A Support Vector Regression Approach for Recursive Simultaneous Data Reconciliation and Gross Error Detection in Nonlinear Dynamical Systems

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Abstract The quality of process data in a chemical plant significantly affects the performance and benefits gained from activities like performance monitoring, online optimization, and control. Since many chemical processes often show nonlinear dynamics, techniques like extended Kalman filter (EKF) and nonlinear dynamic data reconciliation (NDDR) have been developed to improve the data quality. Recently, the recursive nonlinear dynamic data reconciliation (RNDDR) technique has been proposed, which combines the merits of EKF and NDDR techniques. However, the RNDDR technique cannot handle measurements with gross errors. In this paper, a support vector (SV) regression approach for recursive simultaneous data reconciliation and gross error detection in nonlinear dynamical systems is proposed. SV regression is a compromise between the empirical risk and the model complexity, and for data reconciliation it is robust to random and gross errors. By minimizing the regularized risk instead of the maximum likelihood in the RNDDR, our approach could achieve not only recursive nonlinear dynamic data reconciliation but also gross error detection simultaneously. The nonlinear dynamic system simulation results in this paper show that the proposed approach is robust, efficient, stable, and accurate for simultaneous data reconciliation and gross error detection in nonlinear dynamic systems within a recursive real-time estimation framework. It can also give better performance of control.

Key words Support vector regression, data reconciliation, gross error detection, nonlinear estimation

Process data measurements are important for model fitting, process monitoring, control, optimization, and management decision making. Unfortunately, process data measurements usually contain two types of errors, random and gross, which severely impact the effects of process monitoring, control, optimization, and management decision making. Meanwhile, chemical processes usually exhibit nonlinear dynamics. So, online estimation of the process states and removal of random and gross errors from measurements are critical for the application of process monitoring, control, and optimization on dynamic nonlinear processes. This task is termed dynamic data reconciliation (or dynamic data rectification)[1−2], which is especially challenging when the state and/or measurement functions are highly nonlinear.

In order to ameliorate the effect of random errors, several different estimation methods have been proposed. For linear dynamic systems, the Kalman filters (KF) give optimal estimates in the presence of measurement uncertainties. Further, extended Kalman filters (EKF) were developed for nonlinear systems, which were based on linearizing the nonlinear equations and applying the Kalman filter to update equations to the linearized system. The advantages of the KF and EKF and their variants lie in their predictive-corrective form and the recursive nature of estimation, which allows for rapid estimation in real-time. Since the KF and EKF are not specifically designed to detect and remove outliers, a probabilistic formulation was proposed[2], which combined the EKF with the expectation-maximization (EM) algorithm to attain the rectified measurements. However, the KF and all its variants cannot take into account bounds on process variables or algebraic constraints, leading to failure of the EKF in many processes[3]. Furthermore, when the states and/or measurement equations are highly nonlinear, KF and all its variants give unsatisfactory state estimates.

An alternative approach called the recursive nonlinear dynamic data reconciliation (RNDDR) has been proposed[4], which is an extension of EKF. So, the RNDDR is preferable for online applications. Moreover, RNDDR could take account of bounds and algebraic constrains for state estimation at every instant, which has been applied to a CSTR model. However, the covariance calculations encountered in the RNDDR formulation are similar to the EKF, namely, unconstrained propagation and correction involving the Kalman gain, which can affect the accuracy of the estimates. Recently, in order to overcome this disadvantage of the RNDDR, an unscented recursive nonlinear dynamic data reconciliation (URNDDR) technique[5] was proposed, which combined the merits of the unscented Kalman filter (UKF)[6] and the RNDDR to improve accuracy of the estimates. The application of the UKF to chemical processes were recently reported[7−8]. However, both the RNDDR and URNDDR could not reduce the affects of gross errors within the measurements.

More recently, particle filters[9] have attained significant interest with respect to state estimation, and an application of particle filters to dynamic data reconciliation was proposed[10], whose goal was to attain satisfactory state estimates and to detect the presence of gross errors. Though the particle filters approach could achieve more accuracy estimates, it usually takes much time and cannot take account of bounds and algebraic constrains for the state estimation.

Simultaneous data reconciliation and gross error detection can be addressed as a model identification and parameter estimation problem, since gross errors could be considered as parameters in the data reconciliation model, which could be estimated by using the reconciled values of the process variables[11]. Since simultaneous data reconciliation and gross error detection can be addressed as model identification and parameter estimation problem, support vector (SV) regression is introduced. The SV algorithm is a nonlinear generalization of the generalized portrait algorithm developed in Russia in the sixties of last century. As such, it is firmly grounded in the framework of statistical

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learning theory, or Vapnik-Chervonenkis (VC) theory, which has been developed over the last three decades by Vapnik[12] and others. According to statistical learning theory, minimizing empirical risk, which will lead to overfitting and thus bad generalization properties, is replaced by minimizing regularized risk with adding a capacity control term to the objective function[13]. Within the framework of statistical learning theory, or VC theory, the effects of gross errors could be considered as VC dimension, so the effects of gross errors could be eliminated from the estimation of real state variables. With minimizing the regularized risk instead of the maximum likelihood in the RNDDR, our approach could achieve not only recursive nonlinear dynamic data reconciliation but also gross error detection simultaneously. Meanwhile, we use filtered state estimates and measurements to estimate real states at right instant, so the predicted state estimates are not necessary in our approach, which overcomes the effects of the unaccurate covariance calculations in the linearized nonlinear dynamic system model.

In this paper, the merits of the RNDDR and SV regression are combined to obtain an SV regression approach for recursive simultaneous data reconciliation and gross error detection in nonlinear dynamic systems. Since this integration is achieved without sacrificing the recursive nature of the estimation procedure, a more accurate and efficient real-time recursive simultaneous data reconciliation and gross error detection for nonlinear dynamic processes is obtained. The execution of a comparative study between optimization approach RNDDR and our approach is considered in this paper, but probabilistic filtering methods are beyond the scope of this paper.

1 Recursive estimation techniques

In order to motivate the development of our approach, we first give a brief description of two recursive estimation techniques for nonlinear dynamic processes, the extended Kalman filters (EKF), and recursive nonlinear dynamic data reconciliation (RNDDR), which is based on Kalman filter.

Consider a process described by the following continuous-time nonlinear state space model with additive uncertainties (state noise) and discrete measurements sampled data at regular intervals:

$$\begin{aligned} \boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + \int_{k\Delta t}^{(k+1)\Delta t} \boldsymbol{f}\left(\boldsymbol{x}\left(\tau\right), \boldsymbol{u}_k\right) \mathrm{d}\tau + \boldsymbol{w}_k \\ \boldsymbol{y}_{k+1} &= \boldsymbol{g}\left(\boldsymbol{x}_{k+1}\right) + \boldsymbol{v}_{k+1} \end{aligned} \tag{1}$$

In the above model, $\boldsymbol{x}_{k+1}$ is the $n \times 1$ vector of state variables, $\boldsymbol{y}_{k+1}$ is the $m \times 1$ vector of measurements, and $\boldsymbol{w}_k$ and $\boldsymbol{v}_{k+1}$ are mutually independent normally distributed random variables with covariance matrices Q_k and R_{k+1}, respectively. The subscript k represents time instant $t_k = k\Delta t$.

