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非ガウス型状態空間モデルによる時系列データの分解 — 化学プロセスの異常検出への応用 —

Decomposition of Time Series by non-Gaussian State Space Model — Application to Fault Detection in a Chemical Plant —

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Abstract

A novel framework of fault detection of non-stationary chemical process is proposed. This method is based on the following three steps: (1) decomposition of the observed signal into trend and the residual component through the use of the non-Gaussian state space model, (2) modeling of the residual component through the use of an AR model with time varying coefficients, and (3) checking the modeling error of the AR model with a sequential probability ratio test. The proposed framework can isolate the effects of noises and process changes from the changes of operational modes. To demonstrate the method, simulated data from a simple process system with a level control are successfully analyzed.

1. Introduction

To improve process quality, productivity and safety, fault detection is an important problem of practical interest in many chemical process plants. Many algorithms for fault detection have been developed by many researchers. Statistical change detection is a relatively old research field, but recently interest has increased again with the active research for data mining. The problem of detecting a change in the parameters of a static or dynamic stochastic system is well summarized in book[2)] with key mathematical background. It includes Shewhart control charts, geometric moving average charts, finite moving average charts, CUSUM-type algorithms, GLR detector and Bayes-type charts. Chiang *et. al.* also summarizes many approaches for fault detection and isolation, including statistical methods such as SPC, PCA, PLS, FDA, CVA and soft computing methods[3)].

Although these methods are useful, real plant includes various problems to apply these methods and none of the method is sufficient for all the purpose. Before applying the usual methods, decomposition of operational data series into trend signal and the other components can solve the problem in many situations.

Decomposition of process signal into several components has been studied with a primary focus on the problem of sensor validation. Many approaches have been investigated including cluster analysis, pattern recognition, modeling individual sensors, modeling a process including sensors, and statistical analysis[10)]. A linear Gaussian model is one of the powerful approaches for the decomposition with the help of Kalman filter and AIC criteria. However it has the limitation not to apply the process with the abrupt changes of process operational mode.

In this paper, decomposition of the observed time series into trend and the other component is investigated under the changes of process operational mode. To realize this facility, the trend of the observed time series is modeled by the non-Gaussian state space model using the Gaussian mixture approximation. Subsequently, the residual of the trend model is modeled by time varying coefficient AR model. Finally, the residual of the AR model is tested by sequential probability ratio test to detect faults.

2. Method

2.1 Decomposition and Fault Detection

The proposed framework of the fault detection has the following three steps.

- Trend modeling: Modeling the trend of the normal observation signals by non-Gaussian state space model.
- Residual modeling: Modeling the residual of the trend model by time varying coefficient AR model.
- Fault detection: Decision making by sequential probability ratio test on the residual of the AR model.

2.2 Trend Model

The problem of modeling a time series with trend and stationary covariances is described here. Kitagawa proposed a method to decompose an observed time series into local polynomial trend, seasonal, globally stationary autoregressive and observation error components[6)]. In this model, each component is characterized by an unknown variance — white noise perturbed difference equation constraint.

In general, the state space representation for the observations y_n is

$$\begin{aligned} \boldsymbol{x}_n &= \boldsymbol{F}\boldsymbol{x}_{n-1} + \boldsymbol{G}\boldsymbol{v}_n, \\ y_n &= \boldsymbol{H}\boldsymbol{x}_n + w_n, \end{aligned} \tag{1}$$

where $\boldsymbol{x}_n$ is a state vector, $\boldsymbol{F}, \boldsymbol{G}$ and $\boldsymbol{H}$ are $m \times m, m \times \ell$, and $1 \times m$ matrices, respectively. For possibly non-Gaussian white noises $\boldsymbol{v}_n$ and w_n, the recursive formulas for obtaining the densities of the one-step-ahead prediction and filtering are given as follows[7]:

$$p(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1}) \qquad (2)$$
$$= \int_{-\infty}^{\infty} p(\boldsymbol{x}_n|\boldsymbol{x}_{n-1})p(\boldsymbol{x}_{n-1}|\boldsymbol{Y}_{n-1})d\boldsymbol{x}_{n-1},$$

$$p(\boldsymbol{x}_n|\boldsymbol{Y}_n) = \frac{p(y_n|\boldsymbol{x}_n)p(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1})}{p(y_n|\boldsymbol{Y}_{n-1})}, \qquad (3)$$

where $p(y_n|\boldsymbol{Y}_{n-1})$ is obtained by

$$p(y_n|\boldsymbol{Y}_{n-1}) \qquad (4)$$
$$= \int p(y_n|\boldsymbol{x}_n)p(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1})d\boldsymbol{x}_n.$$

