Data-Enhanced Learning Compensation for Linear Predictive Control of Nonlinear Chemical Processes

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June 16, 2022 / DYCOPS22

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Chemical reaction engineering is an engineering activity concerned with the exploitation of chemical reactions on a commercial scale.

Every industrial chemical process is designed to produce economically a desired product from a variety of starting materials through a succession of treatment steps, see Fig. 1.

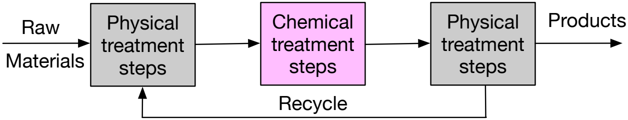

Figure: A simplified illustration of chemical reaction processes

Motivation: Continuous Stirred-Tank Reactor (CSTR)

Consider a CSTR depicted in Fig. 2, where chemical species A reacts to form species B, i.e.,

$$A \rightarrow B$$

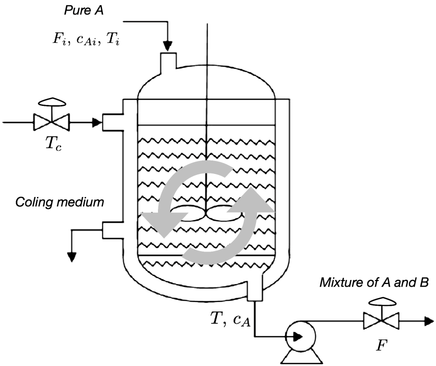

Figure: A simplified illustration of the CSTR

Motivation: Unsteady-State Material Balance

Assumption 1: the rate of reaction is first-order with respect to component A, $r = kc_A$, where $k = k_0 \exp\left(-\frac{E}{RT}\right)$, k_0 is the frequency factor, E is the activation energy, and R is the gas constant.

Assumption 2: i) the CSTR is perfectly mixed; ii) the mass densities of the feed and product streams are equal and constant, denotes as ρ.

Unsteady-state component balances for species A (in molar units) is

$$V \frac{dc_A}{dt} = F\left(c_{Ai} - c_A\right) - Vkc_A$$

Motivation: Unsteady-State Energy Balance

Assumption 3: i) The thermal capacitances of the coolant and the cooling coil wall are negligible compared to the thermal capacitance of the liquid in the tank; ii) All of the coolant is at a uniform temperature as T_c; iii) The rate of heat transfer from the reactor contents to the coolant is given by $Q = UA(T_c - T)$, where U is the overall heat transfer coefficient and A is the heat transfer area. Both of these model parameters are assumed to be constant. iv) The heat of mixing is negligible compared to the heat of reaction. v) Shaft work and heat losses to the ambient can be neglected.

Energy balance for the CSTR is given by

$$V\rho C_p \frac{dT}{dt} = F\rho C_p(T_i - T) + (-\Delta H_R)Vkc_A + Q$$

where ΔH_R is the heat of reaction per mole of A that is reacted.

Process Modeling: Nonlinear State-Space Model

Nonlinear state-space model is finally obtained as

$$\frac{dc_A}{dt} = \frac{F\left(c_{Ai} - c_A\right)}{V} - k_0 \exp\left(-\frac{E}{RT}\right) c_A$$
$$\frac{dT}{dt} = \frac{F\left(T_i - T\right)}{V} - \frac{\Delta H_R}{\rho C_p} k_0 \exp\left(-\frac{E}{RT}\right) c_A + \frac{UA}{V\rho C_p}\left(T_c - T\right)$$