Assume that at time t_k we have filtered state estimates denoted by $\hat{\boldsymbol{x}}_{k|k}$ which have been obtained using all the measurements up to time t_k. From these, the predicted state estimates $\hat{\boldsymbol{x}}_{k+1|k}$ at time t_{k+1} are obtained as

$$\begin{aligned} \hat{\boldsymbol{x}}_{k+1|k} &= \hat{\boldsymbol{x}}_{k|k} + \int_{k\Delta t}^{(k+1)\Delta t} \boldsymbol{f}\left(\boldsymbol{x}\left(\tau\right), \boldsymbol{u}_k\right) \mathrm{d}\tau + \boldsymbol{w}_k \\ \hat{\boldsymbol{x}}_{k|k} &\equiv \hat{\boldsymbol{x}}\left(k\Delta t\right) \end{aligned} \tag{2}$$

The predicted state estimates are corrected using the measurements $\boldsymbol{y}_{k+1}$, and by using the following linear update equation to obtain the filtered state estimates at time t_{k+1}.

$$\hat{\boldsymbol{x}}_{k+1|k+1} = \hat{\boldsymbol{x}}_{k+1|k} + K_{k+1}\boldsymbol{V}_{k+1} \tag{3}$$

where

$$\boldsymbol{V}_{k+1} = \boldsymbol{y}_{k+1} - \boldsymbol{g}\left(\hat{\boldsymbol{x}}_{k+1|k}\right) \tag{4}$$

and matrix K_{k+1} is known as the Kalman gain. The computation of the Kalman gain for the EKF is described in the following section.

1.1 Extended Kalman filter (EKF)

Assume the covariance matrix of errors in the filtered state estimates at time t_k is given by $P_{k|k}$. In EKF, the covariance matrix of errors in the predicted state estimates at time t_{k+1} is approximated by linearizing the nonlinear state space model around $\hat{\boldsymbol{x}}_{k|k}$. The state space matrix for the linearized continuous time model is given by

$$A_k = \frac{\partial \boldsymbol{f}\left(\boldsymbol{x}, \boldsymbol{u}\right)}{\partial \boldsymbol{x}} \Big| \hat{\boldsymbol{x}}_{k|k}, \boldsymbol{u}_k \tag{5}$$

The covariance matrix of estimation errors in the predicted estimates is obtained as

$$P_{k+1|k} = \bar{A}_k P_{k|k} \bar{A}^{\mathrm{T}} + Q_k \tag{6}$$

where $\bar{A}_k = \exp\left(A_k \Delta t\right)$ is the state transition matrix for the equivalent linear discrete system. The Kalman gain matrix is computed using

$$K_{k+1} = P_{k+1|k} G_{k+1}^{\mathrm{T}} \left(G_{k+1} P_{k+1|k} G_{k+1}^{\mathrm{T}} + R_{k+1}\right)^{-1} \tag{7}$$

where G_{k+1} is the linearized measurement model matrix given by $G_{k+1} = \frac{\partial \boldsymbol{g}(\boldsymbol{x})}{\partial \boldsymbol{x}} | \hat{\boldsymbol{x}}_{k+1|k}$. The covariance matrix of errors in the updated state estimates is approximated using

$$P_{k+1|k+1} = \left(I - K_{k+1} G_{k+1}\right) P_{k+1|k} \tag{8}$$

There are several drawbacks associated with EKF, that is, EKF cannot ensure the estimated states to satisfy bounds and other algebraic constraints, and the covariance matrix of estimation errors and Kalman gain are calculated using an approximated linear model of the process which can have an adverse effect on the accuracy of the state estimates. Furthermore, EKF cannot eliminate the effects of gross errors within the measurements.

1.2 Recursive nonlinear dynamic data reconciliation

The update equation for KF as well as EKF can be obtained as the solution of an optimization problem[4]. So the RNDDR method was developed, which can take account of algebraic constraints and bound constraints to be satisfied by state estimates.

Consider the nonlinear dynamic system given by (1). The bounds and algebraic constraints of states are $\boldsymbol{x}_{\mathrm{L}} \leq \boldsymbol{x} \leq \boldsymbol{x}_{\mathrm{U}}$, and algebraic constraints of states are $h\left(\boldsymbol{x}, \boldsymbol{u}\right) \leq 0$, $e\left(\boldsymbol{x}, \boldsymbol{u}\right) = 0$. Let $\hat{\boldsymbol{x}}_{k|k}$ be the filtered estimates at time instant k and the corresponding estimate error covariance matrix be $P_{k|k}$. In the RNDDR method, the predicted state and the covariance matrix of errors in the predicted estimates are obtained as in EKF using (2) and (6), and instead of using (3), the updated state estimates in the RNDDR method are obtained by solving the

following optimization problem:

$$\begin{aligned}\min_{\hat{\boldsymbol{x}}_{k+1|k+1}} & \left(\hat{\boldsymbol{x}}_{k+1|k}-\hat{\boldsymbol{x}}_{k+1|k+1}\right)^{\mathrm{T}}\left(P_{k+1|k}\right)^{-1}\times \\ & \left(\hat{\boldsymbol{x}}_{k+1|k}-\hat{\boldsymbol{x}}_{k+1|k+1}\right)+\left(\hat{\boldsymbol{y}}_{k+1}-\boldsymbol{g}\left(\hat{\boldsymbol{x}}_{k+1|k+1}\right)\right)^{\mathrm{T}} \\ & R_{k+1}^{-1}\left(\hat{\boldsymbol{y}}_{k+1}-\boldsymbol{g}\left(\hat{\boldsymbol{x}}_{k+1|k+1}\right)\right) \\ \text{s.t.} \quad & \boldsymbol{x}_{\mathrm{L}}\leq\hat{\boldsymbol{x}}_{k+1|k}\leq\boldsymbol{x}_{\mathrm{U}} \\ & h\left(\hat{\boldsymbol{x}}_{k+1|k},\boldsymbol{u}_k\right)\leq 0 \\ & e\left(\hat{\boldsymbol{x}}_{k+1|k},\boldsymbol{u}_k\right)=0\end{aligned} \tag{9}$$

Though the above step does not require the measurement model to be linearized, the covariance matrix of the error in the updated estimates in the RNDDR method is still computed using linearized system formulations, which will still be not so accurate. As the same as EKF, the RNDDR could not deal with gross errors within the measurements. We will address these limitations by exploiting the support vector regression approach.

2 Support vector regression approach for gross error detection

2.1 Support vector machines and SV regression

Support vector machines bring out a breakthrough of learning algorithms, which are supported by results of the statistical learning theory. SV regression estimation seeks to estimate function as

$$s\left(\boldsymbol{x}\right)=\left(\boldsymbol{w}\cdot\boldsymbol{x}\right)+B,\quad \boldsymbol{w},\boldsymbol{x}\in\mathbf{R}^N,\ B\in\mathbf{R} \tag{10}$$

based on data

$$\left(\boldsymbol{x}_1,y_1\right),\cdots,\left(\boldsymbol{x}_l,y_l\right)\in\mathbf{R}^N\times\mathbf{R} \tag{11}$$

by minimizing the regularized risk functional

$$\min_{\boldsymbol{w},R_{\mathrm{emp}}^{\varepsilon}}\ \frac{\|\boldsymbol{w}\|^2}{2}+C\cdot R_{\mathrm{emp}}^{\varepsilon} \tag{12}$$

where C is a constant determining the trade-off between minimizing the training error, or empirical risk $R_{\mathrm{emp}}^{\varepsilon}$, and the model complexity term $\|\boldsymbol{w}\|^2$.

The main insight of the statistical learning theory is that in order to obtain a small risk, both training error and model complexity should be controlled.

