Integrated Two-Time-Scale Scheme for Real-time Optimisation of Batch Processes

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Abstract: This paper studies a problem of uncertainties in optimal process control of batch processes. We assume that several batches are processed and that run-to-run optimisation can be performed. We propose an integrated two-time scale that optimises between batches to meet terminal constraints and within batches to improve calculated optimal trajectory for model-mismatch. The results obtained from a batch reactor control indicate that the resulting scheme has better convergence properties than individual schemes dealing either with terminal constraints adaptation or with in-batch neighbouring-extremal (NE) control.

Keywords: dynamic optimisation, neighbouring-extremal control, optimal control, integrated control scheme

1. INTRODUCTION

Chemical processes are subject to large uncertainty during their operation. Common sources of uncertainty include measurement noise, inaccurate kinetic rate parameters, feed impurities, and fouling. This usually give rise to a lower production quality and quantity, and from the quality of the linearisations. This currently limits the application of explicit MPC to problems having no more than a few state variables as well as piece-wise linear dynamics.

This paper presents a two-time-scale approach, whereby a run-to-run adaptation strategy (Bonvin et al., 2006) is implemented at the slow time scale (outer loop) and is integrated with a (constrained) neighbouring-extremal (NE) controller (Bryson and Ho, 1975) that operates at the fast time scale (inner loop). More specifically, run-to-run adaptation of the terminal constraints (Marchetti et al., 2007) is considered for the outer loop. In its original form, this scheme proceeds by re-optimising the batch operation between each run and adapting the terminal constraints based on the mismatch between their predicted and measured values; but no adaptation is made within a run. In order to reject disturbances within each run and at the same time promote feasibility and optimality, a NE controller is here considered as the inner loop. The theory of NE control, which has been developed over the last 4-5 decades to avoid the costly re-optimisation of (fast) dynamic systems, is indeed well-suited for batch process control. The integration between the outer- and inner-loops occurs naturally since the NE controllers are recalculated after each run based on the solution to the outer-loop optimisation problem. The resulting integrated two-time-scale optimisation scheme thus offers promise to enhance performance and tractability.

The paper is organised as follows. Theoretical background on NE control and run-to-run optimisation is provided in Section 2. The proposed integrated two-times-scale optimisation scheme is described in Section 3 and applied in the case study of a semi-batch reactor example in Section 4. Finally, Section 5 concludes the paper.
2. THEORETICAL BACKGROUND

2.1 Problem Formulation

Throughout the paper, the following dynamic optimisation problem with control and terminal bound constraints is considered:

\[
\begin{align*}
\min J &= \phi(x(t_f)) + \int_0^{t_f} L(x(t), u(t))dt \\
\text{s.t.} & \quad \dot{x} = F(x(t), u(t)), \quad 0 \leq t \leq t_f \quad (1) \\
& \quad x(0) = x_0 \quad (2) \\
& \quad \psi(x(t_f), t_f) \leq \psi_{\text{ref}} \quad (3) \\
& \quad u^L \leq u(t) \leq u^U. \quad (5)
\end{align*}
\]

In (1)–(5), \(t \geq 0\) denotes the time variable, with \(t_f\) the final time; \(u \in \mathbb{R}^{n_u}\) the control vector; \(x \in \mathbb{R}^{n_x}\) the state vector, with initial value \(x_0\); \(J, \phi\) and \(L\) the scalar cost, terminal cost, and integral cost, respectively; and \(\psi\) the vector of \(n_\psi\) terminal constraints. All the functions in (1)–(5) are assumed to be continuously differentiable with respect to all their arguments.

2.2 Necessary Conditions for Optimality

Following Bryson and Ho (1975), the Hamiltonian function \(H\) is defined as follows:

\[
H(x, u, \lambda, \lambda^L, \lambda^U) = L(x, u) + F(x, u)^T \lambda^+ + F^L(u^L - u) + F^U(u - u^U), \quad (6)
\]

\(\lambda \in \mathbb{R}^{n_\lambda}\) denotes the so-called adjoint (or costate) vector which satisfies

\[
\dot{\lambda} = -H_x = -F^T \lambda - L_x, \quad 0 \leq t \leq t_f, \quad (8)
\]

with the terminal conditions given by

\[
\lambda(t_f) = [\phi_x + \nu^T \psi_x]_{t=t_f}, \quad (9)
\]

