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Iterative Learning Estimation with Lean Measurements

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Abstract: Precise estimation of parameters has always been an arduous task and parameters estimated at lab scale fail to replicate the output performance at the industrial scale. Also, process models are formulated after a series of assumptions and hence they fail to replicate the plant. Hence, there is a need to refine the parameters using the real time data. Iterative Learning Estimation (ILE) has been proposed in the previous works which updates the parameters using the real time plant output data by minimizing the prediction error. But the real time data is frugal and all the states of the system may not be observable. Thus, we need to improve the established ILE methodology to refine the parameter estimates based on the states which are measurable. In this paper, we develop the ILE methodology for the cases where all the states are not measurable. The effectiveness of ILE has been demonstrated on two case studies; first being the adaptive state estimation of batch reactor and other being the refinement of kinetic parameters of a continuous auto-thermal reformer model. Simulations have been performed to establish the convergence of ILE for both the cases.

Keywords: Iterative Learning, Optimization, Parameter Estimation, Batch Control, Auto-thermal reformer Control

1. INTRODUCTION

A major and common objective felt in the chemical process industry is to manufacture the final product at the lowest cost as well as meet specification requirements. Optimization and process control have been widely used to reduce product variability, improve product quality and reduce production costs. But many of these techniques rely heavily on the accuracy of the process models and thus the product variability is a major function of the model fidelity. Precise model formulations which replicate the plant are difficult to obtain even with considerable effort owing to many shortcomings such as poor first principles knowledge, assumptions made during model formulation and paucity of data. Also, the process models developed at lab scale may have limitations when deployed at commercial scale which leads to sub-optimal control of the processes. For example, the kinetic parameter estimates obtained at the lab scale may not be able to precisely characterize the processes at commercial scale owing to deviations in mixing effects, dead volumes etc. Moreover, the presence of uncertainties and disturbances are not captured in the process models. Hence, there is a need to use real-time data to update the process models so as to achieve better and tighter control of the chemical processes.

Parameter estimation in dynamic models is a well-researched area and most methods employ numerical optimization to determine the parameter values that maximize the predictive ability of the model. However, these methods typically use a batch of data based on which the parameters are estimated. While online recursive parameter estimation approaches have been eminently proposed, these are based on frequent and regular measurement updates. For applications where such measurements are relatively frugal and irregular, iterative learning estimation (ILE) (Konde *et al.*, 2011), posed as a dual of the well-established iterative learning control (ILC), has been shown to be facile. ILE based approaches perform the task of parameter update at the end of an epoch, for e.g. such as end of the batch run, or at the end of a time window of data. Iterative Learning Estimation (ILE) has been extended in previous works by Gupta and Gudi (2015) wherein they integrated the ILE approach with the Iterative Learning Control (ILC) (Lee and Lee, 2007) approach to generate a sequence of batch runs of increasing productivity (due to the ILE parameter update).

In the previous work, ILE has been implemented for the cases where complete measurements of the primary data was assumed to be available. However, real time data is frugal and direct states of interest may not be measurable or are measured at infrequent or irregular times which may pose limitations to this approach. In this paper, we seek to implement ILE for two case studies viz. temperature control of batch reactor and auto-thermal methane reformer where there are limitations to the availability of on-line measurements. Batch processes are finite (but variable) duration processes, with quality measurements

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typically made at the end of the batch. Other secondary measurements could be available during the batch evolution; however some of the key variables are measured either very infrequently or at the end of the batch. Hence an implementation of ILE needs to accommodate this frugal measurement scenario in an overall scheme to update the model parameters and also plan for improved control policies based on the updated parameters. On the other hand, auto-thermal methane reformers form an important part of the fuel cells which witnessed rapid growth in past few years since they offer a promising pathway for the hydrogen operated systems owing to being clean, flexible and efficient. The dynamics of fuel cell and reformer is complex but the response of the fuel cells is an important aspect in many of its applications. There have been many models which have been proposed to capture its dynamics but owing to the complexities, none of the models are able to successfully capture all the nuances of its dynamics. For the reformer as well, data for secondary measurements such as temperature profiles pertaining to different load conditions could be available; however the key variables such as concentrations of H2 and other species are not available. Hence, there is a need to develop methodology to refine the reformer model based on the available measurement data, so that tighter and improved control and optimization can be deployed leading to enhanced performance.