For the dimension value $m = 1, 2$ and 3, Equation (1) represents the polynomial trend, stationary AR, and seasonal effects component models, respectively. The polynomial trend component is represented as a $k-$th order stochastically perturbed difference equation

$$\boldsymbol{\nabla}^k t_n = \boldsymbol{v}_n, \qquad (5)$$

where $\boldsymbol{\nabla}$ denotes the difference operator defined by $\boldsymbol{\nabla} t = t_n - t_{n-1}$.

The corresponding matrices and state vector components are:

$(k = 1)$

$$t_n = t_{n-1} + \boldsymbol{v}_n, \qquad (6)$$
$$\boldsymbol{x}_n = t_n,\ \boldsymbol{F} = \boldsymbol{G} = \boldsymbol{H} = 1.$$

$(k = 2)$

$$t_n = 2t_{n-1} - t_{n-2} + \boldsymbol{v}_n,$$
$$\boldsymbol{x}_n = (t_n,\ t_{n-1})^t, \qquad (7)$$
$$\boldsymbol{F} = \begin{pmatrix} 2 & -1 \\ 1 & 0 \end{pmatrix},\ \boldsymbol{G} = \boldsymbol{H}^t = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Gaussian model:

If the system noise and observation noise have Gaussian densities, that is $\boldsymbol{v}_n \sim N(0, \tau^2)$ and $w_n \sim N(0, \sigma^2)$, the value of $p(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1})$ and $p(\boldsymbol{x}_n|\boldsymbol{y}_n)$ can be effectively estimated through the utilization of the Kalman filter[1].

The best choice of the model can be made by minimizing the value of AIC defined by

$$\text{AIC} = -2\log(\text{maximized likelihood}) + 2(\text{number of free parameters}) \qquad (8)$$

Under the Gaussian assumption, the likelihood is represented by

$$L(\boldsymbol{\theta}, \boldsymbol{x}_{0|0}) \qquad (9)$$
$$= \prod_{n=1}^{N} (2\pi \boldsymbol{r}_{n|n-1})^{-\frac{1}{2}} \exp\left\{ \frac{-\boldsymbol{r}_{n|n}^2}{2\boldsymbol{r}_{n|n-1}} \right\}.$$

where $\boldsymbol{r}_{n|n}$ is the one-step-ahead output prediction error ($\boldsymbol{r}_{n|n} = y_n - \boldsymbol{H}\boldsymbol{x}_{n|n-1}$), $\boldsymbol{r}_{n|n-1}$ is its error covariance matrix and $\boldsymbol{\theta} = (\tau, \sigma)$.

For the evaluation of the AIC criteria, initial value of the variance of the state vector is calculated by applying the estimation filter in reverse. As for the optimization search algorithm, the Pokal-Ribiere-Polyak method is used in the case study experiment.

non-Gaussian model:

If the noise densities are non-Gaussian, Kitagawa developed an algorithm for implementing the non-Gaussian filter by approximating each density function based on a continuous piecewise linear function[7]. The method can be applied to lower order systems, but it is not suitable for higher order state space models due to the huge amount of computation that is requires. Another practical way of performing the computation is the use of a Gaussian-sum filter by using Gaussian mixture approximation to the related densities.