2.2 Gross error detection based on SV regression

The measurement model without gross error can be written as

$$\boldsymbol{y}=\boldsymbol{x}+\boldsymbol{\varepsilon} \tag{13}$$

$$l\left(\boldsymbol{x}\right)=0 \tag{14}$$

where $\boldsymbol{x}$ is the vector of true values of the variables, $\boldsymbol{y}$ is the vector of measurements, $\boldsymbol{\varepsilon}$ is the vector of random errors which is assumed to follow a normal distribution $\mathrm{N_z}\left(0,\boldsymbol{\Psi}\right)$, and $l\left(\boldsymbol{x}\right)$ is the constraints of $\boldsymbol{x}$.

If gross errors are present in process measurements, the measurement bias model for biases of unknown magnitude μ is given by

$$\boldsymbol{y}=\boldsymbol{x}+\boldsymbol{\varepsilon}+\left[b_1\mu_1,b_2\mu_2,\cdots,b_i\mu_i,\cdots,b_n\mu_n\right]^{\mathrm{T}} \tag{15}$$

where n is the number of measurements, and b_i is an indicator, which indicates the location of biases in the model, and can be defined as

$$b_i=\begin{cases}0, & \text{if no gross error presents in the } i\text{th measurement}\\ 1, & \text{if gross error presents in the } i\text{th measurement}\end{cases} \tag{16}$$

The virtual purpose of data reconciliation and gross error detection is to estimate the true values $\boldsymbol{x}$ of the measurements based on the measurements data. If $\boldsymbol{x}$ is also obtained in prior like $\boldsymbol{y}$, the only task remained is to determine the measurement bias model described in (15). Meanwhile, the data reconciliation and gross error detection problem could be addressed as a regression problem, which seeks to estimate the function in (15) based on data set $\left(\boldsymbol{x}_1,\boldsymbol{y}_1\right),\left(\boldsymbol{x}_2,\boldsymbol{y}_2\right),\cdots,\left(\boldsymbol{x}_m,\boldsymbol{y}_m\right)$.

Actually, $\boldsymbol{x}$ could not be obtained in prior, however, the constraints of $\boldsymbol{x}$ can be obtained instead, which are defined by the model of process. Then, a regression problem with a larger degree of freedom is formulated, which aims to estimate the function

$$\boldsymbol{y}=\boldsymbol{x}+\boldsymbol{\varepsilon}+\left[b_1\mu_1,b_2\mu_2,\cdots,b_i\mu_i,\cdots,b_n\mu_n\right]^{\mathrm{T}}$$

$$b_i=\begin{cases}0, & \text{if no gross error presents in the } i\text{th measurement}\\ 1, & \text{if gross error presents in the } i\text{th measurement}\end{cases} \tag{17}$$

based on data

$$l\left(\boldsymbol{x}\right)=0 \tag{18}$$

For the given regression problem proposed in (17) and (18), SV regression is introduced. As the function of (17) is linear, according to Vapnik[12], the VC dimension of (17) is the number of free parameters, which defines the complexity of the measurement bias model and can be written as

$$\sum_{i=1}^{n}b_i \tag{19}$$

So according to (12) and (19), the regularized risk of regression for data reconciliation and gross error detection is

$$\sum_{i=1}^{n}a_ib_i+R_{\mathrm{emp}}^{\varepsilon} \tag{20}$$

We use a_i instead of C to compromise between $\sum_{i=1}^{n}b_i$ and $R_{\mathrm{emp}}^{\varepsilon}$, because the coefficients of b_i relative to the nonredundant measurements should be different to others, as will be discussed in the Subsection 3.2.

3 Proposed support vector regression approach

3.1 Support vector regression recursive nonlinear dynamic data reconciliation and gross error detection

It can be seen from (9) that the RNDDR actually uses empirical risk as the object function. In order to detect gross error in measurements, we replace the empirical risk in the RNDDR with (20). Meanwhile, to avoid calculating $P_{k+1|k}$ by linearizing the system formulation and obtain the constraints described in (18), we use filtered states $\hat{\boldsymbol{x}}_{k|k}$ and $\boldsymbol{y}_{k+1}$ instead of $\hat{\boldsymbol{x}}_{k+1|k}$ and $\boldsymbol{y}_{k+1}$ to estimate states $\hat{\boldsymbol{x}}_{k+1|k+1}$.

Considering the system in (2), we first introduce some new variables $\bar{\boldsymbol{x}}_k$ and $\bar{\boldsymbol{x}}_{k+1}$ as

$$\begin{aligned}\bar{\boldsymbol{x}}_{k|k}&=\hat{\boldsymbol{x}}_{k|k}+\boldsymbol{s}_k\\ \bar{\boldsymbol{x}}_{k+1|k}&=\bar{\boldsymbol{x}}_{k|k}+\int_{k\Delta t}^{(k+1)\Delta t}\boldsymbol{f}\left(\boldsymbol{x}\left(\tau\right),\boldsymbol{u}_k\right)\mathrm{d}\tau\\ \hat{\boldsymbol{x}}_{k|k+1}&=\bar{\boldsymbol{x}}_{k+1|k}+\boldsymbol{w}_k\end{aligned} \tag{21}$$

where we consider $\bar{\boldsymbol{x}}_k$ and $\bar{\boldsymbol{x}}_{k+1}$ to be the true values of states, and S_k is the covariance matrix of $\boldsymbol{s}_k$. Because $\boldsymbol{w}_k$ and $\boldsymbol{v}_{k+1}$ are usually independent identically distribution, we assume S_k, Q_k, and R_{k+1} be diagonal matrices, and $\bar{S}_k$,

$\bar{Q}_k$, and $\bar{R}_{k+1}$ are the vectors constructed of the diagonal elements of S_k, Q_k, and R_{k+1}, respectively. S_k could be determined by

$$\begin{aligned}\min_{\bar{\boldsymbol{S}}_k} \quad & \left(\bar{\boldsymbol{Q}}_k-\bar{\boldsymbol{S}}_k\right)^{\mathrm{T}}\left(Q_k\right)^{-1}\left(\bar{\boldsymbol{Q}}_k-\bar{\boldsymbol{S}}_k\right)+\\ & \left(\bar{\boldsymbol{R}}_{k+1}-G_k\cdot\bar{\boldsymbol{S}}_k\right)^{\mathrm{T}}\left(R_{k+1}\right)^{-1}\left(\bar{\boldsymbol{R}}_{k+1}-G_k\cdot\bar{\boldsymbol{S}}_k\right)\end{aligned} \tag{22}$$

where

$$G_k=\left.\frac{\partial \boldsymbol{g}\left(\boldsymbol{x}\right)}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}=\hat{\boldsymbol{x}}_{k|k}} \tag{23}$$

From (1) and (21), it can be seen that

$$\boldsymbol{y}_{k+1} \quad = \quad \boldsymbol{g}\left(\bar{\boldsymbol{x}}_{k+1|k}+\boldsymbol{w}_k\right)+\boldsymbol{v}_{k+1} \tag{24}$$

where W_k is the addition covariance caused by $\boldsymbol{w}_k$ through the measurement function, which can be calculated by $\boldsymbol{g}\left(\boldsymbol{x}\right)$ and the properties of covariance.

