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# Dynamic Real-time Optimization of Batch Membrane Processes using Pontryagin's Minimum Principle

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## Abstract

This paper studies a dynamic real-time optimization in the context of model-based time-optimal operation of batch processes under parametric model mismatch. A class of batch membrane separation processes is in the scope of the presented applications. In order to tackle the model-mismatch issue, a receding-horizon policy is usually followed with frequent re-optimization. The main problem addressed in this study is high computational burden that is usually required by such schemes. We propose an approach that uses parametrized conditions of optimality in the adaptive predictive-control fashion. The uncertainty in the model predictions is treated explicitly using reachable sets that are projected into the optimality conditions.

**Keywords:** real-time optimization, Pontryagin's minimum principle, membrane processes, parameter estimation

## 1. Introduction

In this paper we consider a real-time implementation of a control policy that optimizes a process by assigning dynamic degrees of freedom such that a certain performance index is optimized:

$$\min_{u(t)\in[u_L,u_U],t_\mathrm{f}} \mathscr{J} := \min_{u(t)\in[u_L,u_U],t_\mathrm{f}} \int_0^{t_\mathrm{f}} F_0(x(t),p) + F_u(x(t),p)u(t)\,\mathrm{d}t \tag{1a}$$

$$\text{s.t. } \dot{x}(t) = f_0(x(t),p) + f_u(x(t),p)u(t), \quad x(0) = x_0, \quad x(t_\mathrm{f}) = x_\mathrm{f}, \tag{1b}$$

where $t$ is time with $t \in [0,t_\mathrm{f}]$, $x(t)$ is an $n$-dimensional vector of state variables, $p$ is an $m$-dimensional vector of model parameters, $u(t)$ is a (scalar) manipulated variable, $F_0(\cdot)$, $F_u(\cdot)$, $f_0(\cdot)$, and $f_u(\cdot)$ are continuously differentiable functions, $x_0$ represents a vector of initial conditions, and $x_\mathrm{f}$ are specified final conditions. We note here that an inclusion of multi-input and/or state-constrained cases is a straightforward extension but it is not considered in this study for sake of simplicity of the presentation. We also note that the specific class of input-affine systems is a suitable representation for a large variety of the controlled objects (Hangos et al., 2006).

The presented problem was studied in many previous works using on-line or batch-to-batch adaptation of the optimality conditions (Francois and Bonvin, 2013) or by design of robust controller for tracking the conditions of optimality (Nagy and Braatz, 2003). Recently, several advanced robust strategies were presented in the framework of model predictive control (Lucia et al., 2013).

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This paper proposes an adaptation of these approaches to the problem of dynamic real-time optimization of batch processes. This task is not straightforward because if one uses a receding-horizon control strategy, the prediction horizons need to be quite long, because of the presence of terminal constraints, which might compromise the real-time feasibility of the scheme.

We base the presented methodology on parameterization of the optimal operation using the conditions of optimality given by Pontryagin's minimum principle. This makes the dynamic decision problem (1) to boil down to identification of switching times of the optimal control policy. Such approach reduces computational burden while allowing for the use of sufficiently long prediction horizons when projecting the parametric uncertainty in controller performance and feasibility, particularly w.r.t. terminal time conditions. Robustness w.r.t. parametric uncertainty is addressed by taking into account the imprecision of parameter estimates such that it is projected into the uncertainty of the switching times. In order to improve performance of such a controller, i.e., to reduce conservatism introduced by uncertain switching times, we use on-line parameter estimation.

## 2. Preliminaries

### 2.1. Conditions for Optimality

Pontryagin's minimum principle can be used (Srinivasan et al., 2003) to identify the optimal solution to (1) via enforcing the necessary conditions for minimization of a Hamiltonian

$$H := \mu_L(u_L - u) + \mu_U(u - u_U) + \underbrace{F_0 + \lambda^T f_0}_{H_0(x(t),\lambda(t),p)} + \underbrace{\left(F_u + \lambda^T f_u\right)}_{H_u(x(t),\lambda(t),p)} u, \tag{2}$$

where $\lambda(t)$ is a vector of adjoint variables, and $\mu_L(t)$ and $\mu_U(t)$ are corresponding Lagrange multipliers. The optimality conditions of (1) can then be stated as (Srinivasan et al., 2003): $\forall t \in [0, t_f]$

$$\frac{\partial H}{\partial u} := H_u(x(t),\lambda(t),p) - \mu_L(t) + \mu_U(t) = 0, \tag{3}$$

$$H(x(t),\lambda(t),p,u(t),\mu_L(t),\mu_U(t)) = 0, \quad H_0(x(t),\lambda(t),p) = 0, \quad x(t_f) - x_f = 0. \tag{4}$$

