Kalman Filtering Approach to Multirate Information Fusion for Soft Sensor Development

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Abstract—Accurate and frequent measurements of quality variables are important for real-time process monitoring and control. However, because online measuring instruments commonly have the limitations of high investment and low accuracy, while offline laboratory analyses are obtained manually and infrequently, neither online instruments nor offline analyses can satisfy the requirements of real-time applications in industries alone. In order to obtain more reliable information of quality variables, this paper develops two kinds of adaptive soft sensors in the framework of Kalman filter. The idea is to take the advantages of fast-rate sampling of online data and high-accuracy of lab data by synthesizing these two sources of measurements at different sampling rates. The CSTR case study and applications in a chemical production process demonstrate the effectiveness of the proposed methods.

Keywords: soft sensor, multirate, Kalman filters, state estimation, dynamic modelling.

I. INTRODUCTION

Hardware sensors are found almost everywhere in industrial processing plants for measuring temperature, flow rate, level, pressure and other process variables. But for some key quality variables such as product composition and molecular weight distribution, the online measuring instruments are usually suffered from high investment, low accuracy and frequent maintenance [1]. Therefore, nowadays measurements of quality variables still rely heavily on offline laboratory analyses. Although this can provide more accurate information, it is not suitable for real-time process monitoring, control and optimization because of the slow sampling rates. For these reasons, soft sensors are desired for prediction of the difficult to measure quality variables in real time by using the easily measurable process variables.

Soft sensors have received much attention over the last two decades, as a powerful tool to improve product quality and production efficiency [2]. One main category of soft sensors is known as first-principle model or white-box model, which is obtained from the fundamental process knowledge, such as constitutive relationships, mass, components and energy balance equations [3]. However, this type of model is difficult to build, requiring considerable time and effort for a large-scale complex process, and is often unavailable due to lack of sufficient process knowledge [4]. On the other hand, distributed control systems have been equipped in many plants, enabling a large amount of process observations to be recorded. As a result, the data-driven model or black-box model becomes a convenient alternative to develop soft sensors, since it relies less on complete process knowledge as opposed to the first-principle model, requires no extra investment, and is costless to implement on the existing systems [5].

Many successful applications of data-driven soft sensors have been reported in various process industries, including steel industry, petrochemical industry, paper manufacturing industry, fermentation industry and so on [6], [7]. A comprehensive review on this topic was conducted by Kadlec and his coworkers [8]. Data-driven soft sensors dedicated to extract mapping relationships between process variables and quality variables based on the historical data. Among the plentiful methods for developing data-driven soft sensors, partial least squares (PLS) is the most popular technique to cope with the problems of large dimension and high correlation involved in process variables [9]. Furthermore, dynamic partial least squares (DPLS) is established by incorporating lagged variables in the input data matrices for capturing process dynamics [10]. Thanks to the inclusion of lagged values, DPLS can greatly improve the model prediction accuracy and is adopted in this paper for modeling due to its simple structure and good performance.

In practical scenarios, development of soft sensors is not a task that can be completed once for all. Time-invariant models are impossible to deal with the drifts of processes resulting from catalyst deactivation, mechanical abrasion, environmental changes and feed materials fluctuation [11]. Therefore, maintenance is necessary to avoid performance degradation and guarantee successful applications of soft sensors. One straightforward way for this purpose is to rebuild a soft sensor periodically, but which is often time consuming and difficult to perform online. Another feasible way is to equip a soft sensor with adaptive capability, allowing the model to update automatically based on the newly obtained measurements [12]. The recursive or moving window based least squares, principal component analysis and PLS algorithms all fall into this category. However, these methods are unable to synthesize observations originated from multiple sources at different sampling rates, so updating of soft sensors seldom performs optimally. In order to make full use of the obtained infor-
mation, this paper adopts Kalman filtering theory to update
the soft sensor and compensate the model mismatch, taking
into account the multiple-source observations with different
sampling frequencies.

The rest of this paper is organized as follows. Section II
briefly introduces Kalman filter (KF) and extended Kalman
filter (EKF) algorithms. Section III states the multirate sam-
pling problem existed in the measurement of quality variables.
Section IV develops two kinds of adaptive soft sensors in the
framework of KF to account for this problem. The proposed
soft sensors are evaluated with a CSTR example and two
case studies in a chemical production process. The applica-
tion results and performance are illustrated and discussed in
section V. Finally, the main conclusions are summarized in
section VI.

