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Supervised linear dynamic system model for quality related fault detection in dynamic processes

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ABSTRACT

Dynamic and uncertainty are two main features of industrial processes data which should be paid attentions when carrying out process monitoring and fault diagnosis. As a typical dynamic Bayesian network model, linear dynamic system (LDS) can efficiently deal with both dynamic and uncertain features of the process data. However, the quality information has been ignored by the LDS model, which could serve as a supervised term for information extraction and fault detection. In this paper, a supervised form of the LDS model is developed, which can successfully incorporate the information of quality variables. With this additional data information, the new supervised LDS model can provide a quality related fault detection scheme for dynamic processes. A detailed industrial case study on the Tennessee Eastman benchmark process is carried out for performance evaluation of the developed method.

1. Introduction

To ensure process safety and improve production efficiency, fault detection has become popular in industrial processes for many years. Compared to traditional model-based fault detection methods which may highly rely on the process knowledge or experience from process engineers, the data-based modeling method is much more flexible, thus has been widely used for fault detection in recent years. This is mainly due to the wide utilization of the distributed control system (DCS) in industrial processes, an enormous number of process data have been collected, which contain useful information for fault detection [1]. Along the past years, a number of data-based fault detection methods have been developed, such as Principal Component Analysis (PCA), Partial Least Squares (PLS), Fisher Discriminant Analysis (FDA), Support Vector Machines (SVM), etc [2–6].

For the purposes of control and optimization in the industrial process, the dynamic relationships among process data should be paid particular attentions. Actually, the dynamic model can provide a powerful tool when the phenomenon of feedback, missing or multiple measurements and noise appears. For fault detection, a data-based dynamic model is also required to capture the serial correlations among the process data. In order to handle the dynamic relationship among process data, several fault detection methods have already been developed [7–14]. For example, a dynamic generalization of the conventional Principal Component Analysis (PCA) method has been developed, which defines an augmented vector that contains time-lagged process measurements [7]. Therefore, the dynamic information can be captured in the subsequent PCA model. To further reduce the false alarms in DPCA, univariate ARMA filters were proposed to remove autocorrelation from the DPCA score variables [8]. Another new dynamic latent variable model has also been developed to improve the monitoring efficiency of the traditional DPCA method [9]. Besides, the state space model has been introduced for dynamical fault detection and diagnosis, most of which are related to the subspace identification methods [10–14].

However, most existing dynamical fault detection methods have not well considered the data uncertainty. Actually, most process variables collected from noisy environments are contaminated by random noises. It is more reasonable to consider that those process variables are inherently random variables. To address both dynamical and uncertain data characteristics, dynamical Bayesian networks (DBNs) have provided an effective modeling framework [15]. There are two well-known modeling tools in DBNs: linear dynamic systems (LDS) for modeling of continuous state sequences and Hidden Markov Model (HMM) for classification of discrete state sequences. For the

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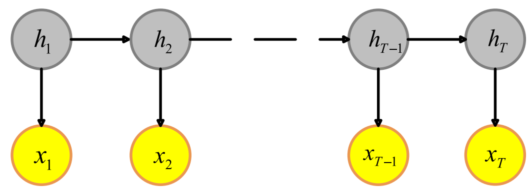
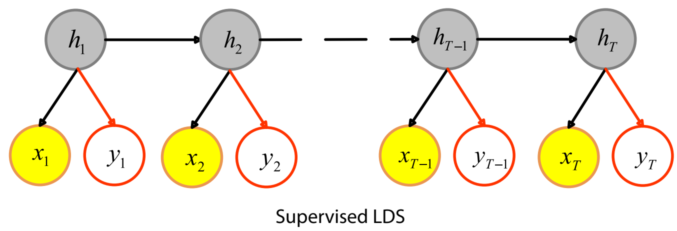


(a)



(b)

Fig. 1. Graphical representation of the LDS and SLDS models, (a) LDS model; (b) SLDS model.

fault detection purpose, the LDS model has already been introduced. For example, a data-based linear Gaussian state-space model was constructed upon the framework of LDS for dynamic process monitoring [16], a switching LDS-based approach has been proposed for fault detection and classification [17].

