Integrating Iterative Learning Estimation with Optimal Control for Batch Productivity Enhancement

Anish Gupta, Ravindra D. Gudi

Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai-400076, India
(e-mail: anish.gupta@iitb.ac.in, ravigudi@iitb.ac.in)

Abstract: Optimal control has wide applications for the control of batch and semi-batch processes to develop an optimum control input policy by extremizing a performance measure. The deployment of optimal control relies heavily on the accuracy of the process models being used for computation of the optimal profile. Often, the process models do not replicate the plants due to various shortcomings such as assumptions made during model formulations, poor first principles knowledge and limited range of experimental data due to short process development cycles. Moreover, scale-up of the processes from lab to manufacturing scale renders the developed models obsolete. The estimated model parameters can significantly differ from their nominal values which calls for the development of a strategy that updates process models so as to achieve an improved and tight control of batch processes. In this paper, we propose a novel methodology based on iterative learning to gradually update models using on-line measurement data at the end of each successive batch run by minimizing the error between plant and model data. In the proposed methodology, we further integrate Iterative Learning Estimation (ILE) with optimal control to update the optimal control input profile with the advent of measurement after each successive batch run. An important aspect of this integration is to ensure that model updates between batch runs generate feasible optimal control trajectories. Simulations are performed for the temperature control of a batch reactor system to validate the proposed methodology.

Keywords: Iterative Learning, Batch Control, Optimal Control, Model-based Control, Optimization, Parameter Estimation

1. INTRODUCTION

Batch processes play a key role in a large number of industries focusing on high value products ranging from traditional polymerization to emerging pharmaceuticals, fine and specialty chemicals, and semi-conductor manufacturing. In spite of such large applications of batch processes, the development of control theory has lagged continuous processes owing to the peculiar complexities of the batch processes. One of the important characteristics of the batch processes is their dynamic operation where the process variable relationships change over the complete batch run. The process dynamics can be highly non-linear with sharp discontinuities owing to the presence of multiple phases/stages during the operation of batch processes. Secondly, most batch processes correspond to a fixed duration of operation which implies that any control strategy needs to be implemented in a shrinking time horizon which is a daunting task due to reduced controllability (Soni and Parker, 2004). These characteristics make the performance control of the batch processes difficult and challenging. Grade transitions between continuous processes such as polymerization have similar characteristics of batch processes and pose a similar set of problems related to optimal control.

Given the deployment of batch processes for the production of high value products, there has been a growing concern in the industry regarding the final product quality which drives profit margins in the high end industries. Process optimization is deployed as a technique to reduce production costs, improve product quality, reduce product variability and for scale up from lab to industrial scale. Therefore, optimal control has been widely used to obtain an input policy which will maximize or minimize a performance measure. Optimal control algorithms rely heavily on the accuracy of the process models and the optimum input trajectories have been found to be highly sensitive to the model uncertainties and disturbances. While the objective function for a typical control problem has to be extremized which critically depend on model fidelity, an often ignored aspect of the optimal control problem is the need to honor constraints on the optimal control trajectory. Since these trajectories are also inferred at optimum values based on the process models, the ability to honor these constraints in a batch run is critically dependent on the model fidelity.

Development of highly accurate models is a formidable task owing to the complexities of the batch processes and availability of frugal data. Precise estimation of model parameters is an arduous task, and parameters estimated
at lab scale generally fail to replicate the output performance at the industrial scale. Computation of optimal input profiles is also affected by uncertainty in the initial conditions, variations across batch and inaccurate measurements. These result in the sub-optimal output profiles, thus making it difficult to achieve the performance objective or a track reference output trajectory. Therefore, it is important to modify the optimal control profile to account for uncertainty.

However, there are many processes where optimal control profiles are obtained offline based on the process models. But, as discussed above, it is imperative to perform an online computation and update of optimal control by taking advantage of the measurement data. In the past, many approaches have been suggested for the on-line update of optimal control profile so as to handle uncertainty. These have been mainly categorized into two approaches, viz. Robust and Measurement based optimization. Robust optimization is performed when measurement data is absent, by considering several possible values of the parameters while the Measurement based optimization takes the advantage of measurements to adjust the optimal profile accounting for parameter uncertainties and disturbances (Srinivasan et al., 2003a). In this paper, an on-line update of the optimal input control policy is attempted using iterative learning of the batch process data refining the model using measurements from each successive batch run.