The condition $H = 0$ arises from the transversality, since the final time is free (Pontryagin et al., 1962), and from the fact that the optimal Hamiltonian is constant over the whole time horizon, as it is not an explicit function of time. The condition $H_0 = 0$ is the consequence of the former two conditions. Since the Hamiltonian is affine in input (see (2)), the optimal trajectory of control variable is either determined by active input constraints or it evolves inside the feasible region.

Assume that for some point $t$ we have $H_u = 0$ and $u_L < u(t) < u_U$. It follows from (3) that the optimal control maintains $H_u(t) = 0$. Such control is traditionally denoted as singular. Further properties of the singular arc, such as switching conditions or state-feedback control trajectory can be obtained by differentiation of $H_u$ with respect to time (sufficiently many times) and by requiring the derivatives to be zero. The time derivatives of $H$ and $H_0$ must be equal to zero as well. Earlier results on derivation of optimal control for input-affine systems (Srinivasan et al., 2003) suggest that it is possible to eliminate $\lambda(t)$ from the optimality conditions and thus arrive at analytical characterization of switching conditions between singular and saturated-control arcs.

As the optimality conditions obtained by the differentiation w.r.t. time are linear in the adjoint variables, the differentiation of $H_u$ (or $H_0$) can be carried out until it is possible to transform the obtained conditions to a pure state-dependent switching function $S(x(t),p)$. It is usually convenient to use a determinant of the coefficient matrix of the equation system $A\lambda = 0$ for this. The singular control $u_s(x(t),p)$ can be found from differentiation of switching function w.r.t. time as

$$\frac{dS}{dt} = \frac{\partial S}{\partial x^T}\frac{dx}{dt} = \frac{\partial S}{\partial x^T}(f_0 + f_u u_s) = 0 \quad \Rightarrow \quad u_s(x(t),p) = -\frac{\partial S}{\partial x^T} f_0 \Big/ \frac{\partial S}{\partial x^T} f_u. \tag{5}$$

The resulting optimal-control policy is then given as a step-wise strategy (Paulen et al., 2015) by

$$u^*(t,\pi) := \begin{cases} u_L, & t \in [0,t_1],\ S(x(t),p) > 0, \\ u_U, & t \in [0,t_1],\ S(x(t),p) < 0, \\ u_s(x(t),p), & t \in [t_1,t_2],\ S(x(t),p) = 0, \\ u_L, & t \in [t_2,t_f],\ S(x_f,p) < 0, \\ u_U, & t \in [t_2,t_f],\ S(x_f,p) > 0, \end{cases} \tag{6}$$

$$x_f = x(t_2) + \int_{t_2}^{t_f} f_0(x(t),p) + f_u(x(t),p)u^*(t)\,dt, \tag{7}$$

where $\pi := (p^T,t_1,t_2,t_f)^T$ is the vector that parameterizes the optimal control strategy. Note that the presented optimal-control strategy determines implicitly the switching times $t_1$, $t_2$ and the terminal time $t_f$ as functions of model parameters $p$.

### *2.2. Set-membership estimation*

In order to estimate model parameters we will assume the model being linear in parameters as

$$\hat{y}(p) = c^T p, \tag{8}$$

where $\hat{y}$ is the prediction of the plant output $y$ and $c$ is a so-called regressor vector. The linearity of the model in parameters is not restrictive, the presented methodology applies to systems that are non-linear in parameters too. We will further assume that the measurement noise is bounded with

$$|y - \hat{y}(p)| \leq \sigma. \tag{9}$$

Under these assumptions a recursive set-membership estimation scheme was presented in Fogel and Huang (1982), which over-bounds the set of all parameter values that satisfy (9) as an ellipsoid