II. KALMAN FILTERING BASED STATE ESTIMATION
A. KF for linear system
Consider the following discrete-time linear system:
\[
\begin{align*}
x_{k+1} &= Ax_k + Bu_k + w_k, \\
y_k &= Cx_k + v_k,
\end{align*}
\]
(1)
where \(x_k \in \mathbb{R}^n\), \(u_k \in \mathbb{R}^m\) and \(y_k \in \mathbb{R}^n\) are the state, input and output variables, respectively; \(A\), \(B\) and \(C\) denote the state transition matrix, control input matrix and observation matrix, respectively; \(w_k\) and \(v_k\) are the process and measurement noises, and further assumed to be mutually independent and drawn from zero mean multivariate Gaussian distributions with covariances \(Q\) and \(R\), respectively.

Observability is a basic prerequisite for state estimation of
any system. The following theorem states the sufficient and
necessary condition for linear systems.

**Theorem 1:** The linear system (1) is observable if and only if the observability matrix
\[
\mathcal{O}(A, C) = \begin{bmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{bmatrix}
\]
has rank equal to \(n\) [13].

For state estimation of linear system (1) in the presence
of Gaussian noise, the well-known KF is able to provide
optimal solutions and has the most wide applications in many
fields [14]. Given the initial state estimation \(\hat{x}_0\) and error
covariance \(P_0\), the KF algorithm is recursively implemented
by two consecutive procedures, namely, **predict** and **update**.
The calculation equations are summarized as below.

- **Predict**
\[
\begin{align*}
\hat{x}_{k+1} &= A\hat{x}_k + Bu_k, \\
\bar{P}_{k+1} &= AP_kA^T + Q,
\end{align*}
\]
(2)
(3)

- **Update**
\[
\begin{align*}
K_{k+1} &= P_{k+1}^{-1}CA\bar{C} + R^{-1}, \\
\hat{x}_{k+1} &= \hat{x}_{k+1} + K_{k+1}[y_{k+1} - C\hat{x}_{k+1}], \\
P_{k+1} &= [I - K_{k+1}C]\bar{P}_{k+1}.
\end{align*}
\]
(4)
(5)
(6)
Here \(K_{k+1}\) is the Kalman gain, and its value determines
the effects that the prior state estimation \(\hat{x}_{k+1}\) and the new
measurement \(y_{k+1}\) respectively take on the generation of the posterior state estimation \(\hat{x}_{k+1}\).

B. EKF for nonlinear system
Practical processes always possess some degree of nonlin-
earity. State estimation in this scenario is out of the capability
of KF. By approximating the nonlinear model with first-
order Taylor expansion, the extended Kalman filter (EKF) was
proposed and served as a suboptimal approach to estimate the
state of nonlinear system:
\[
\begin{align*}
x_{k+1} &= f(\hat{x}_k, u_k), \\
y_k &= h(\hat{x}_k) + v_k,
\end{align*}
\]
(7)
where \(f(\cdot)\) and \(h(\cdot)\) are nonlinear functions. The predict and
update equations of KF in (2) and (5) are accordingly modified as
\[
\begin{align*}
\bar{x}_{k+1} &= f(\hat{x}_k, u_k), \\
\hat{x}_{k+1} &= \bar{x}_{k+1} + K_{k+1}[y_{k+1} - h(\bar{x}_{k+1})],
\end{align*}
\]
(8)
(9)
The matrices \(A\) in (3) and \(C\) in (4) and (6) are replaced with
Jacobian matrices \(F_k\) and \(H_{k+1}\), respectively, given by
\[
\begin{align*}
F_k &= \frac{\partial f}{\partial x}(\hat{x}_k, u_k), \\
H_{k+1} &= \frac{\partial h}{\partial x}(\bar{x}_{k+1}).
\end{align*}
\]
(10)
(11)
Unlike linear systems, it is quite difficult to demonstrate if a
complex nonlinear system is completely observable. However,
a sufficient condition given in Theorem 2 is widely adopted
in practical applications to examine the local observability of
nonlinear systems.

