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# Soft Sensor Model Maintenance: A Case Study in Industrial Processes ⋆

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**Abstract:** One of the challenges of utilizing soft sensors is that their prediction accuracy deteriorates with time due to multiple factors, including changes in operating conditions. Once soft sensors are designed, a mechanism to maintain or update these models is highly desirable in industry. This paper proposes an index that can monitor the prediction performance of soft sensor models and provide guidance about when to update these models. In the proposed approach, a Kalman filter based model mismatch index is developed to monitor the prediction performance of soft sensors with the support of traditional process monitoring indexes, $T^2$ and SPE. Then, the soft sensor model can be updated through partial least squares (PLS) regression by using samples from the off-line training set and new process conditions. The proposed online update method is applied to an industrial process case study and the effectiveness of the proposed approach is demonstrated by comparing with traditional recursive partial least squares (RPLS).

*Keywords:* Soft sensors, Inferential sensors, Kalman filter, Model mismatch index, PLS

## 1. INTRODUCTION

In industry, accurate and reliable measurement and prediction of quality variables play an important role in process control, monitoring, stability and improving product quality (Sharmin et al., 2006; Zhang et al., 2010). Soft sensors are widely used to predict quality variables that are difficult to measure online by using real-time plant data (Bosca and Fissore, 2011; Yu, 2012). An advantage of utilizing soft sensor models is that hardware analyzers can be replaced for these models (Fortuna et al., 2007; Lin et al., 2007).

Soft sensors are traditionally based on first principle models as well as Kalman filter and observers (de Assis and Maciel Fiho, 2000; Heineken et al., 2007; Mangold, 2012). Nevertheless, model based soft sensors require in-depth process knowledge and significant effort for model development. Data-driven techniques can also be utilized to develop soft sensors, which rely mainly on plant data and knowledge of the process (Dufour et al., 2005; Facco et al., 2009). The well-known multivariate statistical methods such as principal component regression (PCR) and partial least squares (PLS) gain some success in building linear inferential models for quality estimates from high-dimensional data with collinearity (Kano and Nakagawa, 2008; Kadlec et al., 2009; Lu et al., 2014). However, the prediction accuracy of soft sensors tends to degrade after a period of their online operation due to process fouling, abrasion of mechanical components, drifted operating conditions, process faults and others (Kadlec et al., 2011). The degradation of soft sensor models may result in a series of issues in process operation with undesirable quality of final products. Therefore, solutions for degradation of soft sensor models are highly desirable in industrial practice. The main contribution of this paper is to provide a mechanism to properly update soft sensor models once they are deployed to online operation.

Various techniques are developed for online adaptation to cope with the issue of degradation in soft sensor models. Block-wise moving window techniques are employed to update the soft sensor model sequentially by retraining the model periodically when a given number of new data samples are collected, such as fast moving window principal component analysis and moving window kernel principal component analysis (Wang et al., 2005; Liu et al., 2009). More recently, a PLS based local learning algorithm is developed to construct an adaptive soft sensor model by using the data in a moving window with different process states (Kadlec and Gabrys, 2011). Nevertheless, the effectiveness of moving window based methods is based on the assumptions that the window size and the intervals between updates are set correctly and the process dynamics do not change within the span of one moving window. If the assumptions do not hold, it is very likely that the soft sensors adapt to noise or have very weak adaptation capabilities. Meanwhile, the recursive partial least squares (RPLS) model is developed by updating the model structure recursively at each sampling instance when the new process and quality measurements are available (Helland et al., 1992; Mu et al., 2006). In addition, recursive methods for PLS are further modified by using the

