# 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

$$A \to B$$
$$B \to C$$
$$2A \to D$$

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 °C. This yields the following dynamic model

$$\dot{c}_A = r_A(c_A, T) + (c_{In} - c_A)u_1 \tag{1a}$$
$$\dot{c}_B = r_B(c_A, c_B, T) - c_B u_1 \tag{1b}$$
$$\dot{T} = h(c_A, c_B, T) + \alpha(u_2 - T) + (T_{In} - T)u_1, \tag{1c}$$

where

$$r_A(c_A, T) = -k_1(T)c_A - k_2(T)c_A^2 \tag{1d}$$
$$r_B(c_A, c_B, T) = \quad k_1(T)(c_A - c_B) \tag{1e}$$
$$h(c_A, c_B, T) = -\delta\Big(k_1(T)\left(c_A \Delta H_{AB} + c_B \Delta H_{BC}\right) + k_2(T)c_A^2 \Delta H_{AD}\Big) \tag{1f}$$
$$k_i(T) = \quad k_{i0} \exp\frac{-E_i}{T + T_0}, \quad i = 1, 2. \tag{1g}$$

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

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

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

The states and inputs are subject to the constraints

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

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

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

$$\text{subject to}$$

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

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

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

with $\gamma \geq 0$.

## Exercise 1 – Steady-State Optimization

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

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

$$\text{subject to}$$

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

$$0 = r_B(c_A, c_B, T) - c_B u_1, \tag{4c}$$

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

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

## Exercise 2 – Stabilizing NMPC

Next, we want to design an NMPC scheme that stabilizes (1) at the optimal set point $(u_\text{s}, x_\text{s})$ computed via (4). If you could not solve this task use $x_\text{s} = [2175.6, 1104.9, 128.53]^\top$, $u_\text{s} = [35, 142.76]^\top$.

a) 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).

b) In order to avoid numerical difficulties first rescale the state and input variables such that they take values between $0$ and $10$.

c) Implement the OCP from part b) using CasADi and compute the solution for a horizon length of $T = 0.2$h. The system parameters from Table 1 are given in the file `parameters.m`. Use the file `rk4.m` to integrate the system dynamics (1).

d) 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`.

e) 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).

a) To this end, consider the finite-horizon version of OCP (3) and reformulate it as a Mayer problem.

b) Before simulating the economic NMPC scheme, solve the single OCP from Ex 1 part a) for the initial condition $[c_A(0), c_B(0), T(0)]^\top = [1500, 1200, 70]^\top$ 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.