**Theorem 2:** If the linearized system is observable, i.e.,
\(\mathcal{O}(F_k, H_{k+1})\) has rank of \(n\), then the nonlinear system (7) is
locally observable [15].

III. PROBLEM STATEMENT

Fig. 1. Multiple measuring approaches with different sampling rates

In order to ensure operation security and product quality
in industries, quality variables are commonly acquired both
from online analyzers as well as lab analyses. As shown in
Fig. 1, the online analyzer is sampled every minute, while the
lab analysis is sampled every 5 minutes. These two measuring
approaches have their own strength and weakness, which are listed as below:

- **Online analyzers**
  
  **Strength:** The online analyzers can provide real-time measurements of quality variables. The tremendous number of observations contain a plentiful information of the process dynamics.
  
  **Weakness:** The measuring instruments are often operated under harsh production environments, such as high temperature, high pressure, excessive dust and strong causticity. Their accuracy and reliability are subject to deterioration over time. As a result, regular maintenance and calibration of the instruments are required, which may not only increase the running cost, but also disrupt the normal operation of the process.

- **Lab analyses**
  
  **Strength:** The lab analyses have characteristics of high precision and high reliability, which can facilitate calibration of the online measuring instruments and rectification of the built soft sensors.
  
  **Weakness:** The sampling frequencies of lab analyses are quite low, which are far from enough to capture the process dynamics. Besides, from an economical point of view, collecting large amounts of samples for lab analysis can greatly increase the labor cost. In addition, sampling manually may expose the operators to the hazardous environments, potentially resulting in physical injuries and property damages.

Therefore, neither online analyzer nor lab analysis alone can meet the requirements of real-time process monitoring and control purpose. It is desired to develop soft sensors for better prediction of the quality variables by combining these two sources of measurements.

IV. ADAPTIVE SOFT SENSOR DEVELOPMENT IN THE FRAMEWORK OF KF

Assume \( U = [u_1, u_2, \cdots, u_n] \) includes the selected \( n \) process variables, \( y^o \) and \( y^r \) represent the online observation and lab analysis of quality variable, respectively. The sampling rate of \( y^r \) is slower than that of \( U \) and \( y^o \), resulting in multirate system with fast-rate sampled-data \( \{U_k, y^r_k, k = 1, 2, \cdots\} \) and slow-rate sampled-data \( \{y^r_{T_j}, j = 1, 2, \cdots\} \), where \( T_j \) is the sampling instant of the \( j \)th lab data. The lifting technique and the polynomial transformation technique are two fundamental tools for multirate systems [16]. But unfortunately they may be impractical for our applications because the lab data is usually sampled rarely and irregularly. Taking into account such multirate sampling situations, this section will present two adaptive soft sensors in the framework of KF to obtain more accurate, reliable and robust predictions of quality variables.

A. Indirect Method Based on EKF

The basic idea of the indirect method is first to build a dynamic model on the basis of the fast-rate sampled-data \( \{U_k, y^r_k\} \). This model is nominal and may not be accurate enough because only online measurement of quality variable \( y^o \) is used to build the fast rate model. To compensate the model mismatch and to adapt for the new operating condition, a scaling parameter and a bias term are introduced into the model. The lab analysis \( y^r_{T_j} \) is further incorporated with \( y^o \) to update the system states and the calibration parameters by means of EKF.

The indirect method based on EKF is summarized as follows:

1.) Based on the historical data of process variables \( \{U_k\} \) and online observations of quality variable \( \{y^r_k\} \), a dynamic model is constructed as

\[
    y^o_{k+1} = g(y^o_k, U_k), \tag{12}
\]

where \( g(\cdot) \) can be either a linear or nonlinear function determined by system identification approach. Considering possible collinearity of the process variables and the model simplicity, the DPLS algorithm can be used to establish a linear model.