\(\lambda^L(t), \lambda^U(t) \in \mathbb{R}^{n_\lambda}\) are Lagrange multiplier vector functions satisfying

\[
\begin{align*}
\mu^L(u^L - u) &= 0; \quad \mu^L, \geq 0 \quad (10) \\
\mu^U(u - u^U) &= 0; \quad \mu^U, \geq 0, \quad 0 \leq t \leq t_f, \quad (11)
\end{align*}
\]

and \(\nu \in \mathbb{R}^{n_\nu}\) are Lagrange multipliers for the terminal constraints such that

\[
0 = \nu_k \forall k, \quad \nu_k \geq 0, \quad \text{for each } k = 1, \ldots, n_\psi. \quad (12)
\]

Provided that the optimal control problem is not abnormal, the first- and second-order necessary conditions for optimality (NCO) read:

\[
\begin{align*}
H_u &= L_u + F^T u \lambda - \mu^L - \mu^U = 0 \quad (13) \\
H_{uu} &\geq 0 \quad (14)
\end{align*}
\]

This latter determines the set of active terminal constraints at the optimum, which is denoted by the vector \(\gamma\) for a given variable denotes partial derivatives of that variable with respect to \(y\).

2.3 Neighbouring-extremal Control

Let’s assume that the optimal control trajectory \(u^*(t)\) for the optimisation problem (1)–(5) consists of a sequence of constrained and unconstrained arcs. The optimal solution then comprises \(x^*(t), \lambda^*(t), \lambda_{\nu}^*, \mu^L, \mu^U, 0 \leq t \leq t_f\). For the control sequence, it is also assumed that the uncertainty is sufficiently small for the perturbed optimal control to have the same sequence of constrained and unconstrained arcs as the nominal solution.

The constrained optimal control problem obtained with a small variation in the initial condition \(x(0) = x_0 + \delta x_0\) and in active terminal constraints \(\psi(x(t_f), t_f) = \delta \psi\) produces variations in optimal control vector \(\delta u(t)\), state vector \(\delta x(t)\), adjoint vector \(\delta \lambda(t)\) and Lagrange multiplier vector \(\delta \nu\) (for the active terminal constraints \(\psi\)). Along unconstrained arcs, these variations can be calculated from the linearisation of the first-order NCO (10)–(12) around the extremal path (Bryson and Ho, 1975):

\[
\begin{align*}
\delta \dot{x} &= \delta F_{xx} \delta x + \delta F_{ux} \delta u \\
\delta \lambda &= -H_{xx} \delta x - F_{xu}^T \delta \lambda - H_{ux}^* \delta u \\
0 &= H_{ux}^* \delta x + F_{xu}^T \delta \lambda + H_{xx}^* \delta u \\
\delta x(0) &= \delta x_0
\end{align*}
\]

with additional conditions:

\[
\begin{align*}
\delta \lambda(t_f) &= [(\delta \phi^T_{xx} + \delta \nu^T \delta \psi_{xx}] \delta x + [\delta \phi^T_{xu} + \delta \nu^T \delta \psi_{xu}]_t = t_f, \quad (19) \\
\delta \nu &= [\delta \phi^T_{xx} \delta x]_t = t_f. \quad (20)
\end{align*}
\]

A superscript * indicates that the corresponding quantity is evaluated along the extremal path \(u^*(t), 0 \leq t \leq t_f\), and corresponding states, adjoints and Lagrange multipliers.

Let us assume that the Hamiltonian function is regular, so that \(H_{xx}^*\) is invertible along \(0 \leq t \leq t_f\). The control variation \(\delta u(t)\) for these unconstrained arcs \(\mu^L = \mu^U = 0\) is then given from (17):

\[
\delta u(t) = -(H_{xx}^*)^{-1} [F_{xu}^T \delta \lambda(t) + H_{xx}^* \delta x(t)]. \quad (21)
\]

Overall, along constrained arcs, the control variation is equal to zero \(\delta u(t) = 0\). Then, \(\delta x(t)\) and \(\delta \lambda(t)\) satisfy the following multi-point boundary value problem (MPBVP):

\[
\begin{align*}
\begin{pmatrix}
\delta \dot{x}(t) \\
\delta \lambda(t)
\end{pmatrix} &= \Delta(t) \begin{pmatrix}
\delta x(t) \\
\delta \lambda(t)
\end{pmatrix}, \\
\delta x(0) &= \delta x_0, \quad \delta \lambda = [\delta \phi^T_{xx} \delta x]_{t = t_f}, \\
\delta \lambda(t_f) &= [(\delta \phi^T_{xx} + \delta \nu^T \delta \psi_{xx}] \delta x + [\delta \phi^T_{xu} + \delta \nu^T \delta \psi_{xu}]_{t=t_f}
\end{align*}
\]

where:

\[
\Delta(t) = \begin{pmatrix}
\alpha(t) - \beta(t) \\
-\gamma(t) - \alpha(t)^T
\end{pmatrix} \quad (22)
\]

and

\[
\begin{align*}
\alpha(t) &:= F_{xx}^* - F_{xx}^* (H_{xx}^*)^{-1} H_{xx}^* \quad (23) \\
\beta(t) &:= F_{uu}^* (H_{xx}^*)^{-1} F_{xu}^T \quad (24) \\
\gamma(t) &:= H_{xx}^* - H_{xx}^* (H_{xx}^*)^{-1} H_{xx}^*. \quad (25)
\end{align*}
\]