Open-loop stable steady-state operating conditions are set as

$$c^s = 0.878 \text{ mol/L},\ T^s = 324.5 \text{ K},\ T_c^s = 300 \text{ K}$$

Process Modeling: Parameters of CSTR

Table: Parameters of the CSTR

Parameter	Explanation	Nominal value	Units
F_i	Inlet flow rate	100	$\mathrm{L/min}$
c_{Ai}	Feed concentration	1	$\mathrm{mol/L}$
T_i	Feed temperature	350	K
V	Volume of CSTR	100	L
k_0	Pre-exponential factor	7.2×10^{10}	min^{-1}
E/R	E/R = Activation energy	8750	K
UA	Heat transfer constant	5×10^{4}	$\mathrm{J/min \cdot K}$
ρ	Density of A-B mixture	1000	$\mathrm{g/L}$
C_p	Heat capacity of A-B mixture	0.239	$\mathrm{J/g \cdot K}$
ΔH_R	Heat of reaction for $A \rightarrow B$	-5×10^{4}	$\mathrm{J/mol}$

Problem Formulation: Mathematical Model

For the state variables:

$$c_A \in [0, 1]\ \mathrm{mol/L}, \quad T \in [0, 400]\ \mathrm{K}$$

They have very large magnitude difference, resulting in difficult control problems.

Define normalized and dimensionless variables x and u as

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \frac{c_A - c^s}{c^s} \\ \frac{T - T^s}{T^s} \end{bmatrix}, \quad u = \frac{T_c - T_c^s}{T_c^s}.$$

Using the model parameters given in Table 1 yields

$$\frac{dx_1}{dt} = -x_1 + 0.1399 - 7.2 \times 10^{10}(x_1 + 1)\exp\left(\frac{-26.9666}{x_2 + 1}\right)$$
$$\frac{dx_2}{dt} = -3.0921x_2 + 1.9342u - 0.0791 + 4.0724 \times 10^{10}(x_1 + 1)\exp\left(\frac{-26.9666}{x_2 + 1}\right)$$

Problem Formulation: Collecting Data

Note that

- A lot of assumptions yield the mathematical model, making it difficult for the model to capture uncertainties inherent to the real plant, such as unmodeled dynamics and uncertainty in parameter values.
- It is best to use historical process data to help us build real-time models and perform optimizations in real-time.

To accomplish this, we examine how historical data can be used to optimize control performance during controller design for the CSTR system.

Since all the historical data such as the inputs and outputs of the reactor are available, i.e.,

$$\mathbb{I} \triangleq \left\{u_0, u_1, \ldots, u_N\right\}$$
$$\mathbb{O} \triangleq \left\{x_0, x_1, \ldots, x_N\right\}$$

Controller Design

We plot uncontrolled response:

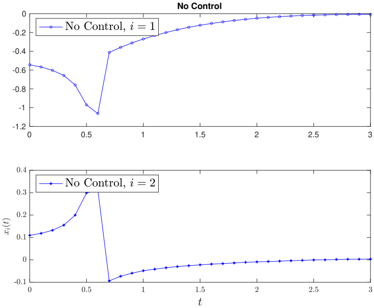

Figure: The uncontrolled response

Controller Design

Using a sampling time of 0.1 min, we obtain the discrete-time state-space model as

$$x(t+1) = Ax(t) + Bu(t))$$

where A and B are given by $A = \begin{bmatrix} 0.8906 & -0.3419 \\ 0.0090 & 0.9067 \end{bmatrix}$ and $B = \begin{bmatrix} -0.0337 \\ 0.1811 \end{bmatrix}$.

Consider the constraints in the following form

$$\mathcal{X} = \left\{ x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} : \begin{cases} -0.5 < x_1(t) < 0.5 \\ -0.4 < x_2(t) < 0.4 \end{cases} \right\}$$

$$\mathcal{U} = \{u(t) : -0.8 < u(t) < 0.8\}$$

Method 1: Linear Quadratic Regulator (LQR)

The optimal control input is obtained by solving the LQR problem:

$$\begin{aligned} \min \quad & \sum_{t=0}^{\infty} x^{\mathrm{T}} Q x(t) + u^{\mathrm{T}} R u(t) \\ \text{s.t.} \quad & x(t+1) = Ax(t) + Bu(t) \end{aligned}$$

without considering constraints.
Assume that (A, B) is stabilizable, then the unique solution to the LQR problem is

$$\begin{aligned} u^{\star}(t) &= Kx(t) \\ K &= -(R + B^{\mathrm{T}} P B)^{-1} B^{\mathrm{T}} P A \\ P &= Q + A^{\mathrm{T}} P A - A^{\mathrm{T}} P B (R + B^{\mathrm{T}} P B)^{-1} B^{\mathrm{T}} P A \end{aligned}$$