Let φ_i be properly defined Gaussian density. The following approximations can be used.

$$p(\boldsymbol{v}_n) = \sum_{i=1}^{K_v} \alpha_i \varphi_i(\boldsymbol{v}_n), \qquad (10)$$

$$p(w_n) = \sum_{j=1}^{K_w} \beta_j \varphi_j(w_n), \qquad (11)$$

$$p(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1}) = \sum_{k=1}^{L_n} \gamma_{kn}\varphi_k(\boldsymbol{x}_n|\boldsymbol{Y}_{\boldsymbol{n-1}}) \quad (12)$$

$$p(\boldsymbol{x}_n|\boldsymbol{Y}_n) = \sum_{\ell=1}^{M_n} \delta_{\ell n}\varphi_\ell(\boldsymbol{x}_n|\boldsymbol{Y}_{\boldsymbol{n}}). \quad (13)$$

Substituting these approximations into Equations (2) and (3), the following one-step-ahead prediction algorithm is derived[8]:

$$p(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1}) \quad (14)$$
$$= \sum_{i=1}^{K_v}\sum_{\ell=1}^{M_{n-1}} \gamma_{i\ell,n}\varphi_{i\ell}(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1}).$$

Here, $\varphi_{i\ell}(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1})$ is the one-step-ahead predictor of $\boldsymbol{x}_n$ under the assumption of Gaussian noise. Therefore, $\varphi_{i\ell}(\boldsymbol{x}_n|\boldsymbol{Y}_{n-1})$ can be estimated by ordinary Kalman filter. Here, one-step-ahead prediction with non-Gaussian white noises can be estimated.

Similarly, the following filtering algorithm is obtained:

$$p(\boldsymbol{x}_n|\boldsymbol{Y}_n) \quad (15)$$
$$= \sum_{j=1}^{K_w}\sum_{k=1}^{L_n} \delta_{jk,n}\varphi_{jk}(\boldsymbol{x}_n|\boldsymbol{Y}_n).$$

In the implementation of the algorithm, reduction of the number of Gaussian components is considered. It was observed that a relatively small number of Gaussian densities can approximate a large class of distributions[9].

2.3 Time varying AR coefficient model

The stationary model was discussed in the previous section. In this section, time varying AR coefficient model is considered, where the coefficient a_{nj} changes gradually with time[4]. The model is

$$z_n = \sum_{j=1}^{m} a_{nj}z_{n-j} + w_n, \quad (16)$$

where w_n is a white noise $N(0, \sigma_a^2)$.

A k-th order difference model for the AR coefficients is defined by

$$\boldsymbol{\nabla}^k a_{nj} = v_{nj}. \quad (17)$$

The state space representation of the time varying coefficient AR model becomes

$$\boldsymbol{x}_n = \boldsymbol{F}\boldsymbol{x}_{n-1} + \boldsymbol{G}\boldsymbol{v}_n, \quad (18)$$

$$z_n = \boldsymbol{H}_n\boldsymbol{x}_n + w_n, \quad (19)$$

where $\boldsymbol{H}_n$ is the km dimensional vector.

For example, if $k = 1$, the state space representation of the model is as follows:

$$\boldsymbol{x}_n = [a_{n1}, a_{n2}, \cdots, a_{nm}]^T, \quad (20)$$

$$\boldsymbol{F}_n = \boldsymbol{I}_m, \quad (21)$$

$$\boldsymbol{G}_n = \boldsymbol{I}_m, \quad (22)$$

$$\boldsymbol{H}_n = [z_{n-1}, z_{n-2}, \cdots, z_{n-m}], \quad (23)$$

where $\boldsymbol{I}_m$ is the unit matrix of $m \times m$.

2.4 Fault Detection

By using the above mentioned decompositions, several kinds of fault detection schematics could be constructed. As an example of the application of the decomposition, a method using the residual of the time varying coefficient AR model is proposed in this section.

If the system is normal, the modeling error of the time varying coefficient AR model can be considered to have a normal Gaussian distribution. Then, a fault can be detected by Wold's sequential probability ratio test (SPRT) on this error signal.

The sequential probability ratio at time n is defined by

$$\lambda_n = \lambda_{n-1} + \log\frac{P(\eta_n|H_1)}{P(\eta_n|H_0)}, \quad (24)$$

where η_n is the modeling error at time n. H_0 is the hypothesis that the system is normal, and H_1 is the hypothesis that the system is faulty. $P(\eta_n|H_0)$ and $P(\eta_n|H_1)$ are the probability density functions for the normal data and abnormal data, respectively. A fault can be detected by monitoring the mean value and the variance of λ_n with the following equations:

$$\lambda_n = \lambda_{n-1} + m_a(\eta_n - \frac{m_a}{2}), \quad (25)$$

$$\lambda_n = \lambda_{n-1} - \frac{\eta_n^2}{2}(\frac{1}{v_a^2} - 1) - \frac{1}{2}\log(v_a^2), \quad (26)$$

where m_a and v_a^2 are the mean and variance of η_n in abnormal situation.