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new process data in either a sample-wise or a block-wise manner to update the current soft sensor model in the form of covariance matrices (Dayal and MacGregor, 1997; Qin, 1998). Compared with moving window techniques, the computational efficiency of recursive adaptation methods is much higher because only covariance or kernel matrix is updated in model adaptation. Nevertheless, choosing an appropriate forgetting factor for previous models is not a trivial task in recursive adaptation methods. Another alternative of performing online parameter estimation of soft sensor models is by utilizing Kalman filters, in which coefficient estimates are calculated by minimizing the noise effects (Rutan, 1990; Teppola et al., 1999). Some effort has been made to employ just-in-time learning (JITL) strategy to construct a local model based on a number of nearest neighbors of the test sample (query data) for adaptive predictions (Ge and Song, 2010). However, JITL methods cannot model the brand new process dynamics between process and quality variables if corresponding data are not stored in the database. The aforementioned dynamic and recursive modeling approaches are not desirable in some industrial applications because the soft sensor model is updated at each sampling instance or each block of sampling instances without considering the necessity of model update. As long as the soft sensor model provides accurate quality predictions, updating the soft sensor model is an unnecessary effort in industry. In addition, updating the soft sensor model at each sampling instance or each block of sampling instances could lead to unstable model parameters with poor interpretability and generalization capabilities.

Table 1. Soft sensor degradation scenarios

| Quality error | Soft sensor degradation | Process faults |
|---|---|---|
| Lab analysis issue for quality | Normal operation condition with drifted process correlation | Process under abnormal condition |
| No effective index | Proposed index | $T^2$ & SPE |
| Not considered | Model Update | No update |

Three relevant scenarios that could lead to soft sensor degradation are listed in Table 1. In this study, it is assumed that quality measurement is correct because identifying abnormalities in quality measurements is a challenging task (Kaneko and Funatsu, 2013). A Kalman filter based model mismatch index is proposed to monitor the soft sensor degradation and provide guidance about when to update the model. The difference from Kalman filter based model update methods (developed in the 90's) is that Kalman filter is utilized to derive a model mismatch index to monitor the soft sensor model performance. With the assistance of traditional $T^2$ and SPE process monitoring indexes, the soft sensor model will not be updated under abnormal process conditions. After the model update decision is made based on the model mismatch index, the regression coefficients can be updated through PLS regression using samples from the training set and the current process conditions. Compared with the model parameters from recursive/block-wise updating or Kalman filtering, the updated soft sensor model parameters updated by the proposed method are more stable with better interpretability.

The remainder of the paper is organized as follows. Section 2 gives preliminaries about PLS regression. Then the proposed online update method is developed in Section 3. The effectiveness of the proposed method is demonstrated in Section 4 utilizing an industrial case study. Finally, concluding remarks are drawn in Section 5.

## 2. PRELIMINARIES

### 2.1 Partial least squares

In this study, the case of a single quality output is considered (PLS1). Given a regressor matrix $\mathbf{X} \in \mathbb{R}^{N\times D}$ consisting of $N$ samples with $D$ selected process variables per sample, and the response matrix $\mathbf{Y} \in \mathbb{R}^{N\times 1}$ of quality outputs, PLS projects $\mathbf{X}$ and $\mathbf{Y}$ onto a lower dimensional subspace defined by a number of latent variables $[\mathbf{t}_1, \ldots, \mathbf{t}_A]$ as follows:

$$\begin{cases} \mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E} \\ \mathbf{Y} = \mathbf{T}\mathbf{Q}^T + \mathbf{F} \end{cases} \tag{1}$$

where $\mathbf{T} \in \mathbb{R}^{N\times A}$ ($A$ is the number of latent variables) is the score matrix representing the projections of the variables on the subspace, $\mathbf{P} \in \mathbb{R}^{D\times A}$ represents the loading matrix for $\mathbf{X}$, and $\mathbf{Q} \in \mathbb{R}^{1\times A}$ defines the loading matrix for $\mathbf{Y}$ (Dayal and Macgregor, 1997; Li et al., 2010). $\mathbf{E}$ and $\mathbf{F}$ denote the modeling residuals. Both $\mathbf{X}$ and $\mathbf{Y}$ matrices are scaled to zero mean and unit variance. The projection matrices in PLS are calculated in an iterative way by solving the following optimization problem:

$$\begin{aligned} &\max \mathbf{w}_a\mathbf{X}_a^T\mathbf{Y}_a\mathbf{q}_a \\ &\text{s.t. } ||\mathbf{w}_a|| = 1, ||\mathbf{q}_a|| = 1 \end{aligned} \tag{2}$$

where $\mathbf{w}_a$ and $\mathbf{q}_a$ are loading vectors for $\mathbf{X}_a$ and $\mathbf{Y}_a$, respectively. Denoting $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_A]$, $\mathbf{T}$ cannot be calculated directly from $\mathbf{X}$ using $\mathbf{W}$ because $\mathbf{X}$ is deflated in each iteration. Instead, $\mathbf{T}$ can be computed from $\mathbf{X}$ directly as follows:

$$\mathbf{T} = \mathbf{X}\mathbf{R} \tag{3}$$

where weighting matrix $\mathbf{R} = [\mathbf{r}_1, \ldots, \mathbf{r}_A]$. Each column of $\mathbf{R}$ can be computed in a recursive manner as follows:

$$\begin{aligned} &\mathbf{r}_1 = \mathbf{w}_1 \\ &\mathbf{r}_a = \mathbf{w}_a - \mathbf{p}_1^T\mathbf{w}_a\mathbf{r}_1 - \ldots - \mathbf{p}_{a-1}^T\mathbf{w}_a\mathbf{r}_{a-1}, \quad (a > 1) \end{aligned} \tag{4}$$

where $\mathbf{p}_a$ is the column vector in $\mathbf{P}$. Based on Eqs. (1) and (3), the PLS regression coefficients $\beta_{PLS}$ between $\mathbf{X}$ and $\mathbf{Y}$ are given by:

$$\beta_{PLS} = \mathbf{R}\mathbf{Q}^T \tag{5}$$

In addition, the number of latent variables for PLS regression is usually determined by cross-validation in order to achieve the optimal prediction performance.

### 2.2 Recursive partial least squares

Recursive partial least squares (RPLS) is one of the most commonly used methods for adaptive online process modeling, especially when the process variables are highly correlated (Qin, 1998; Wang et al., 2003). In RPLS, the old data $\mathbf{X}$ and $\mathbf{Y}$ can be discounted by updating the covariance matrices as new data become available

$$(\mathbf{X}^T\mathbf{X})_k = \lambda(\mathbf{X}^T\mathbf{X})_{k-1} + \mathbf{x}_k^T\mathbf{x}_k \tag{6}$$

$$(\mathbf{X}^T\mathbf{Y})_k = \lambda(\mathbf{X}^T\mathbf{Y})_{k-1} + \mathbf{x}_k^T\mathbf{y}_k \tag{7}$$

where $\mathbf{x}_k$ and $\mathbf{y}_k$ are the new process and quality variables observed at sampling instance $k$, $(\mathbf{X}^T\mathbf{X})_k$ and $(\mathbf{X}^T\mathbf{Y})_k$ are the updated covariance matrices at time $k$. $\lambda$ $(0 < \lambda \leq 1)$ is a forgetting factor that discounts the old data in each sampling instance and $\lambda = 1$ means no discounting of the old data. The widely-used kernel algorithm based RPLS method is employed in this study for comparison purpose (Dayal and MacGregor, 1997).