Clearly, at each switching point between an unconstrained and a constrained arcs, a continuity of control, state and adjoint profiles must be preserved. For example, at a switching point between a lower bound and an interior arc, the value of control on lower bound matches the value of control in the interior arc \(u^L = u^U\). Here, \(u^U\) represents the control obtained from solving the condition \(H_u = 0\).
In addition, state and adjoint trajectories are continuous at this point, too:
\[ x^*(t_{k+}) = x^*(t_{k-}) \]
\[ \lambda^*(t_{k+}) = \lambda^*(t_{k-}) \] (27)

Variations in switching times are difficult to determine and complicate the calculation of the NE control. To make this implementable, it is considered that the switching points are constant at their nominal times. The control values are then updated only between the fixed times. In practice, performance loss is negligible for small variations of switching times.

2.4 Numerical Computation of Neighbouring Feedback Control

The linear MPBVP (22) can be used to calculate the neighbouring-extremal control correction \( \delta u(t) \), \( 0 \leq t \leq t_f \), in either one of two situations:

i. The initial state and (active) terminal constraint variations \( \delta x_0 \) and \( \delta \psi \) are available at discrete time instants, in which case the discrete feedback control can be obtained by directly re-solving the MPBVP. This can be done via a shooting method as described in Pesch (1989);

ii. The variations \( \delta x_0 \) and \( \delta \psi \) are available continuously in time, in which case the backward sweep method (Bryson and Ho, 1975) can be used to derive an explicit feedback control law. This approach is closely explained by Bryson and Ho (1975).

In this paper, we consider the first approach.

2.5 Run-to-run Constraint Adaptation

The principle behind run-to-run optimisation is similar to MPC. But instead of adapting the initial conditions and moving the control horizon as is done in MPC, the adaptation is performed on the optimisation model (e.g., model parameters or constraint biases) before re-running the optimiser. In run-to-run constraint adaptation, more specifically, the terminal constraints (4) in the optimisation model are adapted after each run as (Marchetti et al., 2007):

\[ \psi(x(t_f), t_f) \leq \delta \psi, \] (28)

where \( \delta \psi \) stands for the terminal constraint bias. Such a bias may be directly updated as the difference between the available terminal constraint measurements, \( \psi_{\text{meas}} \), at the end of each run and the predicted constraint values. This simple strategy may however lead to excessive correction when operating far away from the optimum, and it may also exacerbate the sensitivity of the adaptation scheme to measurement noise. A better strategy consists of filtering the bias, e.g., with a first-order exponential filter:

\[ \delta \psi_{k+1} = [I - W] \delta \psi_k + W [\psi_{k\text{meas}} - \psi(x_k(t_f), t_f)] \],

(29)

with \( k \) the run index, and \( W \) a gain matrix—typically, a diagonal matrix.

The constrained dynamic optimisation problem uses the available nominal process model. It is solved between each run, using any numerical procedure, such as the sequential or the simultaneous approach of dynamic optimisation. The optimal control trajectory \( u^*_k(t) \), \( 0 \leq t \leq t_f \), is computed and applied to the plant during the \( k \)th run. The predicted optimal response is denoted by \( x^*_k(t) \). The discrepancy between the measured terminal constraint values \( \psi_{k\text{meas}} \) and the optimiser predictions \( \psi(x^*_k(t_f), t_f) \) is then used to adjust the constraint bias as described earlier, before re-running the optimiser for the next run.

Of course, optimal control trajectory calculated between runs is suboptimal as the real process is never known perfectly.

3. TWO-TIMES-SCALE OPTIMISATION SCHEME

Run-to-run constraint adaptation was shown to be a promising technology in Marchetti et al. (2007). This approach provides a natural framework for handling changes in active constraints in dynamic process systems and it is quite robust towards model mismatch and process disturbances. Moreover, its implementation is simple. Inherent limitations of this scheme, however, are that (i) it does not perform any control corrections during the runs, and (ii) it typically leads to suboptimal performance.