2.) Since the online observations are typically inaccurate, the model identified totally based on which cannot yield satisfactory prediction of the true quality variable. That means it is improper to simply replace \( y^o_k \) in equation (12) by real quality variable \( x_k \), i.e.,

\[
    x_{k+1} = g(x_k, U_k). \tag{13}
\]

To compensate the model mismatch [17], introducing a scaling parameter \( \alpha \) and a bias term \( \beta \) into equation (13) gives

\[
    x_{k+1} = \alpha_k \cdot g(x_k, U_k) + \beta_k + w^\beta_k. \tag{14}
\]

The parameters \( \alpha_k \) and \( \beta_k \) are modeled as random walks and described by

\[
    \alpha_{k+1} = \alpha_k + w^\alpha_k, \tag{15}
\]

\[
    \beta_{k+1} = \beta_k + w^\beta_k. \tag{16}
\]

The augmented state vector \( [x_k, \alpha_k, \beta_k]^T \) is constructed by augmenting the original state \( x_k \) with the parameters \( \alpha_k \) and \( \beta_k \), and the associated process noise vector is \([w^\alpha_k, w^\beta_k, w^\beta_k]^T\).

3.) The observations of online analyzer \( y^o_k \) and lab analysis \( y^r_{T_j} \) can be expressed as

\[
    y^o_k = [1, 0, 0][x_k, \alpha_k, \beta_k]^T + v^\alpha_k, \tag{17}
\]

\[
    y^r_{T_j} = [1, 0, 0][x_T, \alpha_T, \beta_T]^T + v^\beta_{T_j}, \tag{18}
\]

where \( v^\alpha \) and \( v^\beta \) are measurement noises of \( y^o \) and \( y^r \), respectively. Since \( y^o \) is believed to be more accurate than \( y^r \) towards \( x \), the variance of \( v^\beta \) would be much smaller than that of \( v^\alpha \).

Although two measurements are observed at the sampling instant \( k = T_j \), only \( y^o_k \) is used and \( y^r_k \) is discarded to maintain consistency in the dimension of the measurement equation. Thus, the following single-rate measurement equation is obtained by combining (17) and (18),

\[
    z_k = [1, 0, 0][x_k, \alpha_k, \beta_k]^T + (1 - \lambda_k)v^\alpha_k + \lambda_k v^\beta_k, \tag{19}
\]
where $\lambda_k = 1$ and $z_k = y_k'$ when lab data is available; $\lambda_k = 0$ and $z_k = y_k''$ in other cases.

4.) At the sampling instant of lab data (i.e., $k = T_j$), EKF algorithm is applied to (14)-(16) to update the augmented state $[x_k, \alpha_k, \beta_k]'$ based on the observation equation (19). From (10) and (11), the state transition matrix $F_k$ and the observation matrix $H_{k+1}$ are computed by

$$F_k = \begin{bmatrix} \hat{\alpha}_k \cdot g'(\hat{x}_k, U_k) & g(\hat{x}_k, U_k) \\ 0 & 1 & 0 \end{bmatrix} \in \mathbb{R}^{3 \times 3},$$

$$H_{k+1} = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{1 \times 3}.$$

The system models are often slow-varying, it is unnecessary to update the calibration parameters $\alpha_k$ and $\beta_k$ using inaccurate measurement $y_k''$. Therefore, during the interval between two lab data (i.e., $k \in [T_j + 1, T_{j+1} - 1]$), the KF algorithm is applied to (14) based on the observation equation (19) to predict the state $x_k$. The dimension of the state is reduced from 3 to 1; the corresponding state transition matrix and observation matrix are $A = \hat{\alpha}_k \cdot g'(\hat{x}_k, U_k)$ and $C = 1$, respectively. Following this approach, the prediction of quality variable is calculated with a fast rate for any input $U_k$; while the soft sensor model is updated with a slow rate according to the lab data $y_{T_j}'$.

B. Direct Method Based on KF

The direct method based on KF is simpler than the indirect method proposed above. It avoids building a dynamic model using other process variables, and directly rectifies the online measurements using the irregularly sampled lab data to give the prediction of the quality variable. Furthermore, since the associated state equations and observation equations are linear, the KF algorithm is sufficient for solving the state estimation problem, and as a result the errors that come from approximate linearization in the EKF algorithm can be avoided. The specific derivation of this method is as follows:

1.) Model the state $x_k$ of quality variable by a random walk model

$$x_{k+1} = x_k + w_k^x.$$  \hfill (20)

Since the online measurement $y_k'$ is inaccurate, it is reasonable to assume there is a bias $\beta_k$ between $y_k'$ and $x_k$. The following observation equation is obtained,

$$y_k' = x_k + \beta_k + v_k'$$  \hfill (21)

where $\beta_k$ is modeled by random walk

$$\beta_{k+1} = \beta_k + w_k^\beta.$$  \hfill (22)