$$(p-\hat{p})^T V^{-1}(p-\hat{p}) \leq 1, \tag{10}$$

where $\hat{p}$ is the expected true value of the parameters and $V$ is parameter covariance matrix. Upon receiving a new measurement $y$, $\hat{p}$ and $V$ are updated by

$$\hat{p}_+ = \hat{p} + \frac{\beta d}{1+\beta g} V\tilde{c}, \qquad V_+ = \left(1+\beta - \frac{\beta d^2}{1+\beta g}\right)\left(V - \frac{\beta}{1+\beta g} V\tilde{c}\tilde{c}^T V\right), \tag{11}$$

where $\tilde{c} := c/\sigma$, $g := \tilde{c}^T V\tilde{c}$, $d := y/\sigma - \tilde{c}^T\hat{p}$. The parameter $\beta \in (0,1)$ can be selected in order to minimize trace or determinant of the covariance matrix $V$ (Fogel and Huang, 1982). The updated bounds of parameters (parameter confidence intervals) can be found via

$$P_+ := \left[\hat{p}_+ - \mathrm{diag}\left(V_+^{\frac{1}{2}}\right), \hat{p}_+ + \mathrm{diag}\left(V_+^{\frac{1}{2}}\right)\right]. \tag{12}$$

## 3. Dynamic real-time optimization

As the optimal control structure is a function of uncertain parameters, the uncertainty should be taken into account when devising a real-time implementation of the optimal control on the process. We will assume a bounded uncertainty $p \in P := [p^L, p^U]$ with a nominal realization $p_0 := \mathrm{mid}(P)$.

Given the structure of the optimal-control policy (6) one can project the parametric uncertainty into uncertainty of the switching times and singular control as

$$t_i(p) \in [t_i^L(P), t_i^U(P)] := T_i,\ \forall i \in \{1,2,f\}, \tag{13}$$

$$u_s(t,p) \in [u_s^L(t,P), u_s^U(t,P)] := U^*(t), \forall t \in [t_1(p), t_2(p)], \tag{14}$$

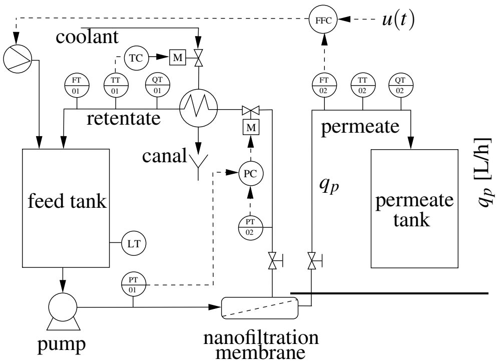


Figure 1: Diafiltration process scheme.

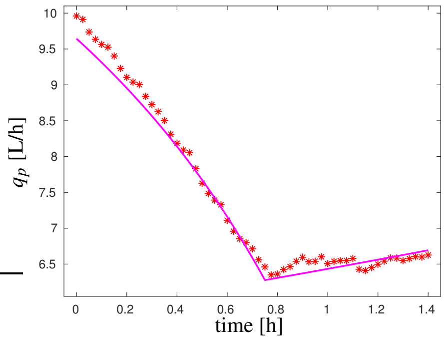


Figure 2: Comparison of data and model predictions.

using some set-theoretic technique for calculating reachable sets (Chachuat et al., 2015). Here a particular technical advantage can be exploited i.e., that the integration of in (7) can be done backwards in time from the final condition. As the batch processes exhibit inherently unstable dynamics, their backward integration is stable. Such a feature can readily be exploited by modern bounding approaches for parametric ordinary differential-algebraic equations.

The result (13) then in practice establishes a parametric solution to the real-time optimization problem. Its implementation can be performed in a robust fashion to determine the parameters of the optimal-control structure that lead to the best performance in the worst case. We can then solve

$$\min_{\substack{u_s(t,p)\in U^*(t), \forall t\in[t_1(p),t_2(p)] \\ t_i\in T_i,\ \forall i\in\{1,2,\mathrm{f}\}}} \max_{p\in P} \|\mathscr{J}(p)-\mathscr{J}(p_0)\|_2^2 \qquad \text{s.t. } (6),(7), \tag{15}$$

for a given $x(0)=x_0$ and $P$, where we propose to minimize variance of the objective under the worst-case realization of $p\in P$.