## 3. ONLINE UPDATE OF THE SOFT SENSOR MODEL

### *3.1 Mismatch detection of the soft sensor model by Kalman filter*

In literature, the decision for soft sensor model update is based on prediction errors. However, having large prediction errors do not necessarily indicate mismatch between the current soft sensor model and actual process dynamics because of faulty conditions or uncertainty in processes. Since the process is subjected to noises and unknown disturbances, the regression parameters may need adjustment to adapt to the current process conditions. As such, the current optimal regression parameters can be treated as hidden states that can be estimated by the Kalman filter. If the difference between the filtered and actual regression parameters (coming from the current soft sensor model) is within a certain range, the soft sensor model can still characterize the variable correlation well and model update is not necessary. Otherwise, the mismatch between the soft sensor model and current variable correlation is severe and the soft sensor model needs to be updated. Note that the regression parameters estimated by the Kalman filter are virtually computed for detection of soft sensor model mismatch and the model updating mechanism of PLS models will be discussed in Section 3.2. The state space model for recursive Kalman estimates can be formulated as follows:

$$\beta_k = \mathbf{F}_k \beta_{k-1} + \mathbf{w}_{k-1} \tag{8}$$

$$\mathbf{y}_k = \mathbf{H}_k \beta_k + \mathbf{v}_k \tag{9}$$

where $\beta_k$ is the regression parameter at time $k$, $\mathbf{F}_k$ is the state transition matrix, $\mathbf{w}_k$ is the Gaussian state noise, $\mathbf{y}_k$ is the quality measurement at time $k$, $\mathbf{H}_k$ is the observation matrix and $\mathbf{v}_k$ is the Gaussian measurement noise. In this study, the regression parameters in the next sampling instance are assumed to be similar with the regression parameters in the last sampling instance, in addition with some disturbance so that $\mathbf{F}_k = \mathbf{I}$ in Eq. (8). $\mathbf{H}_k$ in the measurement equation is given by $\mathbf{x}_k^T$, where $\mathbf{x}_k$ is the process measurement at time $k$. With the initial guess for the state being $\beta_c$ ($\beta_c$ is the regression coefficient vector of the current soft sensor model), the Kalman filter can perform a recursive estimate for the states (Rutan, 1990; Chen, 2003). A prior state estimate based on Eq. (8) can be expressed as:

$$\hat{\beta}_k = \mathbf{F}_k \beta_{k-1}^{KF} \tag{10}$$

where $\beta_{k-1}^{KF}$ is the filtered regression parameters in the last step. Then the prior covariance $\mathbf{P}_{k|k-1}$ of the state is updated as follows:

$$\mathbf{P}_{k|k-1} = \mathbf{F}_k \mathbf{P}_{k-1|k-1} \mathbf{F}_k^T + \mathbf{Q}_k \tag{11}$$

where $\mathbf{Q}_k$ is the covariance of state noise and $\mathbf{P}_{k-1|k-1}$ is the posterior covariance of the state in the last step. The residual $\tilde{\mathbf{y}}_k$ is computed by:

$$\tilde{\mathbf{y}}_k = \mathbf{y}_k - \mathbf{H}_k \hat{\beta}_k \tag{12}$$

Then the posterior state is given by:

$$\beta_k^{KF} = \hat{\beta}_k + \mathbf{K}_k \tilde{\mathbf{y}}_k \tag{13}$$

where $\mathbf{K}_k = \mathbf{P}_{k|k-1}\mathbf{H}_k^T(\mathbf{H}_k\mathbf{P}_{k|k-1}\mathbf{H}_k^T + \mathbf{R}_k)^{-1}$ is the optimal Kalman gain and $\mathbf{R}_k$ is the covariance of measurement noise. Finally, the posterior covariance $\mathbf{P}_{k|k}$ of the state is updated as follows:

$$\mathbf{P}_{k|k} = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k)\mathbf{P}_{k|k-1} \tag{14}$$