3. Case Study

3.1 Simple Tank System

To demonstrate the ability of the method, it is applied to a simple tank system with level control. Figure 1 shows the flow diagram of the simulated system. The tank is modeled with an ordinary differential equation based on the mass balance.

$$\frac{dh}{dt} = \frac{1}{A}F_{\text{in}} - \frac{cu}{A}\sqrt{h} \quad (27)$$

Observation noises are added to each observation variable ($h, F_{\text{in}}, F_{\text{out}}$ and u). The valve characteristics are defined by a first order lag system. In this process, the liquid level h is controlled by a PI controller, parameters of which are tuned by Cohen-Coon method. Runge-Kutta method is used for the integration of the system equation, and the sampling time of the control is 5.0 second.

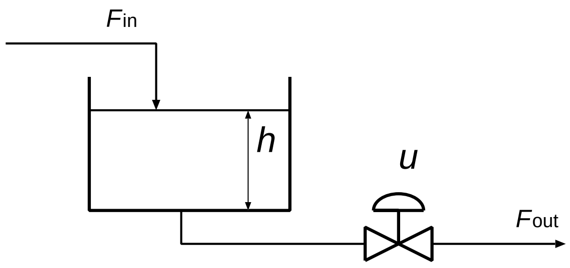

Fig. 1 The example process

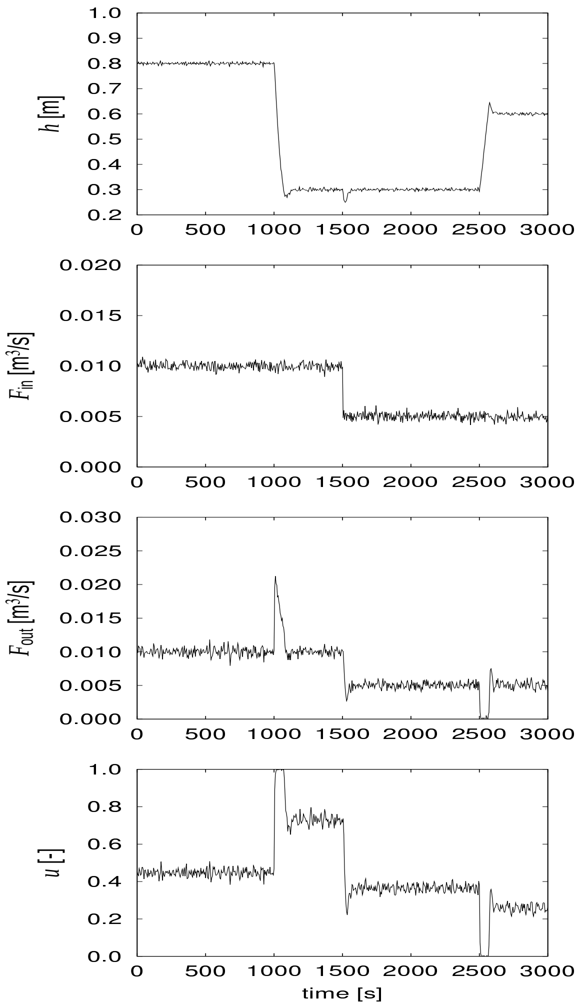

Fig. 2 Simulation run for normal operation

Figure 2 shows an example of the simulation. In this simulation, initial set point of h was 0.8 m. It was changed to 0.3 m at $t = 1000$ seconds, and changed again to 0.6 m at $t = 2500$ seconds. Initial value of the input flow rate F_{in} was 0.01 m^3/S, and the value was changed to 0.005 before $t = 1500$ seconds. Other variables, F_{out} and u, are calculated from the system equations.

