TEMPO Spring School: Theory and Numerics for Nonlinear Model Predictive Control

Exercise 8: Full Information MHE

J. Andersson M. Diehl J. Gillis J. Rawlings M. Zanon

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Consider the following set of reversible reactions taking place in a well-stirred, isothermal, gas-phase batch reactor

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B + C, \qquad 2B \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} C,$$

with constants $k_1 = 0.5$, $k_{-1} = 0.05$, $k_2 = 0.2$ and $k_{-2} = 0.01$. For simplicity, we will omit all units. The states are the concentrations of species in and the measurement is the reactor pressure

$$x = \begin{bmatrix} c_\mathrm{A} \\ c_\mathrm{B} \\ c_\mathrm{C} \end{bmatrix}, \qquad y = RT \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} x,$$

where we assume the ideal gas law in modeling the pressure and $RT = 32.84$.

Material balances lead to the following nonlinear state space model:

$$\frac{\mathrm{d}}{\mathrm{d}t} x = \frac{\mathrm{d}}{\mathrm{d}t} \begin{bmatrix} c_\mathrm{A} \\ c_\mathrm{B} \\ c_\mathrm{C} \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 1 & -2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} k_1 c_\mathrm{A} - k_{-1} c_\mathrm{B} c_\mathrm{C} \\ k_2 c_\mathrm{B}^2 - k_{-2} c_\mathrm{C} \end{bmatrix}.$$

We discretize the system using a sampling time $\Delta = 0.25$ and a fixed-stepsize explicit Runge Kutta integrator with 10 integration steps. In the following, we define the unperturbed discrete-time system as $x_{k+1} = f(x_k)$.

Let us consider an initial state estimate $\bar{x}_0 = \begin{bmatrix} 1 & 0 & 4 \end{bmatrix}^\intercal$ while the real initial state is given by $x_0 = \begin{bmatrix} 0.5 & 0.05 & 0 \end{bmatrix}^\intercal$. The prior density for the initial state, $\mathcal{N}(\bar{x}_0, P)$ with $P = 0.5^2 I$, is deliberately chosen to poorly represent the actual initial state to model a large initial disturbance to the system.

We want to examine how MHE recovers from this large unmodeled disturbance. For the state noise w and measurement noise v we use the following covariance matrices $Q = 0.001^2 I$ and $R = 0.25^2 I$ respectively. We define the perturbed model as

$$\begin{aligned} x_{k+1} &= f(x_k) + w_k, \\ y_k &= RT \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} x_k + v_k. \end{aligned}$$

Tasks:

8.1 Write down on paper the optimization problem that full information MHE solves at each time instant.

8.2 Complete the code that we provided you in order to formulate and solve the MHE problem in CasADi.