0, T] \\
& u_{\max} \leq u(t) \leq u_{\min}, && t \in [0, T] \\
& x(0) = x_0 && (t = 0)
\end{aligned}
$$

where we have i) the terminal-stage cost $E\left(x(T)\right) = \dfrac{1}{2}\left(x(T) - x_{\text{ref}}\right)^T Q_{t_f}\left(x(T) - x_{\text{ref}}\right)$; ii) the running cost $L\left(x(t), u(t)\right) = \dfrac{1}{2}\Big[\left(x(t) - x_{\text{ref}}\right)^T Q\left(x(t) - x_{\text{ref}}\right) + \left(u(t) - u_{\text{ref}}\right)^T R\left(u(t) - u_{\text{ref}}\right)\Big]$. The matrices are $Q_{t_f}, Q \succeq 0$ and $R \succ 0$. The dynamics $f\left(x(t), u(t), d(t)|\theta_x\right)$ are those of a perfectly mixed continuous stirred tank chemical reactor (CSTR) with irreversible first-order reaction $A \to B$ in liquid phase (see Exercise 2 and G. Pannocchia and J.B. Rawlings. Disturbance models for offset-free MPC. *AIChE J.*, 49(2): 426–437, 2003),

$$\frac{dC_A(t)}{dt} = \frac{F_{\text{in}}\left(C_{A_{\text{in}}} - C_A(t)\right)}{\pi r^2 h} - k_0 \exp\left(-\frac{E}{RT(t)}\right) C_A(t) \tag{1a}$$

$$\frac{dT(t)}{dt} = \frac{F_{\text{in}}\left(T_{\text{in}} - T(t)\right)}{\pi r^2 h} + \frac{-\Delta H}{\rho C_p} k_0 \exp\left(-\frac{E}{RT(t)}\right) + \frac{2U}{r\rho C_p}\left(T_c(t) - T(t)\right) \tag{1b}$$

$$\frac{dh(t)}{dt} = \frac{F_{\text{in}} - F(t)}{\pi r^2} \tag{1c}$$

where the state is $x(t) = (C_A(t), T(t), h(t))$ and the controls are $u(t) = (F(t), T_c(t))$. The disturbances $d(t) = (F_{\text{in}}, C_{A_{\text{in}}}, C_{B_{\text{in}}}, T_{\text{in}}) = (0.1, 1, 0, 350)$ can be assumed to be constant. The model parameters θ_x are

$$\theta_x = \begin{bmatrix} F_{\text{in}} \\ T_{\text{in}} \\ C_{A_{\text{in}}} \\ r \\ k_0 \\ E/R \\ U \\ \rho \\ C_p \\ \Delta H \end{bmatrix} = \begin{bmatrix} 0.1 & [\text{m}^3/\text{min}] \\ 350 & [\text{degK}] \\ 1 & [\text{kmol/m}^3] \\ 0.219 & [\text{m}] \\ 7.2 \times 10^{10} & [\text{min}^{-1}] \\ 8750 & [\text{degK}] \\ 54.94 & [\text{kJ / min} \cdot \text{m}^2 \cdot \text{K}] \\ 1000 & [\text{kg/m}^3] \\ 0.239 & [\text{kJ/kg} \cdot \text{K}] \\ -5 \times 10^4 & [\text{kJ/kmol}] \end{bmatrix}.$$

The reference values for the state variable and the controls are $x_{\text{ref}} = (0.878, 324.5, 0.659)^T$ and $u_{\text{ref}} = (0.1, 300)^T$. The system at time $t = 0$ is at $x_0 = \begin{bmatrix} 0.9 & 0 & 0 \\ 0 & 1.1 & 0 \\ 0 & 0 & 1.0 \end{bmatrix} x_{\text{ref}}$. The path constraints for the controls are given in terms of the upper- and lower- bounds $u_{\min} = 0.85 u_{\text{ref}}$ and $u_{\max} = 1.15 u_{\text{ref}}$

Discretise the optimal control formulation in continuous-time by integrating the dynamics of the process over a grid of $K+1$ time-nodes $\{t_k\}_{k=0}^{K}$. Assume that the node are equally distant and assume a constant control u_k over each of the intervals. In each interval, take 25 RK4 steps , to define the discretised dynamics.

- Write the resulting discrete-time optimal control formulation, using the discretised dynamics based on the integration scheme with $\Delta t = t_f/K$;
- Eliminate the state variables from the discrete-time formulation using a forward simulation of the process dynamics, solve the problem using the sequential approach with CasADi/IPOPT, and plot the trajectories obtained for the state and the control variables;
- Keep both the state and the control variables, solve the problem using the simultaneous approach using CasADi/IPOPT, and plot the trajectories obtained from the state and the control variables.

You are free to select the final time t_f, the number K of intervals and the parameters Q_{t_f}, Q, and R.