Method 1: Linear Quadratic Regulator (LQR)

We plot LQR control response:

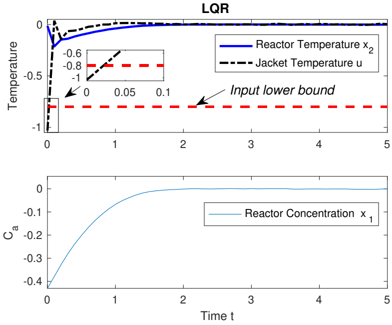

Figure: Performance under the LQR controller.

Note that the jacket temperature is smaller than -0.8, violating the constraints for the CSTR setting.

Preliminary Design for Linear MPC

First, we plot all the constraint polytopes (offline part):

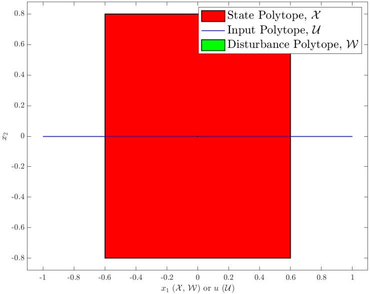

Figure: The constraint polytopes $\mathcal{X}$ and $\mathcal{U}$.

Preliminary Design for Linear MPC

Second, we need the following prior designs (offline part):

1. The terminal set Ω: render the state to stay inside at every end of the prediction horizon, and satisfies
   - Constraint satisfaction: $\Omega \subset \{x : x \in \mathcal{X}, Kx \in \mathcal{U}\}$
   - Disturbance invariance: $(A + BK)\Omega \oplus \mathcal{W} \subset \Omega$
   - Disturbance Tubes $\mathcal{R}_k$: $\mathcal{R}_0 = \{0\}$, $\mathcal{R}_k = \oplus_{j=0}^{k-1}(A + BK)^k \mathcal{W}$, $k = 1, 2, \ldots, N$.

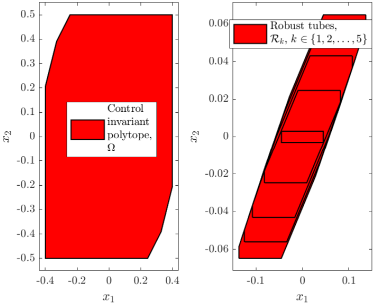

Figure: The control invariant set Ω and the robust tubes $\mathcal{R}_k$.

Method 2: Linear MPC

The linear MPC problem is formulated as

$$
\begin{aligned}
\min \quad & \bar{x}^{\mathrm{T}}(t+N)P\bar{x}(t+N) + \sum_{k=t}^{t+N-1} \bar{x}^{\mathrm{T}}(t)Q\bar{x}(t) + \bar{u}^{\mathrm{T}}(t)R\bar{u}(t) \\
\text{s.t.} \quad & \bar{x}(t) = x(t) \\
& \bar{x}(t+k+1) = A\bar{x}(t+k) + B\bar{u}(t+k) \\
& \bar{u}(t+k) = K\bar{x}(t+k) + c(t+k) \\
& \bar{x}(t+k+1) \in \mathcal{X} \ominus \mathcal{R}_{k+1}, \quad \bar{x}(t+N) \in \Omega \ominus \mathcal{R}_N \\
& \bar{u}(t+k) \in \mathcal{U} \ominus (K\mathcal{R}_k), \quad k = 0, 1, \ldots, N-1.
\end{aligned}
$$

Method 2: Linear MPC

We plot linear MPC control response:

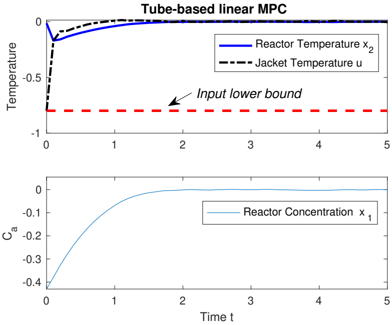

Figure: Performance under the linear tube-based MPC.