If the RNDDR is used to estimate $\bar{\boldsymbol{x}}_{k+1|k}$, it is as

$$\begin{aligned}\min_{\bar{\boldsymbol{x}}_{k|k}} \quad & \left(\hat{\boldsymbol{x}}_{k|k}-\bar{\boldsymbol{x}}_{k|k}\right)^{\mathrm{T}}\left(S_k\right)^{-1}\left(\hat{\boldsymbol{x}}_{k|k}-\bar{\boldsymbol{x}}_{k|k}\right)+\\ & \left(\boldsymbol{y}_{k+1}-\boldsymbol{g}\left(\bar{\boldsymbol{x}}_{k+1|k}\right)\right)^{\mathrm{T}}\left(W_k+R_{k+1}\right)^{-1}\left(\boldsymbol{y}_{k+1}-\boldsymbol{g}\left(\bar{\boldsymbol{x}}_{k+1|k}\right)\right)\\ \text{s.t.} \quad & \bar{\boldsymbol{x}}_{k+1|k}=\bar{\boldsymbol{x}}_{k|k}+\int_{k\Delta t}^{(k+1)\Delta t}\boldsymbol{f}(\boldsymbol{x}\left(\tau\right),\boldsymbol{u}_k)\,\mathrm{d}\tau\\ & \boldsymbol{x}_{\mathrm{L}}\le\bar{\boldsymbol{x}}_{k+1|k}\le\boldsymbol{x}_{\mathrm{U}}\\ & h\left(\bar{\boldsymbol{x}}_{k+1|k},\boldsymbol{u}_k\right)\le 0\\ & e\left(\bar{\boldsymbol{x}}_{k+1|k},\boldsymbol{u}_k\right)=0\end{aligned} \tag{25}$$

From (17), (18), (20), and (25), instead of minimizing the empirical risk, we minimize structural risk considering with the gross errors as

$$\begin{aligned}\min_{\bar{\boldsymbol{x}}_{k|k},\boldsymbol{\mu},\boldsymbol{b}} \quad & \boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}+\left(\hat{\boldsymbol{x}}_{k|k}-\bar{\boldsymbol{x}}_{k|k}\right)^{\mathrm{T}}\left(S_k\right)^{-1}\left(\hat{\boldsymbol{x}}_{k|k}-\bar{\boldsymbol{x}}_{k|k}\right)+\\ & \left(\boldsymbol{y}_{k+1}-\boldsymbol{Y}-\boldsymbol{\mu}\right)^{\mathrm{T}}\left(W_k+R_{k+1}\right)^{-1}\left(\boldsymbol{y}_{k+1}-\boldsymbol{Y}-\boldsymbol{\mu}\right)\end{aligned} \tag{26}$$

s.t.

$$l\left(\boldsymbol{x}\right)=\left\{\begin{array}{c}\bar{\boldsymbol{x}}_{k+1|k}-\bar{\boldsymbol{x}}_{k|k}-\displaystyle\int_{k\Delta t}^{(k+1)\Delta t}\boldsymbol{f}\left(\boldsymbol{x}\left(\tau\right),\boldsymbol{u}_k\right)\mathrm{d}\tau=\boldsymbol{0}\\ \boldsymbol{Y}-\boldsymbol{g}\left(\bar{\boldsymbol{x}}_{k+1|k}\right)=\boldsymbol{0}\\ \boldsymbol{\mu}_{\mathrm{L}}\boldsymbol{b}\le\boldsymbol{\mu}\le\boldsymbol{\mu}_{\mathrm{U}}\boldsymbol{b}\\ \boldsymbol{x}_{\mathrm{L}}\le\bar{\boldsymbol{x}}_{k+1|k}\le\boldsymbol{x}_{\mathrm{U}}\\ \boldsymbol{b}=binary\\ h\left(\bar{\boldsymbol{x}}_{k+1|k},\boldsymbol{u}_k\right)\le 0\\ e\left(\bar{\boldsymbol{x}}_{k+1|k},\boldsymbol{u}_k\right)=0\end{array}\right. \tag{27}$$

where $\boldsymbol{b}$ is a binary vector to indicate which measurement has gross error, $\boldsymbol{a}$ is the coefficient vector of $\boldsymbol{b}$, $\boldsymbol{\mu}_{\mathrm{L}}$, and $\boldsymbol{\mu}_{\mathrm{U}}$ are the lower and upper bounds of gross error value $\boldsymbol{\mu}$. We use $\boldsymbol{Y}$ in order to make (27) easy to be understood in the form of SV regression, and it is just $\boldsymbol{g}\left(\bar{\boldsymbol{x}}_{k+1|k}\right)$.

The integration in the optimization problem of (27) can be dealt with in two ways. One approach is to incorporate the nonlinear differential equations in the solution strategy by embedding — also called the sequential approach — in which only the initial state estimates are treated as decision variables, and the differential equations are integrated using an initial value ordinary differential equation (ODE) solver to generate the estimates for all instants within the time interval[14]. The alternative is to use a simultaneous approach, in which the differential equations are converted to algebraic equations by some form of discretization, and solving the resulting constrained optimization problem[1]. In general, the simultaneous approach is computationally more efficient than the sequential strategy, and it is used in this paper. In this work, we make use a collocation on finite element method based on Lagrangian polynomials to discretize the differential equations. This kind of problem is also an optimization problem of differential algebraic equations (DAE), which has been discussed and solved by sequential quadratic program (SQP)[15]. The optimization problem of (26) and (27) is a mixed integer nonlinear program, which can be figured out by branch-and-bound method with SQP[16] as well. In this paper, we used the Lingo to solve the optimization problem.

From (26) and (27), we can obtain the estimate states $\bar{\boldsymbol{x}}_{k+1|k}$ and $\boldsymbol{\mu}$. As the covariance in (26) is larger than the measurement covariance, the true values of the gross errors estimated $\boldsymbol{\mu}$ should be compensated as

$$\bar{\boldsymbol{\mu}}=\left\{\begin{array}{ll}\boldsymbol{\mu}+\bar{\boldsymbol{R}}_{k+1}, & \boldsymbol{\mu}>0\\ \boldsymbol{\mu}-\bar{\boldsymbol{R}}_{k+1}, & \boldsymbol{\mu}<0\end{array}\right. \tag{28}$$

Then, $\bar{\boldsymbol{x}}_{k+1|k}$, $\boldsymbol{y}_{k+1}$, and $\bar{\boldsymbol{\mu}}$ are used to estimate real states $\hat{\boldsymbol{x}}_{k+1|k}$ as

$$\begin{aligned}\min_{\hat{\boldsymbol{x}}_{k+1|k+1}} \quad & \left(\hat{\boldsymbol{x}}_{k+1|k+1}-\bar{\boldsymbol{x}}_{k+1|k}\right)^{\mathrm{T}}Q_k^{-1}\left(\hat{\boldsymbol{x}}_{k+1|k+1}-\bar{\boldsymbol{x}}_{k+1|k}\right)+\\ & \left(\boldsymbol{y}_{k+1}-\boldsymbol{g}\left(\hat{\boldsymbol{x}}_{k+1|k+1}\right)-\bar{\boldsymbol{\mu}}\right)^{\mathrm{T}}R_{k+1}^{-1}\left(\boldsymbol{y}_{k+1}-\boldsymbol{g}\left(\hat{\boldsymbol{x}}_{k+1|k+1}\right)-\bar{\boldsymbol{\mu}}\right)\\ \text{s.t.} \quad & \boldsymbol{x}_{\mathrm{L}}\le\hat{\boldsymbol{x}}_{k+1|k+1}\le\boldsymbol{x}_{\mathrm{U}}\\ & h\left(\hat{\boldsymbol{x}}_{k+1|k+1},\boldsymbol{u}_k\right)\le 0\\ & e\left(\hat{\boldsymbol{x}}_{k+1|k+1},\boldsymbol{u}_k\right)=0\end{aligned} \tag{29}$$

Finally, we can see that the proposed SV approach is a two-stepped procedure, which first simultaneously estimates $\bar{\boldsymbol{x}}_{k+1|k}$ and detects gross errors $\bar{\boldsymbol{\mu}}$, then uses $\bar{\boldsymbol{x}}_{k+1|k}$, $\bar{\boldsymbol{\mu}}$, and $\boldsymbol{y}_{k+1}$ to estimate $\hat{\boldsymbol{x}}_{k+1|k+1}$. This approach does not need to calculate the predictive covariance matrix $P_{k+1|k}$ and $P_{k+1|k+1}$ by approximating linearized system model, and it is a recursive method for simultaneous data reconciliation and gross error detection which makes it preferable for online application.