This paper is organized as follows: The ILE methodology and its mathematical formulation are briefly discussed in the next section. In Section 3, we present two case studies where ILE methodology is implemented with frugal real time data. Results and discussions are included in this section which validates the proposed methodology followed by conclusions.

2. MATHEMATICAL FORMULATION

In this section, we briefly describe the formulation of Iterative Learning Estimation (ILE) methodology which performs an online update of the parameters using the prediction error. A more complete formulation of the ILE as a dual of the ILC has been presented earlier in Konde *et al.* (2011) and Gupta and Gudi (2015), and we restrict to only the necessary steps here.

2.1 ILE Formulation

The formulation for ILE methodology can be represented as follows. Let $Y^k(N \times 1)$ be the measured output profile, $\hat{Y}^k(N \times 1)$ be the predicted output profile and $\hat{\theta}^k(M \times 1)$ be the vector of model parameters as follows:

$$Y^k = \begin{bmatrix} y^k(1) & y^k(2) & \cdots & y^k(N) \end{bmatrix}^T \tag{1}$$

$$\hat{Y}^k = \begin{bmatrix} \hat{y}^k(1) & \hat{y}^k(2) & \cdots & \hat{y}^k(N) \end{bmatrix}^T \tag{2}$$

$$\hat{\theta}^k = \begin{bmatrix} \hat{\theta}_1^k & \hat{\theta}_2^k & \cdots & \hat{\theta}_M^k \end{bmatrix}^T \tag{3}$$

At the end of each run, the prediction error is defined as follows:

$$\|e_p^k\| = \|Y^k - \hat{Y}^k\| \tag{4}$$

At the end of each run, the prediction error $\|e_p^k\|$ is minimized in the space of parameters $\hat{\theta}^k$ to obtain an updated set of parameters $\hat{\theta}^{k+1}$ which is used to predict the output profile at the end of next run.

$$\min_{\theta} \|e_p^k\| \tag{5}$$

$$\theta^k = \theta^{k-1} + P e_p^k \tag{6}$$

where P can be a learning matrix (Gupta and Gudi (2015)) which can be tuned appropriately. In comparison with well established estimation techniques such as least squares and their recursive variants, the applicability of ILE is particularly suited for the repetitive processes that are poorly modeled. Also, for continuous processes that are required to operate under grade transitions, the ILE approach could help to understand the transition dynamics.

3. CASE STUDIES

Two case studies are presented in this section where we have implemented and validated ILE approach for the case of lean measurements. The first case study is the temperature control of series reaction occurring in a batch reactor and other one is the dynamic response of auto-thermal methane reformer.

3.1 Case Study: Temperature control of batch reactor

The Iterative Learning Estimation (ILE) methodology has been applied to the temperature control of series reactions occurring in the batch reactor where we assume a more realistic measurement scenario; it is assumed that only one state is measured. In this section, we begin with the model description of the process followed by the results obtained after ILE is applied to the system.

Model Description

The series reactions occurring in the batch reactor can be represented in the following form:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

Here, both the reactions follow first order kinetics. The material balance equations for the species $A(x_1)$, $B(x_2)$ and $C(x_3)$ can be written as follows (Ramirez, 1994):

$$\frac{dx_1}{dt} = f_1, \quad f_1 = -k_1 x_1 \tag{7}$$

$$\frac{dx_2}{dt} = f_2, \quad f_2 = k_1 x_1 - k_2 x_2 \tag{8}$$

$$\frac{dx_3}{dt} = f_3, \quad f_3 = k_2 x_2 \tag{9}$$

where

$$k_1 = k_{10} e^{-\frac{E_1}{RT}}; \quad k_2 = k_{20} e^{-\frac{E_2}{RT}} \tag{10}$$

$$x_1(t_0) = 0.53\text{mol/l}; \quad x_2(t_0) = 0.43\text{mol/l} \tag{11}$$

where x_1, x_2 and x_3 are the concentration (mol/L) of species A, B and C respectively. The values of the pre-exponential factors viz. k_{10} and k_{20} are assumed to be known with complete certainty as:

$$k_{10} = 0.535 \times 10^{11} \text{ min}^{-1}$$

$$k_{20} = 0.461 \times 10^{18} \text{ min}^{-1} \tag{12}$$