

Supplementary Material

Details for the two-model linear example

The parameters in the two models used in the example in the introduction are $a = 0.6$ and $b = 10.0$ in Model M_1 and $a = 10.5$ and $b = -5.0$ in Model M_2 . In both models the disturbances w_k are distributed $w_k \sim \mathcal{N}(0, 0.1^2)$. The cost-function parameters are $q = 10$ and $r = 1$ and the time horizon is $N = 20$. For solving the Bellman equation with dynamic programming, the state $x \in [-10, 10]$ and probability $P \in [0, 1]$ are quantized into 21 equally spaced points each, while the control $u \in [-1, 1]$ has 41 equally spaced quantized points. The disturbances are quantized with 9 Hermite-quadrature points. Further increasing the resolutions has no significant effect on the solutions.

Details for the CSTR case study

The model parameters used in the simulations of the CSTR are as follows. The sample time is 0.1 min; in the controller the prediction horizon is 10 samples and the control horizon 5 samples. The cost function weights are

$$Q = \begin{bmatrix} 1/0.5 & 0 \\ 0 & 1/350 \end{bmatrix}, \quad R = \begin{bmatrix} 1/900 & 0 \\ 0 & 1/300 \end{bmatrix}.$$

The initial value of the covariance matrix in the extended Kalman filter is diagonal with diagonal elements 10^{-2} , 10^{-1} , 10^{18} , and 10^{-1} . In the MPC with active learning (Strategy 4), the covariance is reset to a diagonal matrix with diagonal elements 10^{-2} , 10^{-1} , 9×10^{18} , and 10^4 (indicating significant parameter uncertainty) as the probing is induced.

Details for the bioreactor case study

The following parameters are used in the bioreactor case study. The initial conditions are $X(0) = 7.78 \text{ g/dm}^3$, $S(0) = 0.55 \text{ g/dm}^3$, and $P(0) =$

27.50 g/dm³. For μ_{\max} , the initial distribution is $\mu_{\max} \sim \mathcal{N}(\bar{\mu}_{\max}, \sigma_{\mu_{\max}}^2)$, with $\mu_{\max} = 0.3 \text{ h}^{-1}$ and $\sigma_{\mu_{\max}} = \sqrt{0.05} \text{ h}^{-1}$. In the measurements, $v_k \in \mathbb{R}^{2 \times 1}$ and $v_k \sim \mathcal{N}(0, \text{diag}(\sigma_{v_S}^2, \sigma_{v_P}^2))$, with $\sigma_{v_S} = 0.03 \text{ g/dm}^3$ and $\sigma_{v_P} = 1.00 \text{ g/dm}^3$. For the given parameters, optimal productivity occurs when the product concentration is $P_d = 27.5 \text{ g/dm}^3$ and the dilution rate (the control) is $D_d = 0.15 \text{ h}^{-1}$. In all simulations for this case study, the control horizon length is $N = 8$. The input is constrained to $0.0 \leq u_k \leq 0.8 \text{ h}^{-1}$ and the product concentration is constrained to be between 25 g/dm^3 and 30 g/dm^3 with a probability of 90 %. Table 3 lists the nominal parameters.

Table 2: Nominal parameters and operating conditions of the CSTR case study.⁶²

Variable	Nominal value	Units
C_A	0.5	mol/dm ³
\bar{T}_r	350	K
\bar{q}	100	dm ³ /min
\bar{T}_c	300	K
k_0	7.2×10^{10}	min ⁻¹
E/R	8750	K
ΔH	-5×10^4	J/mol
UA	5×10^4	J/(min K)
V	100	dm ³
ρ	1000	g/dm ³
c_p	0.239	J/(g K)
$C_{A,\text{in}}$	1	mol/dm ³
T_{in}	350	K

Table 3: Nominal parameters and operating conditions of the continuous bioreactor case study.^{67,68}

Variable	Nominal value	Units
$Y_{X/S}$	0.4	g/g
α	2.2	g/g
β	0.2	h^{-1}
μ_{\max}	0.48	h^{-1}
K_M	1.2	g/dm^3
S_f	20	g/dm^3
σ_X	0.25	g/dm^3
σ_S	0.25	g/dm^3
σ_P	0.25	g/dm^3