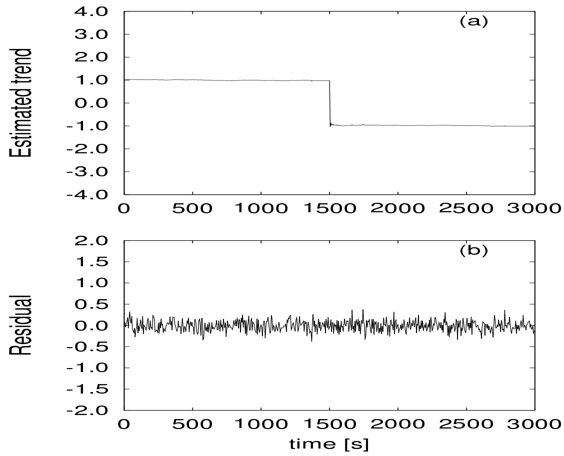

Fig. 3 Estimated trend for F_{in} in Figure 2 (non-Gaussian model)

3.2 Trend Modeling

For the data set of Figure 2, non-Gaussian modeling is applied in order to make the trend model of the normal operation. Based on the algorithm described in the previous section, Figure 3(a) is obtained for the estimated trend component of F_{in}. This result shows that the Gaussian mixture approximation for system noise can handle both the slow shift and the abrupt shift in the process signal. In the same figure, graph (b) plots the residuals, which is the differences between the estimated trend and the observation. Figure 4 shows estimations for the other measurements. As shown in the graph, the residuals do not include any abrupt changes. These graphs show that the non-Gaussian model can decompose the observation signal very well.

For comparison, the result of the decomposition of the observation signal by Gaussian model is shown in Figure 5. The figure shows that, Gaussian model cannot model the abrupt changes, such as the change at 1500 seconds and relatively large residual remains at the point. Also, compared to

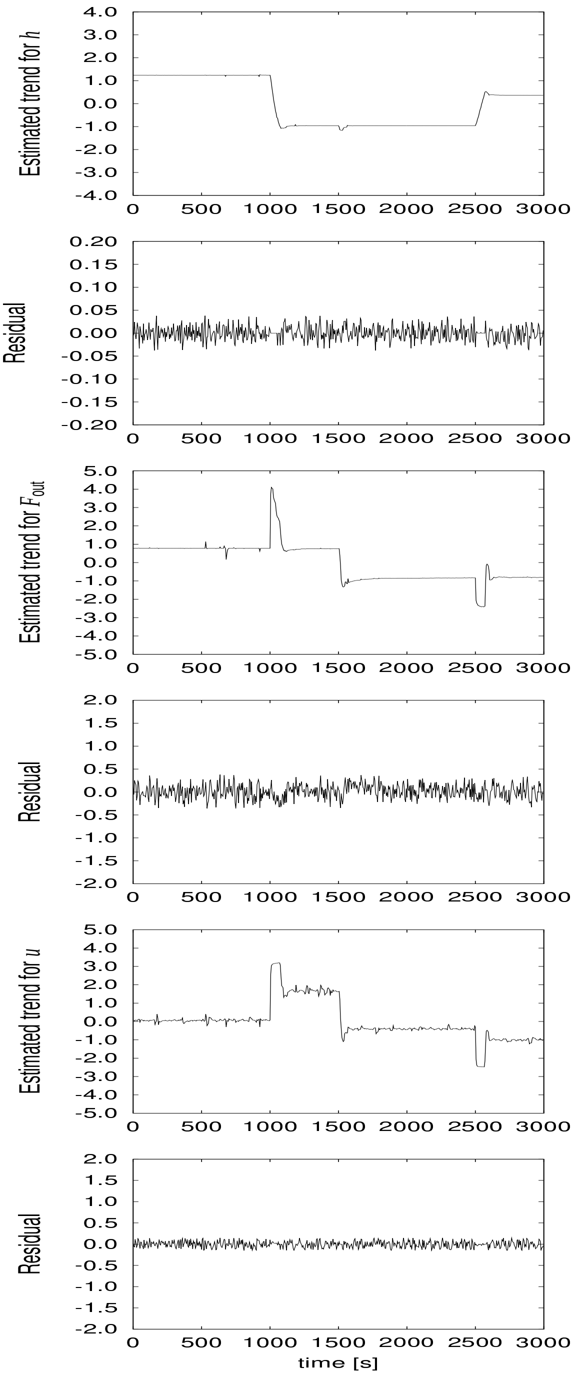

Fig. 4 Estimated trend for h, F_{out}, u in Figure 2 (non-Gaussian model)

