Problem Set #2: Numerical Optimal Control

Exercise 1: Formulation of OCPs

The aim of this exercise is formulate several optimal control problems. We will re-use the results in a later exercise where we implement solutions numerically.

Consider a chemical continuous stirred tank reactor (CSTR) in which the exothermic irreversible reaction

$$A \to B$$

takes place. The dynamics of the CSTR are as follows, see [2] for details.

$$\dot{c}_A = \frac{q}{V}(c_{Af} - c_A) - k_0 e^{\frac{-E}{RT}} c_A \tag{1a}$$

$$\dot{T} = \frac{q}{V}(T_f - T) + \frac{-\triangle H}{\rho C_p} k_0 e^{\frac{-E}{RT}} c_A + \frac{UA}{V\rho C_p}(u_1 - T). \tag{1b}$$

The states c_A and T describe the concentration of subtance A and the reactor temperature in K. The coolant stream temperature u is the considered input variable. The objective is to compute an input signal such that the system reaches the set-point $c_{As} = 0.159[mol/l], T_s = 375[K]$. The coolant stream temperature u is subject to the input constraint $u \in [270, 330]$. The system parameters are listed in the following table.

Table 1: Parameters for CSTR.

q	100	$[L/min]$	C_{Af}	1	$[mol/L]$
T_f	350	$[K]$	V	100	$[L]$
ρ	1000	$[g/L]$	C_p	0.239	$[J/(g \cdot K)]$
$-\triangle H$	$5 \cdot 10^4$	$[J/mol]$	$\frac{E}{R}$	8750	$[K]$
k_0	$7.2 \cdot 10^{10}$	$[min^{-1}]$	UA	$5 \cdot 10^4$	$[J/(minK)]$

a) We want to calculate optimal open-loop inputs which steer the system (1) to the considered set-point. Formulate three different optimal control problem, such that the solution of each of these problems yields the considered open-loop inputs. Justify and explain your choices.

Exercise 2: Direct Discretization

The aim of this exercise is to solve an easy optimal control problem. Specifically, we will use `Yalmip`. It is advisable to install the toolboxes prior to the exercise.

In this exercise we will solve an optimal control problem (OCP) via a (naive) direct simultaneous approach. We consider the following OCP:

$$\min_{u(\cdot)} \int_0^1 \mathbf{x}^T(t)\mathbf{x}(t) + 0.005u^2(t)dt \tag{2a}$$

subject to $\forall t \in [0,1]$:

$$\dot{\mathbf{x}}(t) = \begin{pmatrix} 0 & 1 \\ 0 & c \end{pmatrix} \mathbf{x}(t) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} u(t) \quad c \in \mathbb{R} \tag{2b}$$

$$u(t) \in [-20, 20] \tag{2c}$$

$$g(t, \mathbf{x}) = 8(t-0.5)^2 - 0.5 - x_2 \geq 0 \tag{2d}$$

$$\mathbf{x}(0) = (0, -1)^T. \tag{2e}$$

A simple procedure to integrate an ODE $\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t)), \quad \mathbf{x}(0) = \mathbf{x}_0$ is given by the Euler forward discretization

$$\mathbf{x}(t+h) = \mathbf{x}(t) + h\mathbf{f}(t, \mathbf{x}(t)), \tag{3}$$

where $h > 0$ is the integration step size.

a) Integrate the system (2b) for the given initial condition (2e) from $t = 0$ to $t = 1$. Consider $\forall t \in [0,1]:$ $u(t) = 0, c = 1$ and $h = 0.02$.

b) Assume that you discretized the dynamics (2b) via (3) and the inputs are parametrized as piecewise constant. Furthermore, suppose that the constraints are evaluated the discretization points $t_{k+1} = t_k + h$ and the objective is approximated as $\sum_{k=0}^{N-1} h(\mathbf{x}(t_k)^T \mathbf{x}(t_k) + 0.005u^2(t_k))$. Of which type is the resulting NLP?

c) Solve the OCP (2) via a direct simultaneous approach. Use a piecewise constant parametrization of the input

$$\text{For } t \in [t_k, t_{k+1}]: \quad u(t) = w_{k+1}, \qquad t_{k+1} = t_k + h, \quad k = 0 : N-1$$