The irregularly sampled lab data $y_{T_j}'$ is considered to be more reliable, which is equivalent to the state plus a white noise with small variance, i.e.,

$$y_{T_j}' = x_{T_j} + v_{T_j}'.$$  \hfill (23)

2.) When the lab data is available, two observation equations (21) and (23) are used to update the augmented state $[x_k, \beta_k]'$. The corresponding state transition matrix $A$ and the observation matrix $C$ in the KF algorithm (2)-(6) are

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 1 \end{bmatrix}.$$  \hfill (24)

Using Theorem 1, it is obvious that the system is observable at this sampling instant. However, during the sampling interval between two lab data, only online measurement $y_k'$ is available with observation matrix $C = [1 \ 1]$. If it is used to update the augmented state $[x_k, \beta_k]'$, the observability rank condition of Theorem 1 cannot be satisfied. Therefore, the bias $\beta_k$ has to be kept constant when lab data is unavailable, and only the state $x_k$ is updated based on the observation equation (21). Accordingly, the state transition matrix and the observation matrix are reduced to $A = 1$ and $C = 1$, respectively.

Its simplicity is also a weakness in the direct method. Because no process knowledge is exploited to describe the dynamic of state, its performance is completely dependent on the quality of online measurements and lab analysis. Any outlier or missing data may result in significant deviation. This problem must be well handled during implementation of the proposed soft sensor.

V. CASE STUDIES

First, a simulation of a continuously stirred tank reactor (CSTR) is considered to evaluate and compare the performance of the proposed soft sensors. Then, two case studies in a chemical production process are studied to highlight their effectiveness and practicability.

A. CSTR example

The CSTR system with $A \rightarrow B$ exothermic reaction has been widely used as a benchmark to illustrate nonlinear system modeling and control [18]. Its dynamic behavior can be described by the following first principle model [19]:

\begin{align*}
\dot{C}_A &= \frac{q}{V} (C_{A_f} - C_A) - k_0 \exp(-\frac{E}{RT}) C_A, \quad (24) \\
\dot{T} &= \frac{q}{V} (T_f - T) + \frac{\Delta H}{\rho C_p} k_0 \exp(-\frac{E}{RT}) C_A \\
&+ \frac{UA}{\rho C_p V} (T_c - T), \quad (25)
\end{align*}

where $C_A$ (mol/m³) is the concentration of reagent A, $T$ (K) is the reactor temperature, $T_c$ (K) is the temperature of cooling jacket, and other parameters are listed in Table I with their corresponding steady state values.

Discretize the system (24)-(25) with a sampling interval of 0.1s. Assume $T_c$ is a random input sequence with uniform distribution between 290 and 300. The system is simulated with initial state $[T_0 \ C_{A,0}]^T = [324.48 \ 0.88]^T$ for 500s, the true input-output data are shown in Figure 2.

The output $C_A$ is the quality variable of the interest, which has two measuring approaches, i.e., online measurement
Table I

CSTR Model Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_A$ – Feed concentration (mol/m³)</td>
<td>1</td>
</tr>
<tr>
<td>$q$ – Volumetric flow rate (m³/sec)</td>
<td>100</td>
</tr>
<tr>
<td>$V$ – Reactor volume (m³)</td>
<td>100</td>
</tr>
<tr>
<td>$k_0$ – Pre-exponential factor (1/s)</td>
<td>$7.2 \times 10^{10}$</td>
</tr>
<tr>
<td>$E/R$ – Activation energy term (K)</td>
<td>8750</td>
</tr>
<tr>
<td>$T_f$ – Feed temperature (K)</td>
<td>350</td>
</tr>
<tr>
<td>$\Delta H$ – Heat of reaction for A→B (J/mol)</td>
<td>$5 \times 10^4$</td>
</tr>
<tr>
<td>$\rho$ – Density of A-B mixture (kg/m³)</td>
<td>1000</td>
</tr>
<tr>
<td>$C_p$ – Heat capacity of A-B mixture (J/kg K)</td>
<td>0.239</td>
</tr>
<tr>
<td>$UA$ – Overall heat transfer coefficient (W/K)</td>
<td>$5 \times 10^4$</td>
</tr>
</tbody>
</table>

| \( \hat{y}^o \) with fast sampling rate 0.1s and lab analysis \( y^i \) with slow sampling rate 10s. To overcome the limitations of each approach and obtain more reliable measurements of \( C_A \), the proposed soft sensors are applied to the CSTR system based on the fast rate process variables \( \{ U_k = [T_{c,k}, T_k] \} \) and multirate outputs \( \{ \hat{y}_k^o, \hat{y}_k^i \} \).