Unfortunately, the LDS model can only provide an unsupervised modeling framework for fault detection, which means that only the information of process variables can be incorporated into the model. Here, the unsupervised model means that the model only considers one type of variables, while the supervised model tries to build relationships between two types of variables. More illustrations about unsupervised and supervised learnings can be found in the machine learning community. In practice, data information from quality variables is important and sometimes may play as an essential role in fault detection and diagnosis. To this end, the quality relevant or related process monitoring methods have been developed in recent years. For example, a quality relevant T-PLS modeling and monitoring method has been developed for dynamic processes [18], a concurrent projection to latent structures has been proposed for quality relevant and process relevant fault monitoring [19], a new data-driven process monitoring scheme related to key performance indictors has been developed and applied to hot strip mill process [20], and so on [21–25].

In this paper, the quality data information is incorporated into the traditional LDS model, thus a supervised LDS model will be developed and used for fault detection. With the introduction of the quality data information, the supervised LDS model could be more related to the quality information. Compared to the conventional LDS model based fault detection method, the supervised LDS model can provide more relationships between process variables and the quality variables. The information of quality variables serve as supervised items for the modeling and parameter estimation process of the LDS model. Therefore, the fault detection performance is expected to be improved.

The remainder of this paper is structured as follows. In Section 2, detailed description of the supervised LDS model is presented, including the model structure, learning algorithm, and online inference for the new data. The fault detection scheme is given in Section 3. An industrial case study is carried out in Section 4 to demonstrate the performance of the proposed method. Finally, conclusions are made.

2. Supervised linear dynamic systems (SLDS)

2.1. Model structure

Similar to the traditional LDS model, the supervised LDS model is also a time-series state-space model. The main difference is that the additional quality information has been incorporated into the supervised LDS model, which serves as a supervised item for learning of the LDS model. Therefore, the relationships between quality variables and process variables can be modeled and captured for quality-related fault detection modeling. Generally, the LDS model consists of a latent linear Gaussian dynamic model and a linear Gaussian observation model [15]. The graphical representation of the LDS model is depicted in Fig. 1(a). In contrast, the graphical representation of the supervised LDS model is provided in Fig. 1(b). In these two figures, $\mathbf{h}_t \in R^{H\times 1}$ denotes the latent variable of LDS, which is also known as the state variable in the state space model, $\mathbf{x}_t \in R^{V\times 1}$ is the observed measurement vector of process variables, and $\mathbf{y}_t \in R^{L\times 1}$ is the vector of quality variables, where H, V, and L are numbers of latent variables, process variables and quality variables. It can be seen that additional quality information has been assumed in the supervised LDS model and also connected to the latent variables. Therefore, the supervised LDS model has a latent linear Gaussian dynamic model and two linear Gaussian observation models.

The model structure of SLDS can be described as follows:

$$\mathbf{h}_t = \mathbf{A}\mathbf{h}_{t-1} + \boldsymbol{\eta}_t^h \quad (1)$$

$$\mathbf{x}_t = \mathbf{B}_x\mathbf{h}_t + \boldsymbol{\eta}_t^x \quad (2)$$

$$\mathbf{y}_t = \mathbf{B}_y\mathbf{h}_t + \boldsymbol{\eta}_t^y \quad (3)$$

where $\mathbf{A} \in R^{H\times H}$ is the transition matrix, $\mathbf{B}_x \in R^{V\times H}$ and $\mathbf{B}_y \in R^{L\times H}$ are emission matrices corresponding to $\mathbf{x}_t$ and $\mathbf{y}_t$. $\boldsymbol{\eta}_t^h \in R^{H\times 1}$, $\boldsymbol{\eta}_t^x \in R^{V\times 1}$, and $\boldsymbol{\eta}_t^y \in R^{L\times 1}$ are noises of the latent variables process variables, and quality variables, which are assumed to be Gaussian; thus $\boldsymbol{\eta}_t^h : N\left(\boldsymbol{\eta}_t^h|0, \boldsymbol{\Sigma}_h\right)$, $\boldsymbol{\eta}_t^x : N\left(\boldsymbol{\eta}_t^x|0, \boldsymbol{\Sigma}_x\right)$ and $\boldsymbol{\eta}_t^y : N\left(\boldsymbol{\eta}_t^y|0, \boldsymbol{\Sigma}_y\right)$, where $\boldsymbol{\Sigma}_h$, $\boldsymbol{\Sigma}_x$ and $\boldsymbol{\Sigma}_y$ are noise variances. In order to facilitate the modeling process, the two linear Gaussian observation models can be combined together, which can be described as