In order to reduce conservatism of a robust scheme, parameter estimation can be used for exploitation of data gathered along the process run. The employed parameter estimation scheme should take into account noise in measurements and, if applied recursively for each newly gathered measurement set, it should result in a sequence of the confidence intervals

$$P_k \subseteq P_{k-1} \subseteq \cdots \subseteq P_1 \subseteq P_0 \subseteq P. \tag{16}$$

The problem (15) can then be resolved with the initial state conditions $x(k)=x_k$ and with updated parameter bounds $P_k$ in shrinking-horizon fashion. Once the optimal value of the objective function of (15) reaches $\|\mathscr{J}(P)-\mathscr{J}(p_0)\|_2^2<\varepsilon$, the calculated control actions can be implemented, e.g., with a feedback scheme (Francois and Bonvin, 2013), until the terminal conditions are met. Note that due to the parametrization of the optimal-control policy, the re-estimation and re-optimization do not need to be run at every sampling time but on a much coarser time scale given by range of uncertainty in the sampling times $T_i$. Sophisticated strategies can then be used to evaluate the trade-off between real-time feasibility and performance.

## 4. Case study

We consider a case study of time-optimal control of a batch diafiltration process from Paulen et al. (2012). The scheme of the plant is shown in Fig. 1. The goal is to process a solution with initial volume ($V_0$) that is fed into the feed tank at the start of the batch and that comprises two solutes of initial concentrations $c_{1,0}$ and $c_{2,0}$. At the end of the batch, the prescribed final concentrations

$c_{1,\mathrm{f}}$ and $c_{2,\mathrm{f}}$ must be met. The transmembrane pressure is controlled at a constant value. The temperature of the solution is maintained around a constant value using a heat exchanger. The manipulated variable $u(t)$ is the ratio between fresh water inflow into the tank and the permeate outflow $q_p$ that is given by

$$q_p = \gamma_1 \ln\left(\frac{\gamma_2}{c_1 c_2^{\gamma_3}}\right) = \gamma_1 \left(\ln(\gamma_2) - \ln(c_1) - \gamma_3 \ln(c_2)\right). \tag{17}$$

and is measured at intervals of one minute with the measurement noise that is determined experimentally and bounded by $\sigma = 0.5\mathrm{L/h}$. The model of the permeate flux can be reduced to another widely used *limiting flux model* if $\gamma_3 = 0$, so this example offers to study both parametric and non-parametric plant-model mismatch. The measurement of $q_p$ is used for inferring the values of the parameters $\gamma_1, \gamma_2, \gamma_3$. Note that this leads to linear parameter estimation problem with the regressor $c = (1, \ln(c_1), \ln(c_2))^T$ and parameters $\hat{p} = (\gamma_1 \ln(\gamma_2), \gamma_1, \gamma_1\gamma_3)^T$, from which the values of $\gamma_1, \gamma_2, \gamma_3$ follow directly. Concentrations of both components $c_1(t)$ and $c_2(t)$, where the first component is retained by the membrane and the second one can freely pass through, are measured as well and filtered prior to estimation.

The objective is to find a time-dependent input function $u(t)$, which guarantees the transition from the given initial $c_{1,0}, c_{2,0}$ to final $c_{1,\mathrm{f}}, c_{2,\mathrm{f}}$ concentrations in minimum time. This problem can be formulated as:

$$\mathscr{J}^* = \min_{u(t)\in[0,\infty)} \int_0^{t_\mathrm{f}} 1\,\mathrm{d}t, \tag{18a}$$

$$\text{s.t. } \dot{c}_1 = \frac{c_1^2 q_p}{c_{1,0} V_0}(1-u), \quad c_1(0) = c_{1,0}, \quad c_1(t_\mathrm{f}) = c_{1,\mathrm{f}}, \tag{18b}$$

$$\dot{c}_2 = -\frac{c_1 c_2 q_\mathrm{p}}{c_{1,0} V_0} u, \quad c_2(0) = c_{2,0}, \quad c_2(t_\mathrm{f}) = c_{2,\mathrm{f}}, \tag{18c}$$

$$q_p = \gamma_1 \left(\ln(\gamma_2) - \ln(c_1) - \gamma_3 \ln(c_2)\right). \tag{18d}$$

The parameters of the problem are $c_{1,0} = 50\,\mathrm{g/L}$, $c_{1,\mathrm{f}} = 110\,\mathrm{g/L}$, $c_{2,0} = 5.3\,\mathrm{g/L}$, $c_{2,\mathrm{f}} = 1\,\mathrm{g/L}$, $V_0 = 21\,\mathrm{L}$. The extremal values of $u(t)$ stand for a mode with no water addition, when $u(t) = 0$ and pure dilution, i.e., a certain amount of water is added at a single time instant, $u(t) = \infty$.

