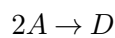
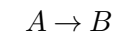


Problem Set #4: Nonlinear Model Predictive Control

Stabilizing and Economic NMPC with CasADi

The aim of this exercise is to design and implement an NMPC controller using Matlab and CasADi (<https://github.com/casadi/casadi/wiki>). See the previous exercise for installation instructions.

Consider a chemical continuous stirred tank reactor (CSTR), in which the reactions



take place. Here, we are only interested in the dynamics of the concentration of the substances A and B , c_A, c_B in mol/m^3 . Since the reactor is non-isothermal we also model the reactor temperature as state variable T in $^\circ\text{C}$. This yields the following dynamic model

$$\dot{c}_A = r_A(c_A, T) + (c_{In} - c_A)u_1 \quad (1a)$$

$$\dot{c}_B = r_B(c_A, c_B, T) - c_B u_1 \quad (1b)$$

$$\dot{T} = h(c_A, c_B, T) + \alpha(u_2 - T) + (T_{In} - T)u_1, \quad (1c)$$

where

$$r_A(c_A, T) = -k_1(T)c_A - k_2(T)c_A^2 \quad (1d)$$

$$r_B(c_A, c_B, T) = k_1(T)(c_A - c_B) \quad (1e)$$

$$h(c_A, c_B, T) = -\delta \left(k_1(T)(c_A \Delta H_{AB} + c_B \Delta H_{BC}) + k_2(T)c_A^2 \Delta H_{AD} \right) \quad (1f)$$

$$k_i(T) = k_{i0} \exp \frac{-E_i}{T + T_0}, \quad i = 1, 2. \quad (1g)$$

The inputs u_1, u_2 are the normalized flow rate through the reactor in $1/\text{h}$ and the temperature in the cooling jacket in $^\circ\text{C}$, respectively. The system parameters are given in Table 1.

Tabelle 1: Parameters for system (1) [1].

α	30.828	$[\text{h}^{-1}]$	k_{20}	$9.043 \cdot 10^6$	$[\text{m}^3/(\text{mol h})]$
δ	$3.522 \cdot 10^{-4}$	$[\text{C m}^3/(\text{kJ})]$	E_1	9578.3	$[\text{C}]$
T_{In}	104.9	$[\text{C}]$	E_2	8560.0	$[\text{C}]$
T_0	273.15	$[\text{C}]$	ΔH_{AB}	4.2	$[\text{kJ/mol}]$
c_{In}	$5.1 \cdot 10^3$	$[\text{mol/m}^3]$	ΔH_{BC}	-11.0	$[\text{kJ/mol}]$
k_{10}	$1.287 \cdot 10^{12}$	$[\text{h}^{-1}]$	ΔH_{AD}	-41.85	$[\text{kJ/mol}]$

The states and inputs are subject to the constraints

$$c_A \in [0, 6000] \frac{\text{mol}}{\text{m}^3}, \quad c_B \in [0, 4000] \frac{\text{mol}}{\text{m}^3}, \quad T \in [70, 200]^\circ\text{C}, \quad u_1 \in [3, 35] \frac{1}{\text{h}}, \quad u_2 \in [100, 200]^\circ\text{C}. \quad (2)$$

We consider the task of optimizing the integral amount of B produced by the reactor. This can be expressed as the following infinite-horizon OCP

$$\min_{u(\cdot)} \int_0^\infty -\gamma c_B(t) u_1(t) dt \quad (3a)$$

subject to

$$\text{system dynamics (1),} \quad (3b)$$

$$\begin{bmatrix} c_A(0) \\ c_B(0) \\ T(0) \end{bmatrix} = \begin{bmatrix} 1500 \\ 1200 \\ 70 \end{bmatrix}, \quad (3c)$$

$$\text{constraints (2),} \quad (3d)$$

with $\gamma \geq 0$.

Exercise 1 – Steady-State Optimization

- a) Solve the steady-state optimization problem that corresponds to the OCP (3), i.e.

$$[u_{ss}, x_{ss}] = \underset{u \in \mathbb{R}^2, x = [c_A, c_B, T]^T \in \mathbb{R}^3}{\operatorname{argmin}} -\gamma c_B u_1 \quad (4a)$$

subject to

$$0 = r_A(c_A, T) + (c_{In} - c_A)u_1, \quad (4b)$$

$$0 = r_B(c_A, c_B, T) - c_B u_1, \quad (4c)$$

$$0 = h(c_A, c_B, T) + \alpha(u_2 - T) + (T_{In} - T)u_1, \quad (4d)$$

$$\text{constraints (2).} \quad (4e)$$

Exercise 2 – Stabilizing NMPC

Next, we want to design an NMPC scheme that stabilizes (1) at the optimal set point (u_s, x_s) computed via (4). If you could not solve this task use $x_s = [2175.6, 1104.9, 128.53]^T$, $u_s = [35, 142.76]^T$.

- Formulate an OCP (without terminal constraints) that can be used to stabilize (1) by means of an NMPC scheme at the optimal setpoint computed via (4).
- In order to avoid numerical difficulties first rescale the state and input variables such that they take values between 0 and 10.
- Implement the OCP from part b) using CasADi and compute the solution for a horizon length of $T = 0.2h$. The system parameters from Table 1 are given in the file `parameters.m`. Use the file `rk4.m` to integrate the system dynamics (1).
- Extend your code from part c) to solve the sequence of OCPs arising in the NMPC scheme. Simulate the NMPC loop using `rk4.m` and Matlab's built-in `ode45` and `ode15s`.
- Compare the control performance with and without a terminal penalty. What can you observe? How does the computation time change? *Hint:* Hotstart the optimization by providing initial guesses.

Exercise 3 – Economic NMPC

Next, we want to design an economic NMPC scheme, which computes a receding-horizon approximation to the infinite-horizon OCP (3).

- To this end, consider the finite-horizon version of OCP (3) and reformulate it as a Mayer problem.
- Before simulating the economic NMPC scheme, solve the single OCP from Ex 1 part a) for the initial condition $[c_A(0), c_B(0), T(0)]^T = [1500, 1200, 70]^T$ and three integration steps per shooting interval. What do you observe?

- c) How can the objective function be extended to penalize chattering? State your proposition mathematically and implement the extended OCP. Plot your optimal trajectories for different lengths of the optimization horizon $T \in \{0.05, 0.1, 0.2\}$ h. What do you observe?
- d) Extend your code from Ex 1 part e) to solve the arising sequence of OCPs. Plot your closed-loop results.

Literatur

- [1] R. Rothfuß, J. Rudolph, and M. Zeitz. Flatness based control of a nonlinear chemical reactor model. *Automatica*, 32:1433–1439, 1996.