3.2 Coefficient selection

According to Vapnik[12], the coefficients, which determine the trade-off between minimizing the empirical risk and the model complexity term, are robust to the result of SV regression problem. In the SV regression approach for data reconciliation and gross error detection, the value of the coefficient $\boldsymbol{a}$ determines how sensitive the SV regression approach is to gross errors, and it is also robust to the result of data reconciliation. So, the value of coefficient $\boldsymbol{a}$ has little impact on reconciled results. However, the smaller the coefficient $\boldsymbol{a}$ is, the more sensitive the SV regression approach is to gross errors. If the coefficient $\boldsymbol{a}$ is too small, then random errors would be reconciled as gross errors by mistake. On the other hand, if the coefficient $\boldsymbol{a}$ is too large, gross errors could not be detected, which would have severe impact on the result of data reconciliation. In this paper, we propose a general method for selecting this coefficient.

If all measurements are redundant, the coefficient can be determined as

$$a_i=2\left(\frac{\lambda_i}{\delta_i}\right)^2 \tag{30}$$

where a_i is the coefficient relative to the i-th measurement, λ_i is the lower bound of the gross error relative to the i-th measurement, and δ_i is the standard deviation of the i-th measurement.

To make our approach reasonable, we set the lower bounds of gross errors to be 3 times the value of standard deviation of measurements.

$$\lambda_i = 3\delta_i \tag{31}$$

Consequently, if the measurements are all redundant, the coefficients are identical to be 18, and $\boldsymbol{a}$ is equivalent to C in (12). However, measurements are usually nonredundant, a case of nonredundant measurements is

$$Y = g(y_m, y_u) \tag{32}$$

where $g(\cdot,\cdot)$ is a measurement function, Y is a measured variable, y_m is a measured state variable, y_u is an unmeasured state variable, so Y, y_m, and y_u are nonredundant. In this case, the gross errors present in Y are equivalent to those in y_m[17].

In order to make the proposed SV regression approach work in this case, the coefficient of Y should be as

$$a_Y = \left(\frac{\lambda_Y + \Delta g_m \cdot \lambda_m + \Delta g_u \cdot \lambda_u}{\delta_Y}\right)^2 \tag{33}$$

where

$$\begin{aligned} \Delta g_m &= \left.\frac{\partial g(y_m, y_u)}{\partial y_m}\right|_{y_u=\hat{x}_{k+1|k,u}} \\ \Delta g_u &= \left.\frac{\partial g(y_m, y_u)}{\partial y_u}\right|_{y_u=\hat{x}_{k+1|k,u}} \end{aligned} \tag{34}$$

where a_Y is the coefficient relative to Y. λ_Y, λ_m, and λ_u are the lower bounds of the gross errors relative to Y, y_m, and y_u, respectively. δ_Y is the standard deviation of the measurement Y. Because y_u is unmeasured, we use $\hat{x}_{k+1|k,u}$, the estimates of y_u, to calculate Δg_m and Δg_u.

Similar to the case of redundant measurements, to make our approach reasonable, we set the lower bounds of gross errors relative to measured variables to be 3 times the values of standard deviation of measurements, and set the lower bounds of gross errors relative to unmeasured variables to be the values of standard deviations of states.

4 Case study

4.1 Continuous-flow stirred tank reactor description

The schematic of the continuous-flow stirred tank reactor (CSTR) system is shown in Fig. 1. The process involves an exothermic reaction $A_{(l)} \rightarrow B_{(l)} + C_{(l)}$. The temperature in the reactor is controlled by manipulating the flow rate of the coolant flowing through the jacket. The level in the reactor is controlled by manipulating the outlet flow rate from the reactor. The pressure in the reactor is controlled by changing the vent gas flow rate. PI controllers are used to control the temperature, volume, and pressure of the reactor. Both the reactor and the jacket are modeled with perfectly mixed tank dynamics.

The reactor holdup at any time is given by

$$\frac{\mathrm{d}V}{\mathrm{d}t} = F_i - F \tag{35}$$

The reactant concentration C_A is given by

$$\frac{\mathrm{d}C_A}{\mathrm{d}t} = \frac{F_i}{V}(C_{Ai} - C_A) - r_A \tag{36}$$

With constant heat capacities and densities, an overall heat balance on the reactor gives the reactor temperature as

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{F_i}{V}(T_i - T) + \frac{r_A(-\Delta H)}{\rho C_P} - \frac{UA(T - T_C)}{V\rho C_P} \tag{37}$$

Overall heat balance on the jacket gives the coolant temperature as

$$\frac{\mathrm{d}T_C}{\mathrm{d}t} = \frac{F_C}{V_j}(T_{Ci} - T_C) + \frac{UA(T - T_C)}{V_j \rho_j C_{Pj}} \tag{38}$$

The pressure in the reactor depends on the number of moles of vapor n. This in turn depends on the rate of reaction and vent (molar) flow rate F_{Vg}. The vapor space V_g is assumed to be constant and vapor is assumed to behave ideally

$$\frac{\mathrm{d}n}{\mathrm{d}t} = r_A V - F_{Vg} \tag{39}$$

$$PV_g = nRT \tag{40}$$

The reaction rate is given as

$$r_A = C_d C_A k_0 \mathrm{e}^{-E/RT} \tag{41}$$

Table 1 Parameters for the CSTR of Fig. 1

Notation	Variable	(Steady state/Constant) Value
V	Volume of liquid in reactor	48 ft^3
C_A	Reactant concentration in reactor	0.2345 lb · mol A/ft^3
T	Reactor temperature	600 °R
n	Number of moles in gas phase of reactor	28.3656 lb · mol C
V_g	Volume of gas phase (constant)	16 ft^3
F_i	Inlet feed flow rate	40 ft^3/h
C_{Ai}	Inlet reactant concentration	0.5 lb · mol A/ft^3
T_C	Jacket temperature	590.51 °R
F_C	Coolant flow rate	56.626 ft^3/h
T_i	Inlet feed temperature	530 °R
V_j	Volume of jacket	3.85 ft^3
k_0	Frequency factor	7.08×10^{10} h^{-1}
C_d	Catalyst activity	1 or 0.7
E	Activation energy	29 900 Btu/lb · mol
R	Universal gas constant	1.99 Btu/lb · mol°R
U	Heat transfer coefficient	150 Btu/h · ft^2°R
A	Heat transfer area	150 ft^2
T_{Ci}	Inlet coolant temperature	530 °R
ΔH	Heat of reaction	−30 000 Btu/lb · mol
C_p	Heat capacity (process side)	0.75 Btu/lbm°R
C_j	Heat capacity (coolant side)	1 Btu/lbm°R
ρ	Density of process mixture	50 lbm/ft^3
ρ_j	Density of coolant for volume	62.3 lbm/ft^3
K_v	PI controller parameter for volume	1
T_v	PI controller parameter for volume	1
K_t	PI controller parameter for temperature	4.3
T_t	PI controller parameter for temperature	0.0541
K_p	PI controller parameter for pressure	0.5
T_p	PI controller parameter for pressure	4