The preliminary run of the laboratory apparatus with $u(t) = 0$ for 0.75 h and $u(t) = 1$ for 0.65 h was used to gathered data which were subsequently used in set-membership estimation to determine the confidence intervals of parameters as $\gamma_1 = [1.86, 3.91]\,\mathrm{L/h}$, $\gamma_2 = [4.1163, 0.6589] \times 10^3\,\mathrm{g/L}$, $\gamma_3 = [-0.11, 0.17]$. The value of $\beta$ used for the estimation is 0.5. Particularly the value of lower bound of $\gamma_3$ points to a potentially strong structural plant-model mismatch. We note for completeness that the particular advantage of used the set-membership estimation is that the assumption $\gamma_3$, which one might like to use in this case, could be easily incorporated in the estimation.

The nominal (parametrized) optimal control of this process can be identified using Pontryagin's minimum principle (Pontryagin et al., 1962) as (6) where the singular control and the respective switching function can be found explicitly (Paulen et al., 2012) as

$$u_s(x(t), p) := \frac{1}{1+\gamma_3}, \qquad S(x(t), p) := \gamma_1 \left(\ln(\gamma_2) - \ln(c_1) - \gamma_3 \ln(c_2) - \gamma_3 - 1\right). \tag{19}$$

For the given nominal parameters of the problem, the optimal control sequence is $u^* = \{0, 0.9333, \infty\}$ with switching times $t_\mathrm{f} = 2.86\,\mathrm{h}$. This operation is taken as a base case for evaluation of the discussed control schemes.

It is clear that the real-time optimality of the operation is strongly influenced by accuracy of the parameter estimates, mostly $\gamma_2$ and $\gamma_3$ since $\gamma_1$ can be factored out from $S(\cdot)$. Preliminary numerical tests with optimal experiment design (OED) methodology (Gottu Mukkula and Paulen, 2017) showed that for the most accurate estimation of $\gamma_2$ the manipulated variable $u(t) = 0$ and, on the other hand, the best estimation accuracy of $\gamma_3$ is reached when $u(t) = 1$. This shows mutual benefit of the optimal control strategy $u^* = \{0, 0.9333, \infty\}$ and estimation of $\gamma_2$, and a potential conflict of accurate estimation of $\gamma_3$ and the optimal control policy. This can also be seen from (17) and (18c), where it is clear that when a controller applies $u(t) = 0$, the parameter $\gamma_3$ is unidentifiable as the concentration $c_2(t)$ remains constant. The OED studies also showed that the best time to measure the plant outputs is in the beginning of the operation. This stems from the absolute error of the measurement (see (9)) and from the that fact the measured permeate flux is highest in the beginning of the operation and drops dramatically with the increase of $c_1(t)$.

The real-time optimal operation using on-line adaptation of parameters reached the final time of operation 2.87 h, which is practically the same performance as the optimal operation, while its counterpart without parameter estimation reached the operation time 4.23 h, which clearly too conservative. This result show the significant benefits of the proposed scheme.

## 5. Conclusion

We have presented a methodology for dynamic real-time optimization of batch processes (with particular application to membrane systems) via parametrization of the optimal controller using Pontryagin's minimum principle. The employed parametrization greatly reduces the computational burden in order to guarantee feasibility of the operation. In order to address parametric plant-model mismatch issue, we have suggested a robust approach, which consisted in projection of the plant uncertainty into optimality conditions. This again greatly reduces computational burden. As the uncertainty in parameters can greatly affect the optimality of the batch, we have proposed an adaptive scheme that makes use parameter estimation and, as shown in the case study, can greatly assist in reducing conservativeness of the real-time scheme.

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