Based on the recursive update procedure of the Kalman filter, the filtered regression parameters are affected by the residual $\tilde{\mathbf{y}}_k$, computed in Eq. (12). In this study, the quality measurement $\mathbf{y}_k$ is assumed to be correct or fault free. If the current soft sensor model can predict the quality variable well, the variation of filtered regression parameters in the next time step will be small. On the other hand, the change of filtered regression parameters in the next time step can be significant based on Eq. (13). If the residual prediction of the current soft sensor model is large, the filtered regression parameters tend to be different from the actual regression parameters $\beta_c$ and the soft sensor model cannot characterize the relationship between process and quality variables well. Given the filtered regression parameters $\beta_k^{KF}$ by Kalman filter at time $k$, the residual between the estimated and actual regression parameters $\tilde{\beta}_k$ is given by:

$$\tilde{\beta}_k = \beta_k^{KF} - \beta_c \tag{15}$$

Then, the model mismatch index is computed as follows:

$$I_k = \tilde{\beta}_k^T \Lambda^{-1} \tilde{\beta}_k \tag{16}$$

where $\Lambda$ is the sample covariance of $\tilde{\beta}_k$. With the developed model mismatch index, a control limit is derived to decide whether the soft sensor model mismatch is severe or not. The probability density of the model mismatch index can be estimated through kernel density estimation using the computed model mismatch index in the training set as follows:

$$\hat{p}(I) = \frac{1}{Nh}\sum_{k=1}^{N} \kappa\left(\frac{I - I_k}{h}\right) \tag{17}$$

where $\hat{p}(I)$ denotes the estimated probability density, $N$ is the number of samples in the training set, $h > 0$ is a smoothing parameter called bandwidth and $\kappa(\cdot)$ represents a Gaussian kernel function (Bowman and Azzalini, 1997). For a given significance level, the control limit for the model mismatch index can be obtained using the estimated probability density. In the test set, the model mismatch index can be calculated every sampling instance when a quality measurement is available. Maximum tolerated alarms are predefined to quantify the necessity of model update and an illustrative diagram is shown in Fig. 1. Once the number of model mismatch index values that are consecutively above the control limit reach the maximum tolerated alarms, the model update shall be performed to recover the mismatch between the current PLS soft sensor model and the actual process variable correlation. However, the Kalman filter based model mismatch index is insufficient to update the soft sensor model, because abnormal conditions in the process can also result in performance degradation of the soft sensor model. Therefore, $T^2$ and SPE indexes are selected to monitor the abnormality in the process. The process is in an abnormal condition if either index exceeds the control limit and the soft sensor model update cannot be performed even

 

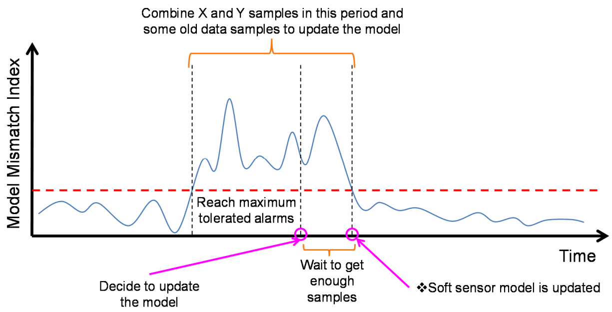


Fig. 1. Illustrative diagram of detecting model mismatch

in the case that the model mismatch index is above the control limit consecutively. Meanwhile, actions should be taken to address the detected process faults. If the model mismatch index is still above the control limit after the process is recovered from the abnormal condition, the soft sensor model will be updated. To summarize, only under the condition that the model mismatch is severe and the process is under normal conditions will the soft sensor model be updated.