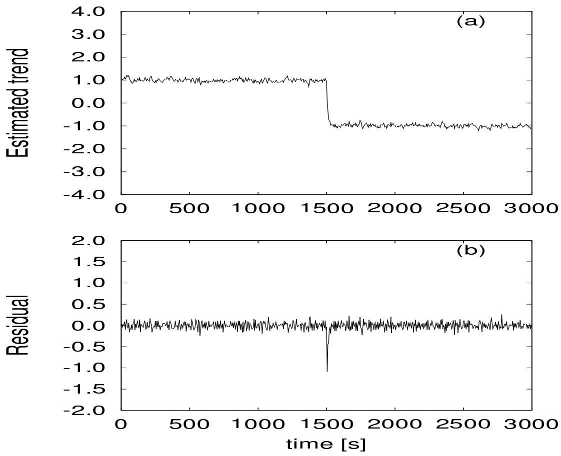

Fig. 5 Estimated trend for Fig. 2 (Gaussian model)

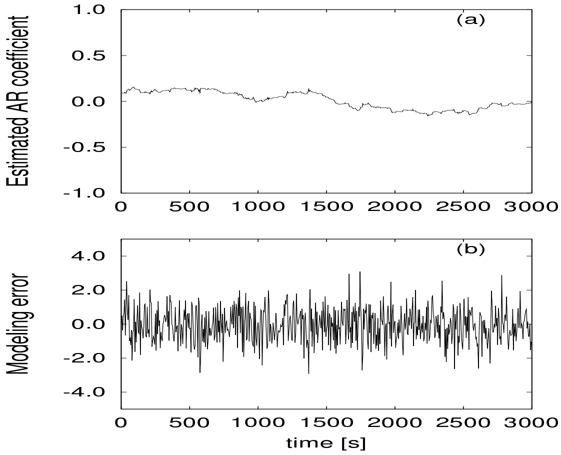

Fig. 6 Estimated AR coefficient and modeling error for the residual

the non-Gaussian model, the trend component is not as smooth.

3.3 Residual Modeling

The residual of the trend model is modeled by time varying coefficient AR model. Figure 6(a) shows the estimated coefficient of the model. The modeling error, which is the difference between the AR estimated value and the residual, is shown in Figure 6(b). In this calculation, model parameters are set to $m = 1, k = 1$, which is decided

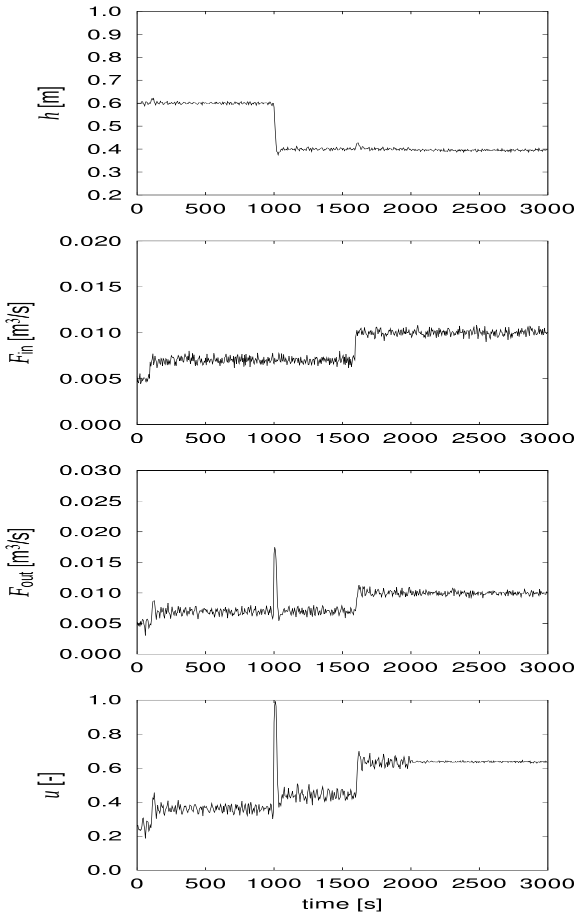

Fig. 7 Faulty operation (valve stuck)

using the AIC criterion. Figure 6(a) shows that AR coefficient changes slowly, which corresponds with the fact that the residual of the trend model does not have strange values. As a result, the modeling error of the AR model, seems to be a white noise (Figure 6(b)).