Iterative learning has been widely established as an emerging technique for the control of repetitive processes. Batch processes fall into this regime and iterative learning has been used to control the input batch trajectories to ensure that the output follows a reference output trajectory. Iterative Learning Control (ILC) algorithm is based on inter-batch learning concept by minimizing the error between the reference and the plant output trajectory. The input trajectory is updated, using the error information, after each batch run so as to achieve convergence. A detailed review of ILC has been performed by Lee and Lee (2007) and Wang et al. (2009). However, one of the limitations of ILC is that the optimal reference output trajectories are computed using the process models, and thus relies heavily on the fidelity of the process models. As already discussed, process models suffer from many shortcomings and hence, there exists a strong reason to refine the reference trajectories so as to enhance the overall performance of the system.

For control, ILC algorithm updates an initially chosen input policy which reduces the error between the reference output trajectory and measured output trajectory. The specification of the reference trajectory could sometimes pose limitations on the tracking ability of ILC. For e.g., various path or input constraints could make it difficult to achieve perfect tracking of reference trajectories. On the other hand, the reference trajectory specified based on an initial approximate model could lead to infeasibility and/or sub-optimal objective function value when the resultant control policy is applied on plant due to model-plant mismatch. It is therefore appropriate to explore the potential of refining the model between batch runs with a view to eventually push the batch closer to optimal operation.

In this paper, we exploit the dual nature of estimation and control and propose Iterative Learning Estimation (ILE) methodology to recursively update the model parameters and reference trajectories so as to achieve feasible and optimal batch operation. While the ILC approach has been proven for the fixed reference trajectory, in this work we have used the traditional time optimal control methods along with Iterative Learning Estimation to progressively improve the batch operation.

The rest of the paper is organized in the following manner. In Section 2, the theory of ILE methodology and its dual relationship with ILC is presented. Section 3 puts forth the aspects of integration of ILE and optimal control methods used to update model parameters and establish optimal control input trajectory. Section 4 discusses about the case study performed for the optimal temperature control of series reactions in the batch reactor. Results which validate the proposed integrated approach are presented in Section 5 followed by conclusions.

2. ITERATIVE LEARNING METHODOLOGY

We begin this section with a brief discussion of the established Iterative Learning Control (ILC) approach. We then proceed to present the dual relationship between Iterative Learning Estimation (ILE) and ILC and develop the formulation of Iterative Learning Estimation (ILE).

2.1 Duality of ILE and ILC

We briefly present the ILC methodology first. Consider a general representation of a system as:

\[
\begin{align*}
\dot{x} &= f(x, u, \theta) \\
y &= g(x, u, \theta)
\end{align*}
\]  

(1)  

(2)

where \( x_{n \times 1}, u_{q \times 1}, \theta_{q \times 1} \) and \( y_{r \times 1} \) represents the vector of state variables, input variables, parameter values and output variables respectively.

Consider a batch run of \( N \) sampling instants which can be represented as:

\[
Y^k = G_p U^k
\]  

(3)

where \( G_p \) is the matrix \((N_p \times N_r)\) defining the input-output relationship, \( Y^k \) is the system output vector of size \( N_r \times 1 \) and \( U^k \) is input process vector of size \( N_p \times 1 \). These vectors can be represented as follows:

\[
Y^k = [y^k(1) \ y^k(2) \cdots y^k(N)]^T
\]  

(4)

\[
U^k = [u^k(0) \ u^k(1) \cdots u^k(N-1)]^T
\]  

(5)

Here, \( k \) represents the batch index.

The reference output trajectory can be represented as follows:

\[
Y^{ref} = [y_r(1) \ y_r(2) \cdots y_r(N)]^T
\]  

(6)

For the \( k^{th} \) batch run, the error between the reference output trajectory and plant output is defined as follows:

\[
||e^k|| = ||Y^{ref} - Y^k||
\]  

(7)

The control errors are then minimized to update the input trajectory:

\[
\min_{u(k)} ||e^k||
\]  

(8)
The objective of the iterative learning control is to update input trajectory $U^k$ such that
\[ \|e^k\| \rightarrow 0 \text{ as } k \rightarrow \infty \] (9)
The input trajectory is updated on a run-to-run basis in the following manner:
\[ U^k = U^{k-1} + He^{k-1} \] (10)
where $H$ is the learning filter matrix (Lee and Lee, 2007).