Plot the optimal input profile. Plot $x_1(t)$ versus t and $x_2(t), g(t, \mathbf{x}) + x_2(t)$ versus t. *Hint: Define the constraints and the objective as* `optivar` *variables.*

d) In order to verify your solution integrate (2b) subject to your optimal solution $u^\star(t)$ with a variable stepsize integrator from `MATLAB`. Add the obtained trajectories to the plots from part c). *Hint: Use the solver* `ode45` *and set the relative and absolute error tolerances to* 10^{-12}. *Integrate over the intervals* $[t_k, t_{k+1}], \quad k = 0 : N-1$ *separately by keeping* u *constant.*

e) Now, set the model parameter set $c = 3$. Repeat c) and d) for this value of c. What do you observe? Try to explain your results. Can you suggest remedies?

f) Now, replace the Euler forward discretization by a second-order Runge-Kutta integration scheme. Use Heun's method[1] which reads

$$\tilde{\mathbf{x}}(t+h) = \mathbf{x}(t) + h\mathbf{f}(t, \mathbf{x}(t)) \tag{4}$$

$$\mathbf{x}(t+h) = \mathbf{x}(t) + \frac{h}{2}\Big(\mathbf{f}(t, \mathbf{x}(t)) + \mathbf{f}(t+h, \tilde{\mathbf{x}}(t+h))\Big). \tag{5}$$

Repeat c) and d) for this value of c. What do you observe? Compare your results to ones obtained in f).

Exercise 3: Direct Collocation

Next, we will try to solve a simple OCP via a simple collocation method. Consider

$$\min_{u(\cdot)} \int_0^1 \frac{1}{2} u^2(t) dt \tag{6a}$$

[1] Heun's method is also known as *trapezoidal rule*.

subject to $\forall t \in [0,1]$:

$$\dot{x}(t) = -x(t) + u(t), \quad x(0) = 1,\ x(1) = 0. \tag{6b}$$

For simplicity, we consider a piecewise constant parametrization of the input

$$\text{for } t \in [t_k, t_{k+1}]: \quad u(t) = w_{k+1}, \qquad t_{k+1} = t_k + h, \quad k = 0 : N-1,$$

where h is the length of each collocation stage. On each stage the state trajectory is to be approximated by Lagrange polynomials of degree 3:

$$x(t) = \sum_{i=0}^{3} \xi_i^k \phi_i^{(3)} \left(\frac{t - t_k}{t_{k+1} - t_k} \right), \quad t \in [t_k, t_{k+1}], k = 0, \ldots, N-1 \tag{7}$$

with

$$\phi_i^{(3)} = \prod_{\substack{q=0 \\ q \neq i}}^{3} \frac{\tau - \tau_q}{\tau_i - \tau_q}$$

and the following collocation points $\{\tau_0, \tau_1, \ldots, \tau_3\} = \{0, 0.25, 0.5, 0.75\}$.

a) Reformulate the OCP in Mayer form. Discretize the reformulated problem via collocation. State the corresponding expressions for states and constraints of the resulting NLP.

b) Write a `MATLAB` script to solve the integration of the reformulated dynamics via `Yalmip`. Consider the given initial condition $x_0 = 1$, $t = 0$ to $t = 1$, the number of stages $N = 10$ and $\forall t \in [0,1]: \quad u(t) = 0$. *Hint: Define the collocation parameters* ξ_i^k *as* `sdpvar` *variables. Use the files* `lagrange.m`, `dlagrange.m` *to evaluate the Lagrange polynomials.*

c) Extend your code in order to solve OCP (6).

d) Compare your results with the analytical solution which can be found in the class textbook [1, Example 4.23 (p. 133-134)]. Consider different numbers of collocation stages $N \in \{5, 10, 20\}$.

References

[1] B. Chachuat. *Nonlinear and Dynamic Optimization: From Theory to Practice*. EPFL, 2009.

[2] M. Henson and D. Seborg. *Nonlinear Process Control*. Prentice Hall, Upper Saddle River, NJ, 1997.