Product quality estimation using multi-rate sampled data

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Abstract

This paper investigates different approaches to develop soft sensors from multi-rate sampled data. The data lifting approach consists of two steps, identifying a model with a slow/lifted sampling period and extracting a fast model. Approaches based on direct extraction and linear regression are briefly reviewed, followed by reformulating the task as an unconstrained optimization problem. An illustrative example concerning design of a free lime soft sensor for cement kiln systems is presented. Using data collected from a simulation system based on first principles models, a weighted partial least squares (WPLS) approach for soft sensor development is compared with data lifting techniques. Case studies reveal the superior performance of the WPLS approach. In addition the product quality for cement kiln systems can be estimated reasonably well, demonstrating the potential to be used for effective quality control.

Keywords: soft sensor, multi-rate data, regression analysis, cement kiln process

1. Introduction

In most chemical processes, quality measurements have slower sampling rate than other process variables. A major obstacle for effective quality control is the lack of frequent or real-time information, due to the time delay associated with lab analysis or slowly processed quality measurements of online analyzers. Therefore, soft sensors that are able to provide a reliable real-time prediction can be essential for effective product quality control. This paper presents a systematic framework to develop soft sensors from multi-rate sampled data.

Plant log systems usually provide the operating data logged with different sampling frequency: high frequency process measurements and low frequency quality measurements. Therefore it is impossible to directly identify a process quality model at the fast sampling rate using the original data. Lu and Fisher (1989) proposed a least squares output estimation approach for multi-rate datasets. A transformation is performed on the original system by multiplying a polynomial such that the inter-sample value of the output is no longer required for identification. Lifting technique is a widely used approach to handle data collected at multiple sampling rates (Wang *et al.*, 2004; Srinivasaro *et al.*, 2005). The data lifting technique transforms multi-rate sampled data into a uniform sampling rate dataset at the lower frequency by stacking the variables with a smaller sampling interval. A model in the lifted time domain is first identified, from which a model of fast sampling domain is extracted. A weighted partial least squares (WPLS) approach has been applied to develop quality estimators from multi-rate data (Lin *et al.*, 2005). A weighting value of 1 is applied to process measurements that correspond to the time instant when a new quality measurement is obtained, 0 to others. A soft sensor with fast sampling period is then directly derived using available process measurements.

For a data lifting technique, the key issue is to reliably extract the fast sampling model. When the ratio of slow/fast sampling period is large, this approach might suffer from high numerical sensitivity or even numerical infeasibility. In addition, the direct extraction of the fast system might also lead to an infeasible system, i.e., with imaginary elements in the system matrix. This paper reformulates the fast model extraction within an optimization framework, in order to minimize the possibility of obtaining infeasible systems. The purpose of this paper is to investigate development of a systematic procedure for multi-rate soft sensor and to illustrate the application on cement kilns, which feature an offline quality measurement. A comparison between an estimator obtained with the lifting technique and WPLS approach is also performed.

Section 2 briefly reviews a data lifting technique and techniques to extract fast models, followed by the proposed optimization framework. Section 3 presents the systematic multi-rate soft sensor development procedure. Case studies for multi-rate soft sensors for cement kiln systems are illustrated in section 4, followed by discussion and conclusions.

2. Lifting technique for multi-rate system

Process measurements $\{u(l)\}$ are sampled with the period T_s, while the quality measurements, $\{y(k)\}$ have a sampling period $p \cdot T_s$. Data lifting technique (Khargonekar et al., 1985) reorganize the original data set by stacking the fast sampled variables. The lifting operator is defined as:

$$\tilde{\mathbf{u}} = L_p \mathbf{u} = \left\{ \underbrace{\begin{bmatrix} u(1) \\ u(2) \\ \vdots \\ u(p) \end{bmatrix}}_{\tilde{\mathbf{u}}(1)}, \underbrace{\begin{bmatrix} u(p+1) \\ u(p+2) \\ \vdots \\ u(2*p) \end{bmatrix}}_{\tilde{\mathbf{u}}(2)}, \cdots, \underbrace{\begin{bmatrix} u(k*p+1) \\ u(k*p+2) \\ \vdots \\ u((k+1)*p) \end{bmatrix}}_{\tilde{\mathbf{u}}(k)}, \cdots \right\} \tag{1}$$

where $p > 1$ is an integer. Therefore, the lifted input sequence $\tilde{\mathbf{u}}$ has the same period as the slowly sampled output. A process model with a slower sampling period, $p \cdot T_s$, can be identified straightforwardly. In order to obtain the inter-sample value of the slow-sampled process measurements, $\{\hat{y}(k)\}$, a fast model is commonly extracted according to the relationship between the slow and the fast system.