$$\begin{bmatrix} \mathbf{x}_t \\ \mathbf{y}_t \end{bmatrix} = \begin{bmatrix} \mathbf{B}_x \\ \mathbf{B}_y \end{bmatrix} \mathbf{h}_t + \begin{bmatrix} \boldsymbol{\eta}_t^x \\ \boldsymbol{\eta}_t^y \end{bmatrix} \rightarrow \mathbf{o}_t = \mathbf{B}\mathbf{h}_t + \boldsymbol{\eta}_t^o \tag{4}$$

From Eqs. (1) and (4), it can be inferred that the conditional probability distributions of latent variable $\mathbf{h}_t$ and observed measurement $\mathbf{o}_t$ are both Gaussians, thus $\mathbf{h}_t|\mathbf{h}_{t-1} : N(\mathbf{h}_t|\mathbf{A}\mathbf{h}_{t-1}, \boldsymbol{\Sigma}_h)$ and $\mathbf{o}_t|\mathbf{h}_t : N(\mathbf{o}_t|\mathbf{B}\mathbf{h}_t, \boldsymbol{\Sigma}_o)$, where $\boldsymbol{\Sigma}_o = \begin{bmatrix} \boldsymbol{\Sigma}_x 0 \\ 0 \boldsymbol{\Sigma}_y \end{bmatrix}$. The prior density of the latent variables $p(\mathbf{h}_1)$ is assumed to be Gaussian with mean $\boldsymbol{\mu}_\pi$ and variance $\boldsymbol{\Sigma}_\pi$, i.e., $\mathbf{h}_1 : N(\mathbf{h}_1|\boldsymbol{\mu}_\pi, \boldsymbol{\Sigma}_\pi)$. Therefore, the joint probability for the sequences of both latent variables $\mathbf{h}_t$ and observed variables $\mathbf{o}_t$ can be formulated as follows:

$$p(\mathbf{o}_{1:T}, \mathbf{h}_{1:T}) = p(\mathbf{h}_1)p(\mathbf{o}_1|\mathbf{h}_1)\prod_{t=2}^{T} p(\mathbf{h}_t|\mathbf{h}_{t-1})p(\mathbf{o}_t|\mathbf{h}_t) \tag{5}$$

where T is the length of the data sequence. Here, we have supposed that the observed dataset has been pre-processed, e.g., auto-scaling.

2.2. Learning supervised LDS model via EM algorithm

According to the model structure of supervised LDS, it can be determined by the parameter set $\boldsymbol{\theta} = \left\{\mathbf{A}, \mathbf{B}, \boldsymbol{\Sigma}_h, \boldsymbol{\Sigma}_o, \boldsymbol{\mu}_\pi, \boldsymbol{\Sigma}_\pi\right\}$. In order to find the maximum-likelihood (ML) estimation for the parameter, the expectation-maximization (EM) algorithm can be used, which is an efficient two-step iteration method [26]. In the expectation step (E-step), the posterior distribution of the latent variables is calculated according to the current parameter values. In the maximization step (M-step), the values of all parameters are updated by maximizing the expected log-likelihood function.

For a given measurement data $\mathbf{o}_{1:T}$, the log-likelihood function of the SLDS model can be written as:

$$L(\boldsymbol{\theta}) = \ln p\left(\mathbf{o}_{1:T}, \mathbf{h}_{1:T}|\boldsymbol{\theta}\right) = \ln p(\mathbf{h}_1)p(\mathbf{o}_1|\mathbf{h}_1)\prod_{t=2}^{T} p(\mathbf{h}_t|\mathbf{h}_{t-1})p(\mathbf{o}_t|\mathbf{h}_t) \tag{6}$$

In the M-step, the new parameters θ^{new} can be calculated by maximizing the expectation of $L\left(\theta\right)$

$$\boldsymbol{\theta}^{\text{new}} = arg\max_{\boldsymbol{\theta}} E\{L\left(\theta\right)\} = arg\max_{\boldsymbol{\theta}} E\{\ln p\left(\mathbf{o}_{1:T}, \boldsymbol{h}_{1:T}|\theta\right)\}_{p\left(\mathbf{h}_{1:T}|\mathbf{o}_{1:T}, \boldsymbol{\theta}^{\text{old}}\right)} \tag{7}$$