The observations of \( \hat{y}^o \) and \( \hat{y}^i \) are given by

\[
\begin{align*}
\hat{y}_k^o &= C_{A,k} + \epsilon_k^o, \\
\hat{y}_k^i &= C_{A,T} + \epsilon_k^T,
\end{align*}
\]

where \( \epsilon_k^T \) is assumed to be a white noise with variance 0.01², but different and more challenging scenarios of \( \epsilon_k^o \) will be considered to test the developed soft sensors.

**Case 1:** \( \epsilon_k^o \) is a Gaussian noise with a mean value of 0.01 and variance 0.1².

**Case 2:** \( \epsilon_k^o \) is a colored noise and described by

\[ \epsilon_k^o = \frac{1}{1 - 0.6q^{-1} n_k^o}, \]

where \( n_k^o \) is a white noise with variance 0.1².

Divide the available multirate data into two segments, the first 3/5 and the rest 2/5 data are used for identification and cross validation, respectively. The DPLS algorithm is employed to identify the following model,

\[ y_{k+1}^o = [1, \hat{y}_k^o, T_k, T_{c,k}] \times D, \]

where \( D = [d_1, d_2, d_3, d_4]^T \in \mathbb{R}^{4 \times 1} \) is the parameter vector. Based on the modeling data of **Case 1** and **Case 2**, we obtain

\[ D = [1.6689, 0.1115, -0.0026, -0.0001]^T \] and \( D = [0.7658, 0.6154, -0.0012, -0.0001]^T \), respectively. The built model is applied to the cross validation data sets, the prediction results are shown in Figure 3. From this figure, we can see that the variance of the model prediction \( \hat{y}^o \) is smaller than that of \( y^o \). However, the mismatch between \( \hat{y}^o \) and \( C_A \) is still large.

To compensate the model mismatch and improve the prediction performance, the multirate extended Kalman filter is applied to (14)-(16) based on measurement equation (19) to update the augmented state \( [x_k, \alpha_k, \beta_k]^T \), where \( x_k \) indicates the real output \( C_A, g(x_k, U_k) = [1, x_k, T_k, T_{c,k}] \times D \). Before implementation of this method, we first examine the observability of the concerned system.

The linearized state transition matrix and observation matrix are given by

\[
F_k = \begin{bmatrix}
\hat{\alpha}_k d_2 & g(\hat{x}_k, U_k) & 1 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix} \in \mathbb{R}^{3 \times 3},
\]

\[
H_{k+1} = \begin{bmatrix}
1 & 0 & 0
\end{bmatrix} \in \mathbb{R}^{1 \times 3}.
\]

The observability matrix is

\[
\mathcal{O}(F_k, H_{k+1}) = \begin{bmatrix}
\hat{\alpha}_k d_2 & 0 & 0 \\
\hat{\alpha}_k d_2 & g(\hat{x}_k, U_k) & 1 \\
(\hat{\alpha}_k d_2)^2 & g(\hat{x}_k, U_k)(\hat{\alpha}_k d_2 + 1) & \hat{\alpha}_k d_2 + 1
\end{bmatrix}.
\]

Since \( \text{rank}[\mathcal{O}(F_k, H_{k+1})] = 2 < 3 \), Theorem 2 is failed to determine the observability of our system, we have to seek help from Theorem 3 which is a more efficient alternative.

**Theorem 3:** The nonlinear system (7) is locally observable if
the observability matrix

\[
\mathbf{O}^* = \begin{bmatrix}
\frac{\partial h}{\partial \mathbf{x}} | \mathbf{x}_k \\
\frac{\partial h}{\partial \mathbf{x}} | \mathbf{x}_{k+1} \\
\vdots \\
\frac{\partial h}{\partial \mathbf{x}} | \mathbf{x}_{k+n-1} \\
\frac{\partial f}{\partial \mathbf{x}} | \mathbf{x}_k \\
\vdots \\
\frac{\partial f}{\partial \mathbf{x}} | \mathbf{x}_{k+n-2} \\
\frac{\partial f}{\partial \mathbf{x}} | \mathbf{x}_{k+n-1}
\end{bmatrix}
\]

has full rank [20].