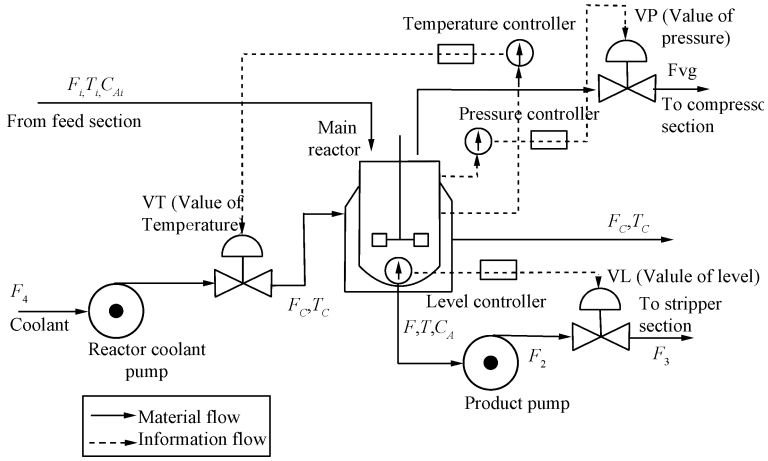

Fig. 1 Continuous flow stirred tank reactor (CSTR)

Without no accumulation in the pumps, valves, and jacket, the following relations are obtained:

$$F_3 = F_2 = F \tag{42}$$

$$F_4 = F_C = F_{Ci} \tag{43}$$

It is assumed that in addition to the three controlled variables, the reactor concentration and coolant outlet temperatures are also measured using a regular sampling period of 3 min. It should noted that the four state variables — V, T, T_C, and C_A — are measured directly.

Whereas the measured pressure is a nonlinear function of the state variables n and T. Therefore, this is an nonredundant nonlinear measurements case. The parameters for the CSTR are shown in Table 1. More details of the case study can be found in Vachhani[4].

For both the RNDDR and the SV regression approaches, we used the same parameters of the CSTR, the same standard deviations, the same PI controllers, and the same controller set values. States noise with standard deviations $0.5\,\mathrm{ft}^3$, $0.1\,\mathrm{lb}\cdot\mathrm{mol}\cdot\mathrm{C}$, $0.708\,^\circ R$, $0.005\,\mathrm{lb}\cdot\mathrm{mol\,A/ft}^3$, and $0.708\,^\circ R$ for V, n, T, C_A, and T_C were introduced. Measurements noises with standard deviations $0.5\,\mathrm{ft}^3$, $2\,\mathrm{lb}\cdot\mathrm{mol\,A/ft}^3$, $0.708\,^\circ R$, $0.005\,\mathrm{lb}\cdot\mathrm{mol\ A/ft3}$, and $0.708\,^\circ R$ were added to the measurements for V, n, T, C_A and T_C. We simulated the process of the CSTR within 5 hours, which generated 100 sampling instants. In every simulation, 10 % measurements were corrupted by gross errors, and the corrupted measurements were chosen randomly with an equal probability. The sign of the gross errors were randomly assigned either "+" or "−" with an equal probability. The magnitudes of the gross errors were taken to be between 10 times and 40 times the value of the standard deviations with an equal probability. We used a collocation method based on 3-order Lagrangian polynomials to discretize the differential equations. The CSTR was controlled by PI controller and we used the estimates as the feedback values to the controller, and the controller set values of V, T, and P were 48, 600, and 2 116, respectively, for both the RNDDR and the SV regression approaches in all the simulations.

For implementing the RNDDR, the initial estimation error covariance matrix P_0 was chosen to be diagonal. The standard deviations of the errors in the initial estimates of state variables V, n, T, C_A, and T_C were chosen to be equal to the standard deviations of their respective states errors. The application used to generate data of the simulations was developed in Matlab. The support vector regression problems and the RNDDR were solved using LINGO optimization software invoked by Visual Basic.

4.2 Comparison between the RNDDR and the SV regression approaches

First, we used the same random and gross errors to study the performances of the RNDDR and the SV regression approaches. The simulations were carried out with the Catalyst activity C_d as a constant, which was equal to 1. Meanwhile, in order to reveal the robustness of the coefficient in the SV regression approach, we used the controller set values to calculate the coefficient vector $\boldsymbol{a}$, which was a constant, $\boldsymbol{a} = [18, 18, 18, 18, 99.89]^{\mathrm{T}}$ relative to V, C_A, T, T_C, and P, respectively.

Figs. 2 ∼ 7 show the simulation results of the RNDDR, and Figs. 8 ∼ 13 display the results of SV regression approach for data reconciliation and gross error detection. From the figures we can observe that the estimates of the RNDDR method are corrupted by gross errors heavily because the RNDDR could not detect any gross error in measurements. With the corrupted estimates by the RNDDR as the feedback values to controllers, the states fluctuated tempestuously and they began to deviate from the set values. Especially, the pressure deviated much far away from the set value, which was 1 782.398 at the end time, whereas the set value was 2 116. Furthermore, the curve of pressure indicates a further deviation from the set value at the end time.