On the other hand, neighbouring-extremal control is able to correct small deviations around the nominal extremal path in order to deliver similar performance as with re-optimisation. Since no costly on-line re-optimisation is needed, this approach is especially suited for processes with fast dynamics. However, the performance of NE control typically decreases dramatically in the presence of large model mismatch and process disturbances, and it requires a full-state measurement. This leads to suboptimality or, worse, infeasibility when constraints are present or limited measurements are available.

Our proposal is to combine the advantages of these two approaches: Run-to-run constraint adaptation is applied at a slow time scale (outer loop) to handle large model mismatch and changes in active constraints, based on run-end measurements only. Further, NE control is applied at a fast time scale (inner loop) and uses measurement information available within each run, in order to enhance convergence speed and mitigate sub-optimality. It need to be stated that full-state measurement is required even in case of integrated scheme. The proposed integrated two-time-scale optimisation scheme is depicted in Figure 1.

The implementation procedure is as follows:

**Initialisation:**

(0) Initialise the constraint bias \( \delta \psi = 0 \), select a gain matrix \( W \) and set the run index to \( k = 1 \)

**Outer Loop:**

(1) Determine \( u^*_k \) by solving the optimal control problem (1)–(5), then obtain the corresponding states \( x^*_k \) and adjoints \( \lambda^*_k \), with the active terminal constraints \( \psi \) and Lagrange multipliers \( \mu^*_k \), and together with Lagrange multipliers for boundary constraints \( \mu^L \) and \( \mu^U \) that satisfy NCO (10)–(12).

(2) Design a NE controller around the extremal path \( u^*_k \), either by using the backward sweep approach (continuous measurements), or by applying the shooting method (discrete measurements).

(3) **Inner Loop:**

Implement the NE controller during the \( k \)th run in order to calculate the corrections \( \delta u_k(t) \) to \( u^*_k(t) \)
based on the available (continuous or discrete) process measurements.

(4) Update the constraint bias $\delta \psi_{k+1}$ as the filtered difference between the measured values of the terminal constraints and their predicted counterparts.

(5) Increment the run index $k \leftarrow k + 1$, and return to Step 1.

4. CASE STUDY

4.1 Semi-Batch reactor model

A semi-batch reactor example taken from Chen and Hwang (1990) is considered to illustrate the proposed integrated two-times-scale approach. The goal is to maximise the yield of ethanol using the feed rate $u(t)$ as the control variable, while keeping the liquid volume below some maximum threshold. Simple bound constraints are imposed on the feed rate. The mathematical formulation of this problem is:

$$\max \ J = c_E(t_f)V(t_f) - 0.1 \int_{t_0}^{t_f} u^2 dt$$  \hspace{1cm} (30)

subject to

$$\dot{c}_\text{MS}(t) = p_1(t)c_\text{MS}(t) - u(t) \left( \frac{c_\text{MS}(t)}{V(t)} \right)$$  \hspace{1cm} (31)

$$\dot{c}_S(t) = -10p_1(t)c_\text{MS}(t) + u(t) \left( \frac{150 - c_S(t)}{V(t)} \right)$$  \hspace{1cm} (32)

$$\dot{c}_E(t) = -p_2(t)c_\text{MS}(t) - u(t) \left( \frac{c_E(t)}{V(t)} \right)$$  \hspace{1cm} (33)

$$\dot{V}(t) = u(t)$$  \hspace{1cm} (34)

where:

$$p_1(t) = \left( \frac{0.408}{1 + \frac{t}{16}} \right) \left( \frac{c_S}{0.22 + c_S} \right)$$  \hspace{1cm} (35)

$$p_2(t) = \left( \frac{1}{1 + \frac{t}{16.5}} \right) \left( \frac{c_S}{0.44 + c_S} \right).$$  \hspace{1cm} (36)

The state values $c_\text{MS}(t)$, $c_S(t)$, $c_E(t)$ and $V(t)$ are the cell biomass, substrate, and ethanol concentrations [g/L], and the volume [L]. The final time is set to $t_f = 60$ h. The reactor container is initially fed by $V(0) = 10$ L of reaction mixture with biomass and substrate concentrations $c_\text{MS}(0) = 1$ g/L and $c_S(0) = 150$ g/L. No ethanol is initially present in the reaction mixture. The feed rate [L/h] is bounded as:

$$0 \leq u \leq 12 \frac{[L]}{[h]}.$$  \hspace{1cm} (37)

The liquid volume is limited by $V_{\text{max}} = 200$ L, so the terminal condition reads:

$$V(t_f) \leq V_{\text{max}} \frac{[L]}{[h]}.$$  \hspace{1cm} (38)

Note that the integral term $\int_{t_0}^{t_f} u^2 dt$ augments the original objective function in order to make the control problem non-singular. This way $\bar{H}_u$ depends on the control variable and Hamiltonian $H$ is regular.