Method 3: Data Compensation for Linear MPC

The data compensation for linear tube-MPC is formulated as

$$
\begin{aligned}
\min\ & \tilde{x}^{\mathrm{T}}(t+N)P\tilde{x}(t+N) + \sum_{k=t}^{t+N-1} \tilde{x}^{\mathrm{T}}(t)Q\tilde{x}(t) + \bar{u}^{\mathrm{T}}(t)R\bar{u}(t) \\
\text{s.t.}\ & \bar{x}(t) = x(t) \\
& \tilde{x}(t+k+1) = A\tilde{x}(t+k) + B\bar{u}(t+k) + \mathcal{O}_t(\tilde{x}(t+k), \bar{u}(t+k)) \\
& \bar{x}(t+k+1) = A\bar{x}(t+k) + B\bar{u}(t+k) \\
& \bar{u}(t+k) = K\bar{x}(t+k) + c(t+k) \\
& \bar{x}(t+k+1) \in \mathcal{X} \ominus \mathcal{R}_{k+1}, \quad \bar{x}(t+N) \in \Omega \ominus \mathcal{R}_N \\
& \bar{u}(t+k) \in \mathcal{U} \ominus (K\mathcal{R}_k), \quad k = 0, 1, \ldots, N-1.
\end{aligned}
$$

The variable $\tilde{x}$ is used in adaptive model with data compensation, thereby yielding more accurate predictions for the actual state trajectory.

Method 3: Data Compensation for Linear MPC

By comparing the unknown part

$$\begin{aligned} g(x(t), u(t)) &= f(x(t), u(t)) - Ax(t) - Bu(t) + d(t) \\ &= x(t+1) - Ax(t) - Bu(t) \end{aligned}$$

with the data-compensated prediction model

$$x(t+1) = Ax(t+k) + Bu(t) + \mathcal{O}_t(x(t), u(t))$$

we would want that, with more data collected for compensation,

$$\mathcal{O}_t(x(t), u(t)) \rightarrow g(x(t), u(t))$$

Method 3: Data Compensation for Linear MPC

Now, design the $\mathcal{O}_t(x(t), u(t))$ as

$$\mathcal{O}_t(x(t), u(t)) \triangleq \mathcal{O}_t(x, u) = P_x^{\mathrm{T}} \overrightarrow{m}_{[0,r_1]}(x) + P_u^{\mathrm{T}} \overrightarrow{m}_{[0,r_2]}(u)$$

where $\overrightarrow{m}_{[0,r_1]}(x)$ and $\overrightarrow{m}_{[0,r_2]}(u)$ with two positive integer r_1 and r_2 denote the polynomials of the vector $x \in \mathbb{R}^n$ and $u \in \mathbb{R}^m$ with the order at least 0 and at most r_1 and r_2, respectively, i.e.,

$$\overrightarrow{m}_{[0,r_1]}(x) = \begin{bmatrix} 1 \\ x(t) \\ \vdots \\ x^{r_1}(t) \end{bmatrix}, \quad \overrightarrow{m}_{[0,r_1]}(u) = \begin{bmatrix} 1 \\ u(t) \\ \vdots \\ u^{r_2}(t) \end{bmatrix}$$

and, p_x, p_u denote two vectors that need to be identified using the available data.

Method 3: Data Compensation for Linear MPC

Writing in a compact form results in

$$\mathcal{O}_t(x(t), u(t)) = \Xi^{\mathrm{T}} \begin{bmatrix} \overrightarrow{m}_{[0,r_1]}(x(t)) \\ \overrightarrow{m}_{[0,r_2]}(u(t)) \end{bmatrix}.$$

Next, collecting the data $\{x(k)\}_{k=1}^{t}$ and $\{u(k)\}_{k=1}^{t}$, and construct the data

$$y(t) \triangleq x(t+1) - (Ax(t) + Bu(t))$$

and then, form $\overrightarrow{m}_{[0,r_1]}(x)$ and $\overrightarrow{m}_{[0,r_1]}(u)$ for $t = 1, 2, \ldots, k$.