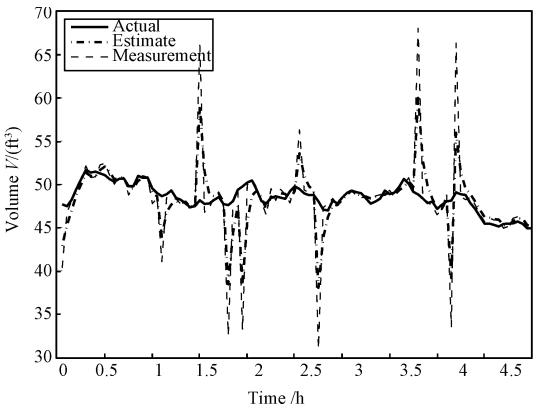

Fig. 2 The state V estimates by RNDDR

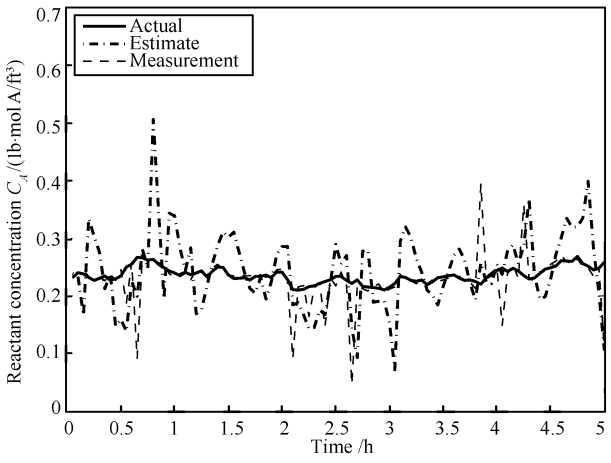

Fig. 3 The state C_A estimates by RNDDR

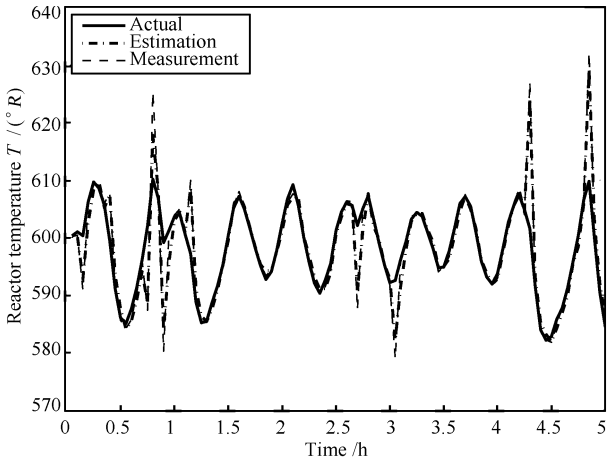

Fig. 4 The state T estimates by RNDDR

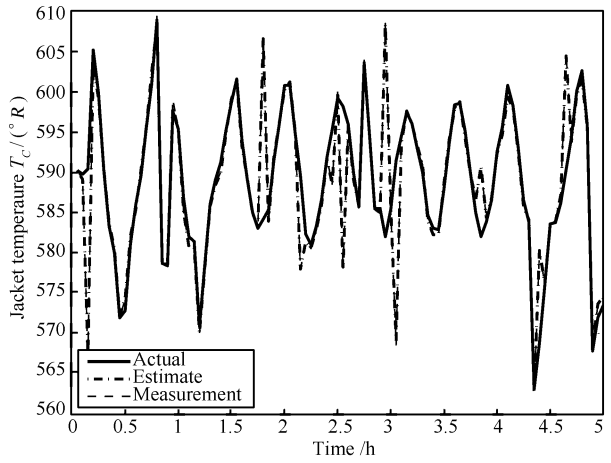

Fig. 5 The state T_C estimates by RNDDR

From the results of our approach, it is clear that the SV regression data reconciliation and gross error detection can detect most of the gross errors and estimate the values of gross errors accurately. The states are more smooth and nearer to the set point. It can provide a better control performance of the states. Though our approach cannot detect all gross errors in the measurements of pressure P, the performance of controlled pressure P is better than the performance of RNDDR, and it shows a trend to follow the set value opposite to the RNDDR.

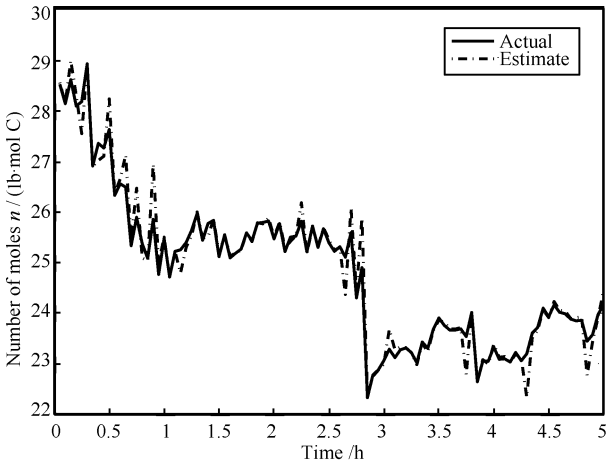

Fig. 6 The state n estimates by RNDDR

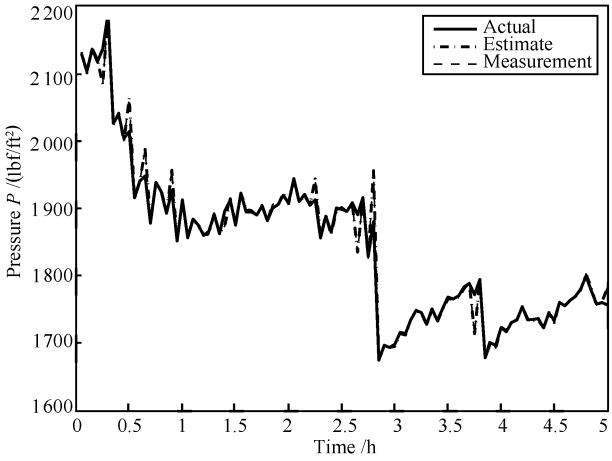

Fig. 7 The state P estimates by RNDDR

The root-mean square (RMS) errors in the estimates (difference between estimated and true values) and the controller set values (difference between controller set values and true values) are shown in Table 2 (see page 715).

It can be seen in Table 2 that our approach gives more accurate estimates in all states and measurements. The RMS errors of the estimates and the controller set values of the pressure P are a little bit larger than others because P is a nonlinear nonredundant measure of T and n, and the covariance of P is much larger. Furthermore, our approach gives a more smooth control performance. The RMS error of the state of pressure in our approach is much smaller than that in the RNDDR, and the pressure estimated and controlled with our approach could follow the controller set value, whereas the pressure estimated and controlled with the RNDDR begins to deviate, which can be seen in Fig. 7.