### *3.2 Online model update*

When it is time to update the soft sensor model based on the criteria described in Section 3.1, $M$ process measurements $\mathbf{X}_{new} \in \mathbb{R}^{M\times D}$, and quality measurements $\mathbf{Y}_{new} \in \mathbb{R}^{M\times 1}$ in the new condition are collected and combined with $M$ samples in the training data to update the regression coefficients ($M \ll N$). In order to make sure that the samples from the training data, $\mathbf{X}_{old} \in \mathbb{R}^{M\times D}$ and $\mathbf{Y}_{old} \in \mathbb{R}^{M\times 1}$, represent the distribution of the whole model generation data set, those samples can be obtained through equidistant sampling of the whole training data set. For the industrial case study, multiple values of $M$ were tested and 20 was found to lead to best prediction performance. The actual value of $M$ depends on the change rate of process. In parallel, $\mathbf{X}_{new}$ is automatically validated online through the PLS monitoring model while $\mathbf{Y}_{new}$ is validated through the quality control procedure in lab analysis. Given the combined input process data matrix $\mathbf{X}_u = [\mathbf{X}_{old}^T \quad \mathbf{X}_{new}^T]^T$ and output data matrix $\mathbf{Y}_u = [\mathbf{Y}_{old}^T \quad \mathbf{Y}_{new}^T]^T$, the linear regression model in the new process condition can be described as follows:

$$\mathbf{Y}_u = \mathbf{X}_u\beta_u + \mathbf{E}' \tag{18}$$

where $\beta_u$ is the updated regression coefficient vector computed via PLS regression and $\mathbf{E}'$ denotes the prediction residual. Then, the quality will be predicted through the updated soft sensor model.

## 4. AN INDUSTRIAL PROCESS CASE STUDY

A simplified process diagram of the industrial process is shown in Fig. 2. The industrial process has three unit operations and 61 measurable process variables. Units A, B and C are distillation columns, in which temperatures, pressures, flows and calculated variables are measured and stored. This industrial process has one quality variable, which is associated with the final product of Unit C. The process variables are measured online every hour while the quality variable is measured through off-line laboratory analysis approximately every six hours. The main

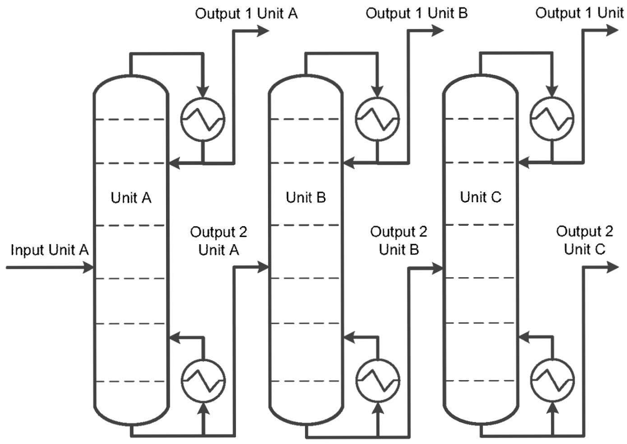


Fig. 2. Process diagram of the industrial process

objective is to build and maintain a reliable soft sensor model by using some of the 61 process measurements to predict the quality variable. 735 samples collected from January 2011 to February 2012 are used for training the soft sensor model while another 750 samples collected from February 2012 to May 2013 are employed as an online test to demonstrate the effectiveness of the proposed online update method. The process undergoes different operating conditions with various disturbances during the 29 months. The training data does not include all possible scenarios in the online test so that the online update for the soft sensor model is necessary. The PLS soft sensor

Table 2. Comparison of computational results between RPLS and the proposed method in the online test for the industrial process

| Method | RMSE | MAPE | $R^2$ |
|---|---|---|---|
| No Update | 0.7499 | 15.78% | 0.6110 |
| The proposed method | 0.6443 | 12.86% | 0.7093 |
| RPLS ($\lambda = 0.9$) | 0.6297 | 11.57% | 0.7220 |

model is built upon 4 process variables (25, 42, 51 and 52), where those variables are chosen based on engineering knowledge and an optimization procedure. The model mismatch index is shown in Fig. 3(b), where the PLS model is updated 10 times during the online test. Note in Fig. 3(a) that the predicted quality values of the updated PLS model properly follow the actual quality values. Utilizing $T^2$ and SPE indexes, Figs. 3(c) and (d) show that an abnormal condition happens between the 140th and 160th sampling instances. Though the model mismatch index also exceeds the control limit between the 140th and the 160th sampling instances, the soft sensor model is not updated during that period because it is experiencing an abnormal condition. The original PLS model predictions and the PLS model with an online update are depicted in Fig. 4. The quality predictions from the original soft sensor model cannot characterize the trend in the quality variable, while the predicted values of the soft sensor model with an online update closely follow the actual trend of the quality variable. A strong offset between the actual quality measurements and the predicted values from the 1st to the 320th sampling instances is observed, indicating