Given a discrete linear system with a sampling period of T_s:

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{A}\mathbf{x}_k + \mathbf{B}\mathbf{u}_k \\ \mathbf{y}_k &= \mathbf{C}\mathbf{x}_k \end{aligned} \tag{2}$$

A new discrete linear system is obtained using lifted data:

$$\begin{aligned} \mathbf{x}_{k+1}^L &= \bar{\mathbf{A}}\mathbf{x}_k^L + \bar{\mathbf{B}}\mathbf{u}_k^L \\ \mathbf{y}_k^L &= \bar{\mathbf{C}}\mathbf{x}_k^L \end{aligned} \quad (3)$$

where the parameter relations can be derived:

$$\begin{aligned} \bar{\mathbf{A}} &= \mathbf{A}^p \\ \bar{\mathbf{B}} &= \begin{bmatrix} \mathbf{A}^{p-1}\mathbf{B} & \mathbf{A}^{p-2}\mathbf{B} & \cdots & \mathbf{AB} & \mathbf{B} \end{bmatrix} \\ \bar{\mathbf{C}} &= \mathbf{C} \end{aligned} \quad (4)$$

It is straightforward to extract matrices $\mathbf{B}$ and $\mathbf{C}$ from the lifted system. The system matrix $\mathbf{A}$ can be obtained using at least one of the following two approaches:(Wang *et al.*, 2004)

The first approach starts from the equation $\bar{\mathbf{A}} = \mathbf{A}^p$ where $\mathbf{A}$ is calculated directly as $\mathbf{A} = \bar{\mathbf{A}}^{\frac{1}{p}}$. It is necessary to obtain a real-valued matrix. Therefore, $\mathbf{A}$ is approximated with the real part of $\bar{\mathbf{A}}^{\frac{1}{p}}$. That is, $\mathbf{A} = \mathrm{Re}(\bar{\mathbf{A}}^{\frac{1}{p}})$.

The second approach derives $\mathbf{A}$ through a linear regression. Given $\bar{\mathbf{B}} = \begin{bmatrix} \mathbf{A}^{p-1}\mathbf{B} & \cdots & \mathbf{A}^1\mathbf{B} & \mathbf{B} \end{bmatrix}$,

$$\bar{\mathbf{B}}_i = \mathbf{A}^{i-1}\mathbf{B} \quad i = 1, 2, \cdots, p \quad (5)$$

which is the i^{th} block of $\bar{\mathbf{B}}$. The following relationship holds:

$$\bar{\mathbf{B}}_{i+1} = \mathbf{A}\bar{\mathbf{B}}_i \quad i = 1, 2, \cdots, p-1 \quad (6)$$

and

$$\bar{\mathbf{A}}\mathbf{B} = \mathbf{A}\bar{\mathbf{B}}_p \quad (7)$$

rewrite in a matrix form:

$$\underbrace{\begin{bmatrix} \bar{\mathbf{A}}\mathbf{B} & \bar{\mathbf{B}}_p & \bar{\mathbf{B}}_{p-1} & \cdots & \bar{\mathbf{B}}_2 \end{bmatrix}}_{\mathbf{\Gamma}} = \mathbf{A}\underbrace{\begin{bmatrix} \bar{\mathbf{B}}_p & \bar{\mathbf{B}}_{p-1} & \bar{\mathbf{B}}_{p-2} & \cdots & \bar{\mathbf{B}}_1 \end{bmatrix}}_{\mathbf{\Psi}} \quad (8)$$