For this particular system, the observability matrix \( \mathbf{O}^* \) is computed as

\[
\mathbf{O}^* = \begin{bmatrix}
1 & 0 & 0 \\
\hat{\alpha}_k d_2 & 0 & 1 \\
(\hat{\alpha}_k d_2)^2 & \Pi & \hat{\alpha}_k d_2 + 1
\end{bmatrix},
\]

where \( \Pi = d_1 + 2\hat{\alpha}_k d_2 g(\hat{x}_k, \mathbf{U}_k) + \hat{\beta}_k d_2 + \mathbf{U}_{k+1}[d_3, d_4]^T \), which has full rank if

\[
(\hat{\alpha}_k d_2 - 1) g(\hat{x}_k, \mathbf{U}_k) + [1, \hat{\beta}_k, \mathbf{U}_{k+1}] \mathbf{D} \neq 0.
\] (28)

According to our calculations, the above inequality is always satisfied so that the concerned system is locally observable.

The initial guess of the state is set as \([0.92, 1, 0]^T\), the noises are chosen as \(w_k^0 \sim N(0, 0.1^2)\), \(w_k^1 \sim N(0, 0.1^2)\), \(w_k^3 \sim N(0, 0.1^2)\), \(v_k^0 \sim N(0, 0.1^2)\), \(v_k^1 \sim N(0, 0.1^2)\), and \(v_k^2 \sim N(0, 0.01^2)\), respectively. The soft sensor prediction results of the indirect method based on EKF is shown in Figure 4.

Fig. 4. Soft sensor prediction of indirect method (a) Case 1; (b) Case 2

Applying the direct method based on KF to the cross validation data sets, the soft sensor prediction results are shown in Figure 5.

The prediction performance of different methods is compared in Table II in terms of rooted mean square error (RMSE). From Figures 4-5 and Table II, we can see that the proposed soft sensors can provide more accurate measurements of \( C_A \) than the online analyzer. Furthermore, the indirect method is superior to the direct one for both Case 1 and Case 2. While the direct method is much simpler, and its performance is also satisfactory especially for Case 1.

<table>
<thead>
<tr>
<th></th>
<th>Online analyzer</th>
<th>Indirect method</th>
<th>Direct method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.0142</td>
<td>0.0028</td>
<td>0.0054</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.0120</td>
<td>0.0018</td>
<td>0.0039</td>
</tr>
</tbody>
</table>

Table II: RMSE comparison of different measurements

B. N/C ratio soft sensor of an industrial process

Process description

High Pressure (HP) synthesis loop is a critical component in urea production process, which is mainly comprised of HP reactor, HP stripper, HP condenser and HP scrubber. The inlet of the loop is feed CO\(_2\) gas, feed NH\(_3\) solution, and recycled carbamate solution; the outlet is urea solution and purge gas stream. The main reaction taken in the HP synthesis loop is CO\(_2\) and NH\(_3\) converting to urea. In order to minimize consumption of energy and maximize yield of urea, the molar ratio between NH\(_3\) and CO\(_2\) in the reactor termed as N/C ratio needs to be controlled within a tight range. Hence, real-time measurement of the N/C ratio with high accuracy is essential to achieve this purpose.

The N/C ratio has been continuously measured by an N/C meter, utilizing the density of the urea reactor effluent stream. The online measurements are recorded every 10 minutes, but they are most of time unreliable because of temperature and pressure disturbances. Therefore, lab analysis is still conducted once a week for determining the N/C ratio. However, the deviation between these two sources of measurements is large,
which can be seen clearly from the historical data.

Due to complexity of the process, it is difficult and costly to build a first-principle model. Therefore, the data-driven approach will be investigated to develop the soft sensor for obtaining more accurate real time prediction of N/C ratio.