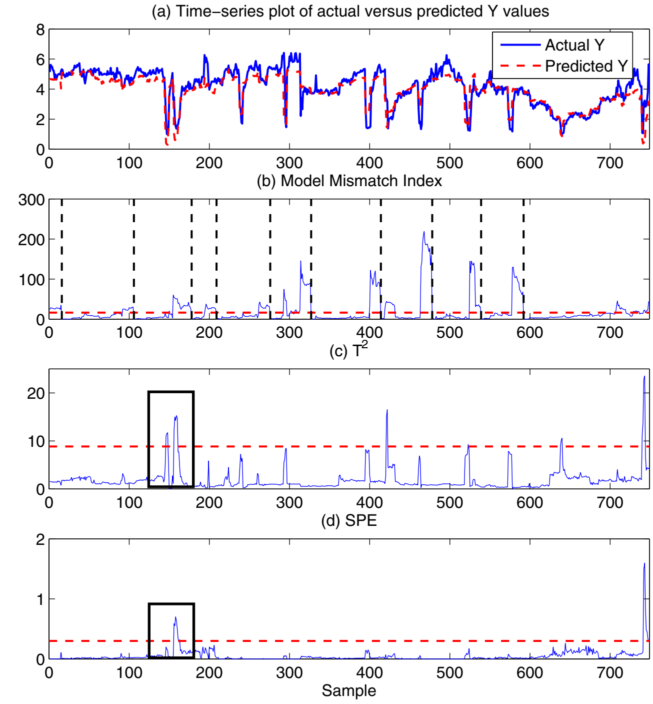


Fig. 3. Online test for the industrial process

that the soft sensor model is not well suited to predict the quality variable under the current process conditions. The prediction accuracy metrics are also listed in Table 2, where the RMSE and MAPE values without model update are as high as 0.7499 and 15.78% and $R^2$ value is as low as 0.6110. In comparison, the soft sensor with an online update leads to more satisfactory prediction results, with the RMSE and MAPE values being 0.6443 and 12.86% and $R^2$ value of 0.7093. Such comparison demonstrates that the proposed update method can make the soft sensor model adaptive with improved prediction accuracy.

The PLS model with the proposed online update method is compared against the RPLS model with the optimal forgetting factor $\lambda = 0.9$, which is determined through a grid search. Although the RPLS model with $\lambda = 0.9$ achieves slightly better performance than the proposed method (as shown in Fig. 4 (b)), the oscillation in its regression coefficients in Fig. 5 is strong. The RPLS method updates regression coefficients at each sampling instance, while the majority of updates in RPLS are not necessary. Furthermore, there is not a reasonable explanation for the sign changes of the regression coefficients of the RPLS model. If a process variable is positively correlated to the quality variable based on statistical analysis of historical data, they should not be negatively correlated for several samples in the online operation. Hence, the regression coefficients of RPLS lack consistency and interpretability. In contrast, the signs of regression coefficients in the proposed method never change, which leads to a stable model structure and better interpretability. Consequently, the proposed method provides a desirable advantage in industrial practice.