4.2 Open-loop optimal control

Solving the optimisation problem (30)–(38), with the sequential method (Edgar and Himmelblau, 1988; Guntern et al., 1998), the piecewise constant control profile (see Figure 2) shows the presence of one interior arc and two boundary arcs. Further analysis of this solution indicates that optimal control consists of a lower bound, an interior arc and another short lower bound. As the problem is regular, the control action along interior arc can be explicitly determined from the necessary conditions of optimality. Note that along boundary arcs, the control action is determined by a lower bound hence the control variations are simply $\delta u = 0$. The switching times $t_1$ and $t_2$ between these arcs are not explicitly known and they need to be estimated, too. The switching times from piecewise constant control profile give good initial guess for these switching times. Overall, the optimal control solution is given as:

(1) $t \in (t_0, t_1)$, the control remains on its lower bound $u^*(t) = 0$

(2) $t \in (t_1, t_2)$, the control is given as a solution of a differential-algebraic system of equations:
The case study compares the performance of the two-time-scale integrated solution with a pure constraint adaptation control scheme and a pure neighbouring-extremal controller.

The integrated two-time-scale scheme is applied using a nominal model perturbed by varying the initial values and adding measurement noise. While the NE controller is designed using the nominal mathematical model, the simulations use measured outputs from the perturbed model. We consider full-state measurements and measured outputs are states with added white noise. We consider the following variations in initial conditions $\delta x = [0.17 -6 0.9 0.8]$. These variations are chosen to cause a performance loss and terminal constraint violation, when applying the open-loop control profile. Run-to-run constraint adaptation is initialised with a constraint bias of $\delta \nu = 0$ and considers a filter gain of $W = 0.2$. The filter parameters were chosen so as to achieve the terminal constraint as fast as possible while avoiding oscillations during the adaptation.

Figure 4 compares the evolution of the performance during the first 20 batches. The evolution of the terminal constraint is presented in the left plot. Observe that the pure NE controller does not violate the terminal constraint, but on the other hand this constraint is inactive in all batches. In contrast, pure constraint adaptation violates the terminal constraint in the most of the batches. In the last 5 batches, the method almost reaches the terminal constraint. Note that this approach seems to be more sensitive to measurement noise than other two. The integrated scheme remains in close proximity of terminal constraint for all batches. Due to the fact that control corrections are applied during each batch as well, this approach is able to correct the control profile with lower sensitivity to measurement noise. The middle plot of Figure 4 shows the evolution of terminal constraint bias. This bias varies a little for the integrated scheme, because the NE controller in the inner loop is able to recover a large portion of optimality loss. In contrast, constraint adaptation requires heavier bias adaptation since no correction is made during the batch. The right plot shows evolution of the performance index. The worst average case is for pure NE control. In contrast, the pure constraint adaptation exhibits the highest values. The cost function of the proposed integrated approach stays between them and is very close to the optimal solution for perturbed system.

The resulting control profile after adaptation within 20 batches is shown in right plot in Figure 5. The control still consists of the tree same arcs, but the switching times have changed compared to nominal solution displayed in Figure 2, as a result of the constrained adaptation. The corresponding measured output of liquid volume is presented in the left plot in Figure 5. It can be seen that the measured output of perturbed process is in good agreement with re-optimised solution.

5. CONCLUSIONS

In this paper, an integrated two-times-scale control scheme for batch processes has been proposed. It improves the performance of dynamic real-time optimisation applied to batch processes. The combination of two approaches, namely run-to-run adaptation and neighbouring-extremal control, allows to complement the benefits of each other, while mitigating some of their deficiencies. On the other hand, run-to-run adaptation allows to deal with large model mismatch and handles better terminal constraints. Advantages of the integrated scheme have been demonstrated on the case study for a semi-batch reactor. As part of future work, an extension of the current scheme to singular control problems is currently under investigation, as well as the ability to handle problems with state path constraints.
Fig. 4. Dotted lines with circles: constraint adaptation alone, dash-dotted lines with crosses: neighbouring extremal control alone, dashed lines: optimal solution for perturbed system, solid lines with diamonds: integrated two-time-scale scheme control. Left plot: evolution of the terminal constraint; Middle plot: evolution of the terminal constraint bias; Right plot: evolution of the performance index.

Fig. 5. Performance with perturbed initial conditions after 20 run of adaptation. Left plot: control trajectory; Right plot: state trajectory of liquid volume; Solid line: perturbed system with two-time-scale integrated scheme; Dashed line: optimal solution for perturbed system.

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