### Soft sensor development

The indirect method based on EKF is adopted to develop the soft sensor. First, a dynamic model is built to map the relationship between the NC meter readings $y_k$ and the measurements of 14 process variables $U_k \in \mathbb{R}^{1\times14}$, including inlet flow rates of CO$_2$ gas and NH$_3$ solution, outlet flow rate of urea solution, and several temperature measurements at different locations within the HP synthesis loop. Because the process variables are highly correlated, ordinary least squares algorithm has the problem of ill-condition and cannot obtain a robust model. Thus, the DPLS algorithm is applied to estimate the parameter vector $D \in \mathbb{R}^{16\times1}$ of the following model:

$$y_k = [1, y_{k-1}, U_k] \times D.$$  \hspace{1cm} (29)

The number of latent variables is found by cross validation to avoid model over-fitting and enhance extrapolation property. From the auto-validation and cross validation results of the DPLS model, we observe that the model prediction follows quite well the trend of the N/C meter readings, but the difference between the prediction and the lab data is still large. Therefore, the built DPLS model should be further calibrated by combining the online analyzer data with the lab data.

Considering the scaling and bias correction strategies to compensate the model mismatch, the following state-space model is constructed:

$$\begin{align*}
  x_{k+1} &= \alpha_k [1, x_k, U_k] \times D + \beta_k + w_k^x, \\
  \alpha_{k+1} &= \alpha_k + w_k^\alpha, \\
  \beta_k &= \beta_k + w_k^\beta, \\
  y_k &= x_k + v_k, \\
  y_k^O &= x_k^O + v_k^O,
\end{align*}$$  \hspace{1cm} (30)

where $x_k$ represents the real state of N/C ratio, $\alpha_k$ and $\beta_k$ are the calibration parameters, $D$ is the estimated parameter vector of (29), $y_k$ and $y_k^O$ are the online data and lab data of N/C ratio, respectively, $w_k^x, w_k^\alpha, w_k^\beta, v_k$ and $v_k^O$ are assumed to be mutually independent white noises with variances $0.2^2, 0.2^2, 0.2^2, 5.0^2$ and $5.0^2$, respectively.

According to Step 4 of the indirect method proposed in section IV, the augmented state is updated when the lab data is available by using the EKF algorithm. Otherwise, $\alpha_k$ and $\beta_k$ are kept as their previous values, and only $x_k$ is updated based on the online data by using the KF algorithm, where the dimension of the state vector is reduced to 1.

The soft sensor prediction results are shown in Figures 6 and 7. For proprietary reason, all industrial data presented in this paper have been normalized. As it was expected, the soft sensor can provide much more accurate measurements than the online N/C meter.
where $x_k$ is the real state of $O_2$ composition, $y_k$ is the online data, $y_{Tj}^L$ is the lab data, $\beta_k$ is the bias term to palliate the mismatch between the state and online data, $w_k^T, w_k^B, v_k^T$, and $v_k^B$ are assumed to be mutually independent white noises with variances $0.1^2, 0.1^2, 1.0^2$ and $0.01^2$, respectively.

The KF algorithm is applied to update the prediction $x_k$ and the bias $\beta_k$. According to the availability of lab data, the dimension of the observation equation changes as well. The soft sensor prediction results are shown in Figures 8 and 9, we can see that the prediction is much closer to the lab data compared with the online data, in the mean time, which also keeps the time trend of the online data so that the process dynamic is reflected.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig8.png}
\caption{Soft sensor prediction of the $O_2$ composition}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig9.png}
\caption{Scatter plot comparison of soft sensor prediction and online data of the $O_2$ composition}
\end{figure}

VI. Conclusions

This paper develops two adaptive soft sensors for prediction of the quality variables based on multirate data provided by online analyzers and lab analyses, where the Kalman filter or extended Kalman filter is used to integrate these two sources of measurements. The proposed soft sensors have been evaluated using a CSTR example for prediction of the reagent concentration; and practical data sets of a urea production process for prediction of the N/C ratio in a HP synthesis loop and the $O_2$ composition in a $H_2$ combustion tank. The application results show that the performance of the soft sensors is superior to the existing online analyzers.

In some chemical processes, the lab data is available with a significant time delay due to manual analysis or complexity of computation. How to appropriately handle the delay in multirate state estimation to improve the soft sensor prediction performance requires further study, especially when the exact delay is unknown.

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REFERENCES