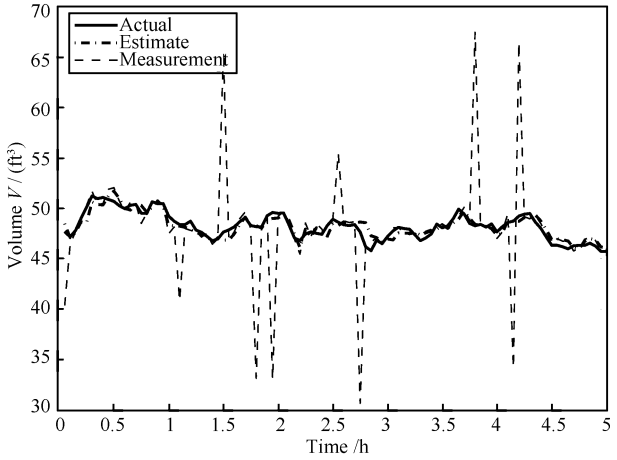

Fig. 8 The state V estimates by the SV regression regression

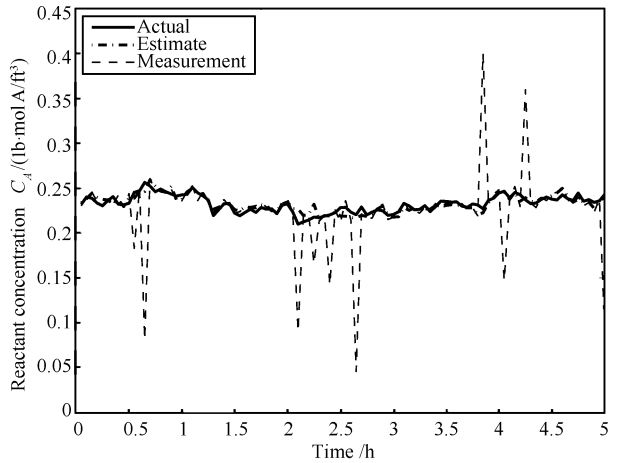

Fig. 9 The state C_A estimates by the SV regression regression

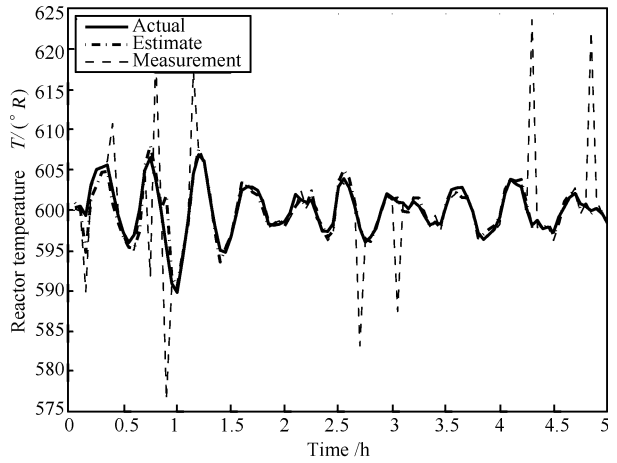

Fig. 10 The state T estimates by the SV regression regression

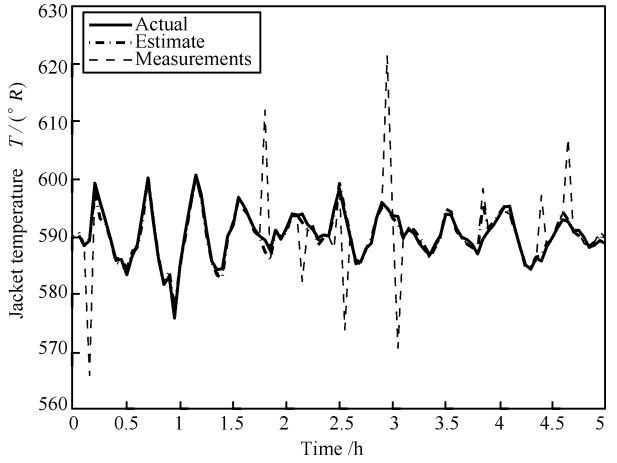

Fig. 11 The state T_C estimates by the SV regression regression

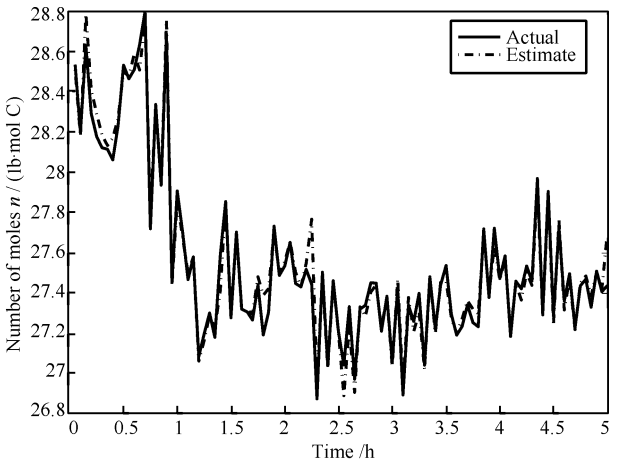

Fig. 12 The state n estimates by the SV regression regression

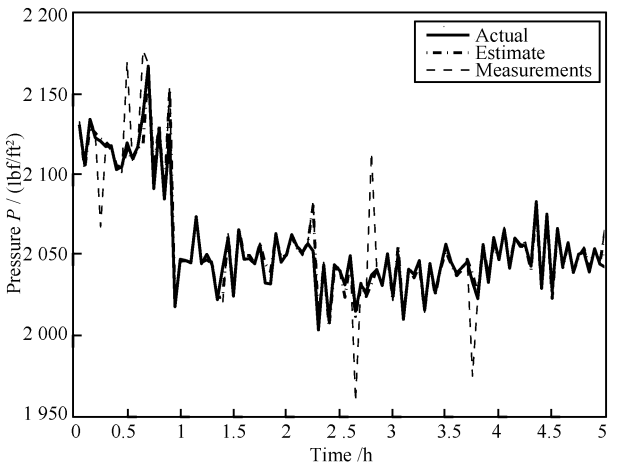

Fig. 13 The state P estimates by the SV regression regression

Table 2 RMS errors of estimates and controller set values

	RNDDR		SV regression approach	
	Estimates	Controller set values	Estimates	Controller set values
V	2.9544	4.9720	0.5927	1.2507
C_A	0.0633	–	0.0050	–
T	4.5188	9.5302	1.0947	3.1357
T_C	5.7258	–	0.9760	–
n	0.2752	–	0.0702	–
P	14.9855	209.9326	6.0697	67.1516

4.3 The performance with model parameter and controller set values changing

In this case, in order to study the robustness and stableness of the SV regression approach, the simulation was carried out with the catalyst activity C_d changing from 1 to 0.7 at sampling instant 20, and at the same time, the controller set values changed from 600 to 550 and from 2 116 to 1 900 for T and P, respectively. The random and gross errors were generated randomly as described above. The coefficient vector $\boldsymbol{a}$ was still a constant as $\boldsymbol{a} = [18, 18, 18, 18, 99.89]$ relative to V, C_A, T, T_C, n, and P, respectively.

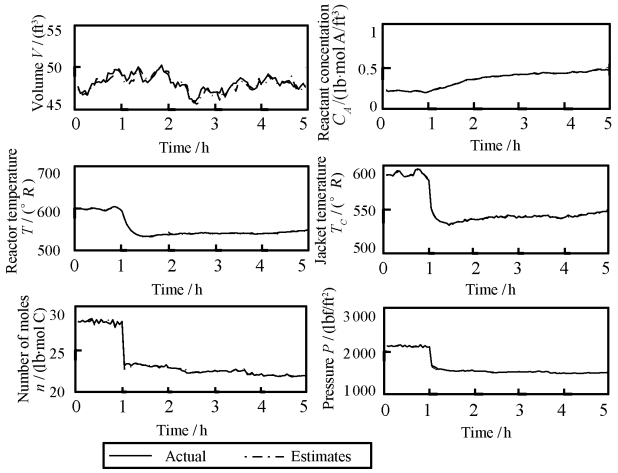

Fig. 14 The state estimates by the SV regression approach with model parameter changing

Fig. 14 shows the simulation results. From the Fig. 14, it can be seen that the SV regression approach could remove gross errors and provide accurate estimates even when the controller set values and the model parameter changed during the process. In this study, the coefficient vector was also a constant and both the model parameter and the controller set values changed, but the SV regression approach could remove the gross errors and provided accurate reconciled values as well, because the coefficient in the SV regression is robust to reconciled result. Meanwhile, the SV regression could follow the step change of the controller set values even after the model parameter changed. The stable results shown in Fig. 14 reveal the stableness of using estimates reconciled by the SV regression approach as feedbacks to controllers.

5 Conclusion

An SV regression approach for recursive simultaneous data reconciliation and gross error detection in nonlinear dynamic system was presented in this paper. The SV regression approach is found to be robust and have superior performance. This approach considers the statistical learning theory as the framework of data reconciliation and gross errors detection instead of the empirical risk, so it can detect gross errors and estimate gross error values. At the same time, it is based on a recursive estimation framework, which makes it preferable for online application. Another advantage of our approach is that no linearized system model is needed, which eliminates the adverse effect on the accuracy of the state and the covariance matrix estimates by an approximate linear model of the process. The nonlinear dynamic system simulation results in this paper show that the SV regression approach is robust, stable, and accurate for simultaneous data reconciliation and gross error detection in nonlinear dynamic systems within a recursive real-time estimation framework. It can also give better performance of control.

The SV regression approach proposed in this paper was applied to a widely used model defined in (1) which constitutes the constraints $l(\boldsymbol{x})$ in the SV regression approach. Furthermore, more complex models could be used instead of the model defined in (1) to constitute the constraints $l(\boldsymbol{x})$, then the SV regression approach proposed in this paper could be extended to more complex models, which shall be addressed in future works.

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