## 5. CONCLUSIONS

With the objective of detecting soft sensor degradation in industrial processes, a Kalman filter based soft sensor

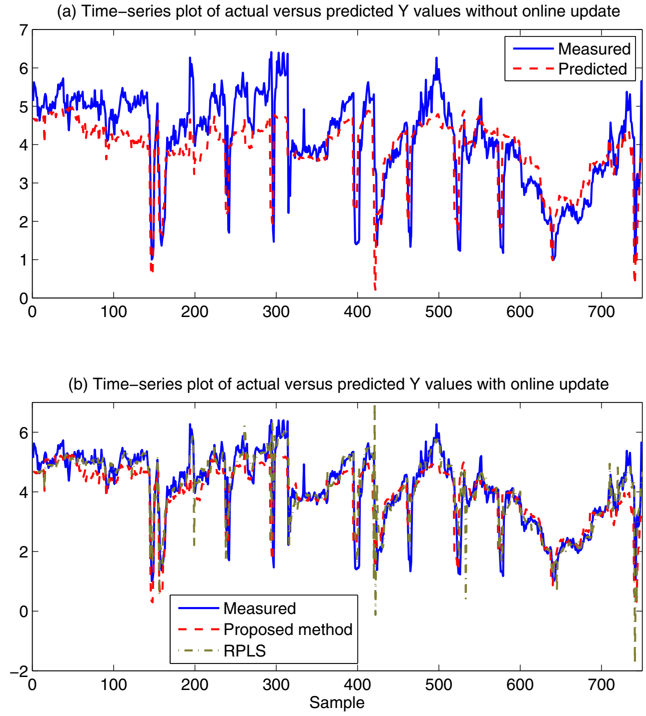


Fig. 4. Comparison of soft sensor prediction performance for the industrial example

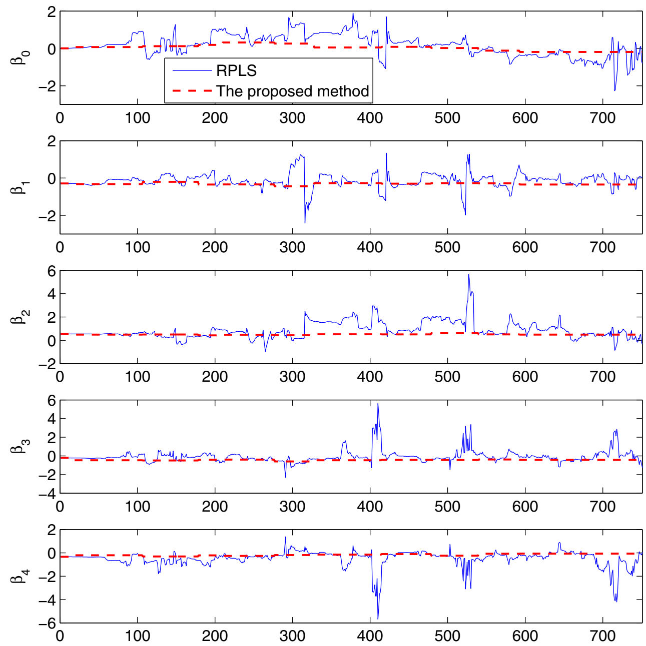


Fig. 5. Comparison of regression coefficients between the proposed approach and RPLS method

model mismatch index and a corresponding contribution plot for diagnosis are developed in this paper. Benefiting from filtering capabilities of the Kalman estimates, the mismatch index provides accurate information on whether the soft sensor model is in need of maintenance. Based on the statistical properties of the model update index in the training set, the control limit (denoting the red line for severe model mismatch) is obtained through kernel density estimation. Integrated with the process monitoring indexes, the Kalman filter based model mismatch index is employed to determine when to update the soft sensor model. With the decision to update the soft sensor model, the new regression parameters are computed by using samples in the training set and the current conditions. Consequently, the soft sensor model is updated only when significant degradation occurs, improving prediction performance of the soft sensor model.

The proposed approach is applied to an industrial process case study and compared against the RPLS method. The computational results indicate that the proposed index can capture the model mismatch of the soft sensor model in the early stages and the online updated soft sensor model leads to accurate quality predictions. In addition, the comparison with the RPLS method demonstrates that the proposed approach is more desirable in industrial applications because model degradation can be tackled without frequently updating the model parameters.

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