ILE algorithms gradually improves the input profile by learning from control errors in each batch run. Taking advantage of iterative learning for batch processes, we have propose an integrated ILE methodology which performs an online update of the parameters by using prediction error information from each batch run.

The problem formulation for ILE can be represented as follows. Let $Y^k$ be the measured output profile and $U^k$ be the optimal control input profile as represented in eqn(4) and eqn(5) respectively. The predicted output profile using the process models can be represented as follows:
\[ \hat{Y}^k = \hat{y}^k(1) \hat{y}^k(2) \cdots \hat{y}^k(N)^T \] (11)
We define the prediction error at the end of the $k^{th}$ batch run, $\|e^k_p\|$, as
\[ \|e^k_p\| = \|Y^k - \hat{Y}^k\| \] (12)
Let $\hat{\theta}^k (M \times 1)$ be a vector of model parameters obtained after $k^{th}$ batch run:
\[ \hat{\theta}^k = [\hat{\theta}^k_1 \hat{\theta}^k_2 \cdots \hat{\theta}^k_M]^T \] (13)
In each batch run the error $\|e^k_p\|$ is minimized in the space of parameters $(\hat{\theta}^k_{M+1})$ to obtain an updated set of the parameters $(\hat{\theta}^k_{M+1})$. The updated input trajectory $(U^{k+1})$ for the $(k+1)^{th}$ batch is computed using model based on the updated parameters $(\hat{\theta}^k)$ at the end of $k^{th}$ batch run.
\[ \min_{\hat{\theta}} \|e^k_p\| \] (14)
\[ \theta^k = \theta^{k-1} + P_{\theta}e^k_p \] (15)

3. INTEGRATING ILE AND ILC

The integration of ILE and ILC at the end of each batch run needs to recognize and honor several practical constraints on batch operation. Firstly, in ILC the corrections of control trajectories between batches need to ensure feasibility of the new profile relative to the earlier one. The corrections to earlier control profile need to be conservative and as such must also respect path and end point constraints. Given that the model plant model mismatch could be quite significant, the corrections in the input profiles need to be regulated by explicitly posing constraints on the profiles in the optimal control problem.

3.1 Optimal Control: General Formulation

We first briefly explain the mathematical formulation of the optimal control. An additional constraint on the change in input variables (as in eqn. 19) is incorporated in the optimal control formulation (Srinivasan et al., 2003b) to reflect its integration with ILE as follows:
\[ \min_{t_f,u(t)} J(t_f,x(t_f)) \] (16)
such that
\[ \dot{x} = F(x,u); \ x(0) = x_0 \] (17)
\[ S(x,u) \leq 0; \ T(x(t_f)) \leq 0 \] (18)
\[ \|u^k - u^{k-1}\| \leq \Delta u^{max} \] (19)
where $J$ is the scalar performance measure to be minimized, $x$ represents the $n \times 1$ vector of state variables with initial conditions $x_0$, $u$ is the $m$-dimensional input vector, $S$ is a $q$-dimensional vector of path constraints which include state constraints and bounds on the input vector, $T$ represents the $r$-dimensional vector of endpoint constraints and $t_f$ is the final time which can be either fixed or free. The inequality path constraints can be handled by transforming them into end-point constraints (Vassiliadis et al., 1994).

Figure 1 represents the integration of ILE and optimal control used in this paper. It is important to note that in the proposed approach ILC is replaced by optimal control algorithm and ILE task is performed using nonlinear constrained optimization. For the $k^{th}$ batch run, the optimal input control profile is established based on the model parameters obtained at the end of previous run by minimizing the prediction error.