4. Fault Detection

Now, let us consider about the fault in another simulation run (Figure 7). Let us suppose that a valve stuck at 2000 seconds. In this simulation, initial value of the set point of the level was 0.6 m. It was changed to 0.4 m at 1000 seconds, and changed again to 0.7 m at 2500 seconds. Although the valve stuck at 2000 seconds, the level h vir-

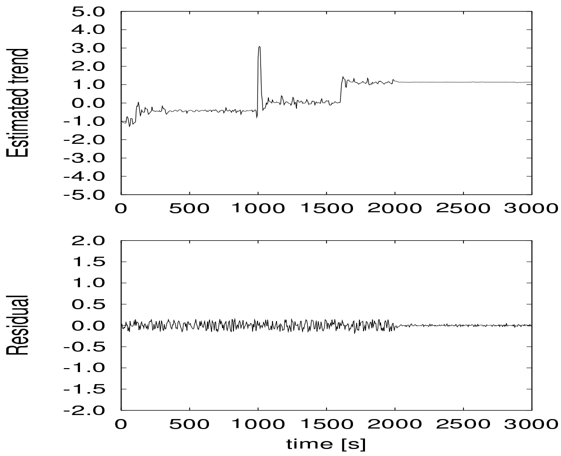

Fig. 8 Estimated trend for u in Fig. 7 (non-Gaussian model)

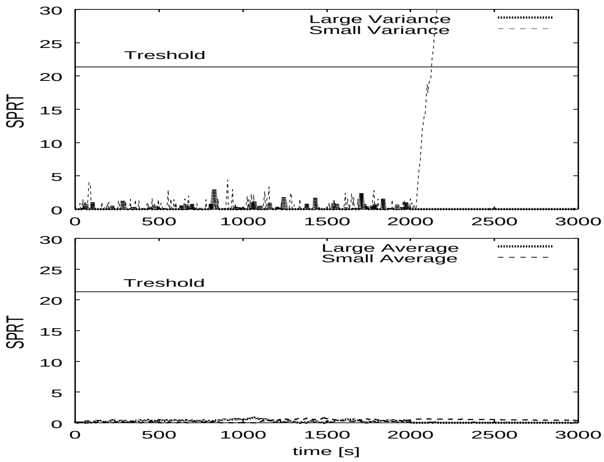

Fig. 9 Result of Fault Detection by SPRT

tually seems to be controlled normally until 2500 seconds.

The proposed framewrok is applied to this faulty data. Figures 8 and 9 show the estimated trend and SPRT value for the fault detection respectively. As shown in the figure 9, the SPRT value of the variance suddenly becomes large at 2000 seconds, which corresponds to the occurrence of the valve stick. A sudden change in the variation of residual is also shown in the Figure 8. In normal data, u should include both the process noise and observation noise, but in this data, only the observation noise is included after 2000 seconds. With the existence of changes in the set-point of liquid level or changes of the process disturbance, the method detects the real fault with considerable accuracy. This result shows that the proposed framework provides an excellent tool for fault detection of non-stationary chemical process.

5. Conclusions

In this paper, we have proposed a novel method for the decomposition of process time series data into the trend and the residual component. The method is based on the non-Gaussian state space model and can deal with the changes of operating conditions. As an application of the decomposition, a method of fault detection is shown by using the modeling error of the time varying coefficient AR model, which models the decomposed residual from the trend.

The method is applied to a simple tank system with liquid level control. The example process has several operational changes, such as the set-point changes; additionally, a valve stick error is successfully detected by the sequential probability ratio test of the modeling error. The example shows that the proposed method add a powerful tool for the decomposition of process trend. Our method is also useful for the detection of fault in the process having changes in operation mode. Future direction will likely include the use of the other decomposed components for fault detection.

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