Then,

$$\mathbf{A} = \left(\mathbf{\Gamma}\mathbf{\Psi}^T\right)\left(\mathbf{\Psi}\mathbf{\Psi}^T\right)^{-1} \quad (9)$$

A third approach is proposed here in which the extraction of fast models is reformulated within an optimization framework. Assume the system matrix of the fast system $\mathbf{A}$ is expressed as:

$$\mathbf{A} = \mathrm{Re}(\mathbf{A}) + i\,\mathrm{Im}(\mathbf{A}) \quad (10)$$

the objective function is expressed as the deviation between $\mathbf{A}^p$ and $\bar{\mathbf{A}}$, plus the norm of the imaginary part of $\mathbf{A}$:

$$\arg\min_{\mathbf{A}}\left(\left\|\mathbf{A}^p - \bar{\mathbf{A}}\right\|_l + \left\|\mathrm{Im}(\mathbf{A})\right\|_l\right) \quad (11)$$

where $\|\ \|_l$ can be taken as 1, 2 or the ∞ norm.

The objective function can also be defined as the deviation between the impulse response of the lifted and fast models:

$$\arg\min_{\mathbf{A}} \sum_i (h^p(i) - h(p \cdot i))^2 \tag{12}$$

An unconstrained optimization problem is then formulated, and solved, e.g. with the "*fminsearch*" function of MATLAB or any other unconstrained minimizer. *fminsearch* finds the minimum of an unconstrained nonlinear scalar function with simplex search.

Since the quality measurements are sampled at a slower rate than other process measurements, the same value is inserted in the log system till a new lab analysis is obtained. Therefore, a weighting vector $\{w(k)\}$:

$$w(k) = \begin{cases} 1 & y(k) \neq y(k-1) \\ 0 & otherwise \end{cases}$$

is used to downweight the inter-sample value of the quality measurement. A soft sensor is then developed using weighted partial least squares (WPLS) approach, which is compared with soft sensors developed by extracting the fast model from a lifted system.

3. Case studies

The proposed approaches to design data driven soft sensors from combining fast process measurements with slowly sampled quality data are compared for a cement kiln simulation system.The product quality of a cement kiln is indicated by the amount of CaO (free lime) in clinker. The direct measurement is generally only available every 1 or 2 hours with a time delay of about 40 minutes. It is desirable to develop a soft sensor that can accurately predict the content of CaO in real time for effective quality control.

Data collected from a Cemulator® simulation system which originally was based on a first principles model (Delfter, 1982), are used in this study. The free lime content of the clinker is available every hour, while other process measurements are logged every 10 minutes, which include kiln speed, kiln feed, position of the tertiary air damper, induced draft fan (IDFan) power, fuels to calciner and kiln, plus several temperature measurements within the kiln system. A data block of 2000 samples is selected: 1800 samples to derive the model (300 quality measurements) and 150 samples for validation.

Pseudo Random Binary Sequence (PRBS) signals are applied to the kiln speed, feed, tertiary air damper and IDFan power to excite the process. A state space model is identified from lifted data using the identification toolbox of MATLAB.

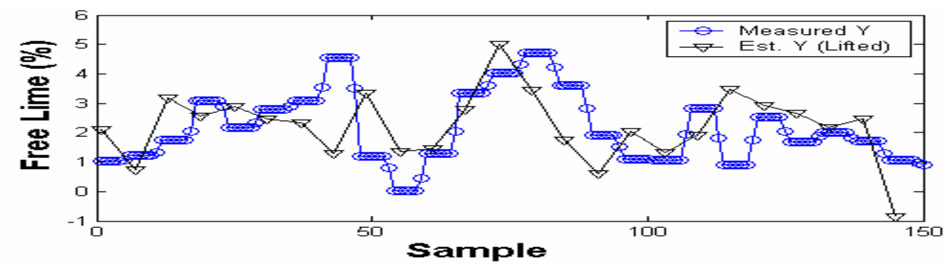

Figure 1. Free lime estimation obtained with quality measurements and lifted data

As shown in Figure 1, the free lime soft sensor obtained with lifted data is able to predict the trend of the quality measurement reasonably well. In order to estimate a model for the intersample behaviour the three approaches described above are investigated. The fast model obtained from the first approach is unstable, due to the omission of imaginary part of $\overline{\mathbf{A}}^{1/p}$. The second approach yields a solution, however, the validation shows significant sensitivity as seen in Figure 2.