3.2 ILE with constraints on parameter change

In a similar manner as in Section 3.1, the updates on the parameters also need to be regulated. Since the evaluated optimal control trajectory calculated on the updated model needs to be feasible, explicit constraints on the incremental parameter updates need to be imposed. The ILE problem formulation is thus posed as follows:
\[ \min_{\theta} \|e^k_p\| \] (20)
with constraints
\[ \|\theta^k - \theta^{k-1}\| \leq \Delta \theta^{max} \] (21)

4. CASE STUDY

The proposed integrated Iterative Learning Methodology (ILE) is applied to the temperature control of series reactions occurring in batch reactor. We begin with a model description of the batch process in this section.

4.1 Model Description

The series reactions occurring in the batch reactor can be represented in the following form:
Here, both the reactions follow first order kinetics. The material balance equations for the species $A(x_1)$ and $B(x_2)$ can be written as follows (Ramirez, 1994):

\[
\frac{dx_1}{dt} = f_1, \quad f_1 = -k_1 x_1
\]
\[
\frac{dx_2}{dt} = f_2, \quad f_2 = k_1 x_1 - k_2 x_2
\]
\[
\frac{dx_3}{dt} = f_3, \quad f_3 = k_2 x_2
\]

where

\[
k_1 = k_{10} e^{-\frac{x_1}{T}}
\]
\[
k_2 = k_{20} e^{-\frac{x_2}{T}}
\]

$x_1(t_0) = 0.53 \text{mol/L}; \quad x_2(t_0) = 0.43 \text{mol/L}$

\[(22)\]
\[(23)\]
\[(24)\]
\[(25)\]
\[(26)\]
\[(27)\]

The parameter values which are assumed to have uncertainty are $E_1$ and $E_2$. Their nominal values are as follows:

$E_1 = 18000 \text{ cal/mole}$

$E_2 = 30000 \text{ cal/mole}$

\[(28)\]
\[(29)\]

### 4.2 Optimal Control Formulation

As is well known, optimal control problem performs a dynamic optimization to generate an input profile which extremizes a performance measure in the space of the control variables. The optimal control considered here has a specified final time and initial state values. For the problem above, the optimum temperature profile is obtained so as to maximize the yield of the species $B(x_2)$ at the final time which is chosen to be 8 min.

\[
\max_{T(t)} \int_{t_0}^{t_f} f_2 dt
\]

\[(30)\]

\[u = T(t)\]

\[(31)\]

The control vector iteration approach using the modified gradient method (Ray, 1981) is used to compute the optimal control input profile.

### 4.3 Parameter Uncertainty

For the case study, we consider that the parameter values ($E_1$ and $E_2$) are assumed to have an offset of 8.33% and 6.67% respectively. Thus, the initial values of the parameters $E_1$ and $E_2$ are as follows:

$\hat{E}_1 = 16500 \text{ cal/mole}$

$\hat{E}_2 = 28000 \text{ cal/mole}$

\[(32)\]

A suboptimal input control profile would be obtained with these parameter values and our objective is to minimize the error ($\|e_p\|$) in the space of $E_1$ and $E_2$ to get an updated value of the parameters.

\[\|e_p\| = \|y - \hat{y}\|\]

\[(33)\]

where $y$ and $\hat{y}$ corresponds to plant and model output respectively.

The state variables ($x_1$ and $x_2$) are measured and a 2% measurement noise is assumed for the case study.

\[y = [x_1 \ x_2 \ x_3]^T; \quad \hat{y} = [\hat{x}_1 \ \hat{x}_2 \ \hat{x}_3]^T\]

\[(34)\]

Here, $x_1, x_2$ and $x_3$ corresponds to the measured reactant concentrations, and $\hat{x}_1, \hat{x}_2$ and $\hat{x}_3$ represents the concentrations of reactants $A, B$ and $C$ estimated using the process model.

### 4.4 Constraints on parameter change

Integrated ILE and optimal control approach is also implemented on the batch reactor system in the presence of constraints on the change in the parameter values ($E_1$ and $E_2$) in between batch runs. For the present case study, we have assumed that both the parameters can differ by 600 cal/mol in successive batch runs as follows:

$\hat{E}_1 - \hat{E}_{1k-1} \leq 600$ \hfill (35)

$\hat{E}_2 - \hat{E}_{2k-1} \leq 600$ \hfill (36)

Thus, the prediction error ($\|e_p\|$) is minimized in the ILE step so that the above constraints on the parameters are satisfied.