Method 3: Data Compensation for Linear MPC

Finally, given two integers r_1 and r_2, using the least-squares method, we can optimize the parameter Ξ by solving the least-squares problem

$$\hat{\Xi} = \arg\min_{\Xi} \quad \sum_{k=0}^{t} \left\| \left(y(k) - \Xi^{\mathrm{T}} \begin{bmatrix} \overrightarrow{m}_{[0,r_1]}(x(t)) \\ \overrightarrow{m}_{[0,r_2]}(u(t)) \end{bmatrix} \right) \right\|^2$$

Note that the $\mathcal{O}_t(x(t), u(t))$ is linear in the coefficients Ξ, where $\overrightarrow{m}_{[0,r_1]}(x)$ and $\overrightarrow{m}_{[0,r_1]}(u)$ are two sets of polynomial vectors.

Summary of the Main Results

We highlight that the data-enhanced learning function has two different meanings.

1. Data-enhanced compensation allows for corrections to be made to the nominal prediction model:
    - The second element modifies the A, B matrices of the nominal model;
    - The remainder produces a more accurate model than the nominal one.
2. The coefficients of data compensation are characterized as unique optimizers of the least-squares problem.
    - Using data-enhanced learning compensation for the nominal model provides specific predictions of future behaviors, resulting in more accurate inputs and outputs for minimization of the performance function in solving OCP.

Our proposed method describing the data-enhanced learning compensation for tube MPC is summarized in Algorithm 1.

Algorithm 1: Data-Enhanced Learning Predictive Controller

Data: Collect histrotical input and output data
Input: r_1, r_2
Output: $\zeta(t)$ for every t

$k \leftarrow t$;
while $k \geq \max(r_1, r_2)$ **do**
  if $t \geq 0$ **then**
    Form extend data vectors $\overrightarrow{m}_{[0,r_1]}(x)$ and $\overrightarrow{m}_{[0,r_1]}(u)$;
    Solve the least-squares problem to obtain an estimate of Ξ;
    Solve the data-compensated MPC problem to obtain $\zeta(t+k)$, $k = 0, 1, \ldots, N-1$;
  end
  Apply $\tilde{u}(t) = K\bar{x}(t) + \zeta(t)$ to the system;
  $t \leftarrow t + 1$;
end

Method 3: Data Compensation for Linear MPC

We plot data-compensated MPC control response:

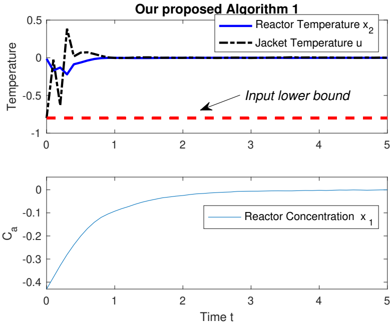

Figure: Performance under our proposed Algorithm 1.

Comparison results

We compare accumulated costs associated with LQR, linear MPC, and Algorithm 1.

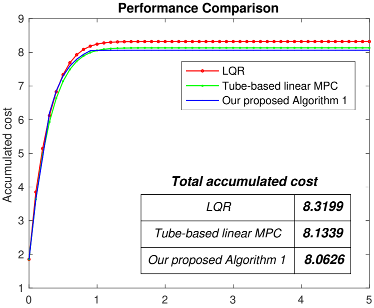

Figure: System performance under our proposed Algorithm 1.

Conclusions

Conclusions:

1. A data-enhanced learning compensation for linear MPC with closed loop performance improvement.
2. Some limitations of LQR and linear MPC formulations for nonlinear chemical processes.
3. A method for tuning the prediction model used in linear MPC while also ensuring the robustness and performance of the closed-loop system.
4. A method for handling situations when engineering constraints must be satisfied by a system with nonlinearities or unknown dynamics that render conventional control methods ineffective.

Thanks for listening!

Questions?