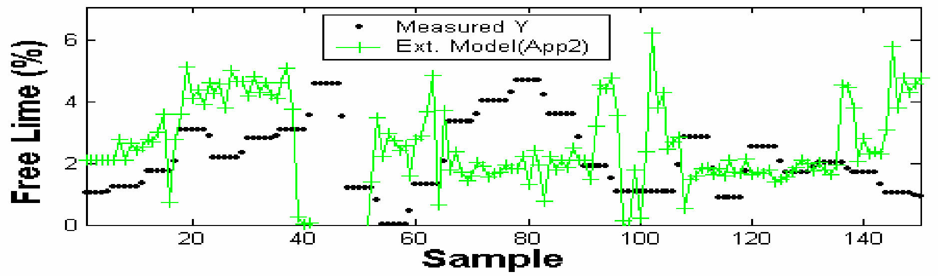

Figure 2. Free lime estimation with fast model extracted by approach 2

Since the simplex search method is a local optimization approach, the final result depends on the initial guess. 10 runs are performed for approach 3 using both objective functions (eqs. 11 and eq12). The best solution of 10 runs performs similarly to the 2nd approach. However, large variations are observed in the results of 10 tests, which indicate the high probability of arriving at a locally optimal solution. Therefore, a more reliable algorithm is desirable to obtain a consistent solution.

A CaO soft sensor is developed using WPLS approach. As mentioned before, weighting vectors are multiplied onto inter-sample inputs and outputs of modelling data. During the model validation phase, this regression model is applied to all input samples. Therefore, the intersample behaviour of the soft sensor can be calculated.

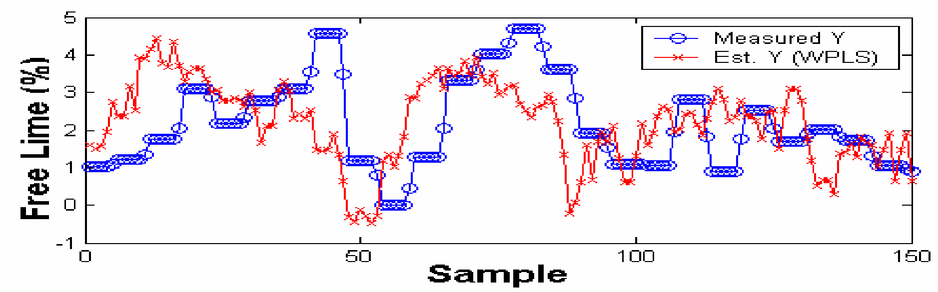

Figure 3. Free lime estimation with WPLS approach during validation period

As shown in Figure 3, the soft sensor follows the trend well, however, deviations are observed in a couple of periods. Comparing with the lifting technique based approaches, WPLS approach shows improved performance for providing inter-sample estimation. Therefore lifting with regularization should be developed to investigate which regularization is to be preferred.

4. Conclusions

This paper investigates the approaches of developing soft sensors from multi-rate sampled data sets. Since product quality is normally infrequently sampled and only available with a time delay, inter-sample information is most valuable. A two-step approach based on data-lifting techniques is investigated: the identification of a system with slow sampling rate followed by the extraction of a fast model. An optimization reformulation is provided to overcome the shortcomings associated with direct extraction methods. The proposed approach is applied to design a free lime soft sensor for product quality. Data collected from a simulator based on first principle models are used to compare the approaches based on data-lifting techniques and WPLS method.

Preliminary results reveal that the soft sensor from the WPLS approach outperforms those of the investigated data-lifting techniques. One reason might be the large number of samples (12) between product quality and standard measurements. More importantly, the soft sensor developed with the WPLS approach is able to provide reasonable prediction for the free lime, demonstrating potential of using regularization combined with lifting to provide estimates for effective quality control and optimizing process operation.

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