### 4.5 Optimization

While earlier approaches in Iterative Learning use a sequential update after every batch run that generates a correction to the policy used in the earlier batch run, in this paper an explicit optimization has been used to minimize the prediction errors. The optimization has been performed in TOMLAB operating in MATLAB environment 7.4 using the CONOPT solver.

### 5. RESULTS AND DISCUSSIONS

The integrated approach of ILE and optimal control has been formulated in the Section 2. In this section, we demonstrate the effectiveness of this integrated approach by implementing it for the temperature control of series reactions in a batch reactor.
number of iterations

FIG. 7. Change in the optimal profile with constraints on parameter change

The parameter values ($E_1$ and $E_2$) converge within 0.5% of the nominal values after both the parameter values are converged. The final converged values of the parameters are as follows:

$$E_{1}^{\text{conv}} = 18015.84 \text{ cal/mole}$$  \hspace{1cm} (37)

$$E_2^{\text{conv}} = 30150.72 \text{ cal/mole}$$  \hspace{1cm} (38)

Figure 5 shows the change in the output reactant concentration profile ($C_b$). It can be seen that the measured output concentration profile matches well with the optimal concentration profiles after 5 iterations which depicts the success of the integrated ILE and optimal control approach. After the parameters are converged, the measured value of the objective function ($J$) is 0.691 mol/l which is in close agreement with the objective function ($J = 0.679$ mol/l) obtained using the nominal parameter values.
The simulations have also been performed on the temperature control of series reactions in the batch reactors with a constraint on the maximum modification possible for the parameter values ($E_1$ and $E_2$) in between the batch runs. Hence, the integrated ILE and optimal control, approach has been validated in the presence of constraints on the modifications of parameters. Figure 6 depicts the change in parameter values in between batch runs and convergence for the both the parameters is obtained after 9 batch runs. The converged parameter values for this case are:

\[ \hat{E}_{\text{conv}}^1 = 18011.18 \text{ cal/mol} \]
\[ \hat{E}_{\text{conv}}^2 = 30105.97 \text{ cal/mol} \]

Figure 8 shows the change in the reactant concentration profiles ($C_b$) for the case where parameter constraints are imposed in ILE step at end of each batch run. The measured objective function value ($J$) obtained after the parameters are converged is 0.691 mol/l which is in close agreement to the value of the objective function obtained using the nominal values of the parameters. ($J = 0.679$ mol/l). Figure 7 depicts the refinement in the optimal control input profile when the constraints on the parameters have been imposed. This represents the success of the ILE in a scenario when the constraints on the change in the parameter values are imposed thus updating the optimal profile such that it is feasible to implement in between the batch runs. This is of utmost importance since large variations in between the batch (as in Figure 5) would not be acceptable from a batch operation perspective.

Remark: It may appear that the proposed iterative and integrated ILE approach of model refinement and control is similar to the run-to-run optimization as proposed in the literature (Srinivasan et al., 2001). It is important to point out a fundamental difference between the two approaches. In the run-to-run optimization, measurements are only available at the end of the batch run and thus the model refinement is based on the prediction error at the final time. On the other hand, in ILE, the measurements are available over the complete batch horizon and thus the prediction error is evaluated and minimized using all the available measurements. Thus using only the single point measurements at final time may slow down the convergence or may also lead to a sub-optimal parameter estimate. ILE attempts to overcome this problem by using the prediction errors over the entire batch duration and minimizing it which ensures the parameter convergence based on the entire optimal trajectory.

6. CONCLUSIONS

In this paper, we have considered an integrated approach of Iterative Learning Estimation (ILE) and optimal control to enhance the batch productivity. We have implemented it on a case study to perform a temperature control of series reaction in a batch reactor. The integrated approach is proposed to update the model used for computation of the optimal input profile by taking advantage of measurement obtained at the end of successive batch runs. The results obtained validate this approach. The model parameters converge to their nominal values and the measured reactant concentration profile matches the optimal output concentration profiles. This methodology highlights the need for updating the model parameters to establish optimal control profiles so as to enhance the final batch productivity. Developing a framework for integrating ILE and ILC so as to include constraints on input and output as well as an analysis of the joint convergence of the integrated approach will be a subject matter of a future study.

REFERENCES