Notice that $p(\mathbf{h}_1)$, $p(\mathbf{h}_t|\mathbf{h}_{t-1})$ and $p(\mathbf{o}_t|\mathbf{h}_t)$ are all Gaussian, given as follows:

$$p(\mathbf{h}_1) = \frac{1}{(2\pi)^{H/2}|\boldsymbol{\Sigma}_\pi{}^{1/2}|} \exp\left\{-\frac{1}{2}(\mathbf{h}_1 - \boldsymbol{\mu}_\pi)^T \boldsymbol{\Sigma}_\pi^{-1}(\mathbf{h}_1 - \boldsymbol{\mu}_\pi)\right\} \tag{8}$$

$$p(\mathbf{h}_t|\mathbf{h}_{t-1}) = \frac{1}{(2\pi)^{H/2}|\boldsymbol{\Sigma}_h{}^{1/2}|} \exp\left\{-\frac{1}{2}(\mathbf{h}_t - \mathbf{A}\mathbf{h}_{t-1})^T \boldsymbol{\Sigma}_h^{-1}(\mathbf{h}_t - \mathbf{A}\mathbf{h}_{t-1})\right\} \tag{9}$$

$$p(\mathbf{o}_t|\mathbf{h}_t) = \frac{1}{(2\pi)^{(V+L)/2}|\boldsymbol{\Sigma}_o{}^{1/2}|} \exp\left\{-\frac{1}{2}(\mathbf{o}_t - \mathbf{B}\mathbf{h}_t)^T \boldsymbol{\Sigma}_o^{-1}(\mathbf{o}_t - \mathbf{B}\mathbf{h}_t)\right\} \tag{10}$$

Hence, the expectation of the log-likelihood function can be derived as [26]:

$$\begin{aligned} E\{L\left(\theta\right)\} &= E\{\ln p(\mathbf{h}_1) + \sum_{t=2}^{T}\ln p(\mathbf{h}_t|\mathbf{h}_{t-1}) + \sum_{t=1}^{T}\ln p(\mathbf{o}_t|\mathbf{h}_t)\} \\ &= -\frac{1}{2}\left\{\ln|\Sigma_\pi| + T\ln|\Sigma_o| + (T-1)\ln|\Sigma_h| + tr\left(E(\mathbf{h}_1\boldsymbol{h}_1^T)\boldsymbol{\Sigma}_\pi^{-1}\right) - 2E(\boldsymbol{h}_1)^T\boldsymbol{\Sigma}_\pi^{-1}\mu_\pi + \boldsymbol{\mu}_\pi^T\boldsymbol{\Sigma}_\pi^{-1}\mu_\pi\right\} \\ &-\frac{1}{2}\sum_{t=2}^{T}\left\{tr\left(E(\mathbf{h}_t\boldsymbol{h}_t^T|\mathbf{o}_{1:T})\boldsymbol{\Sigma}_h^{-1}\right) - 2tr\left(E(\mathbf{h}_t\boldsymbol{h}_{t-1}^T|\mathbf{o}_{1:T})\boldsymbol{A}^T\boldsymbol{\Sigma}_h^{-1}\right) + tr\left(E(\mathbf{h}_{t-1}\mathbf{h}_{t-1}^T|\mathbf{o}_{1:T})\boldsymbol{A}^T\boldsymbol{\Sigma}_h^{-1}\mathbf{A}\right)\right\} \\ &-\frac{1}{2}\sum_{t=1}^{T}\left\{tr\left(\mathbf{o}_t\boldsymbol{o}_t^T\boldsymbol{\Sigma}_o^{-1}\right) - 2tr\left(\mathbf{o}_tE(\boldsymbol{h}_t|\mathbf{o}_{1:T})^T\boldsymbol{B}^T\boldsymbol{\Sigma}_o^{-1}\right) + tr\left(E(\mathbf{h}_t\boldsymbol{h}_t^T|\mathbf{o}_{1:T})\boldsymbol{B}^T\boldsymbol{\Sigma}_o^{-1}\mathbf{B}\right)\right\} + \text{constant} \end{aligned} \tag{11}$$

where $E(\mathbf{h}_t|\mathbf{o}_{1:T})$, $E(\mathbf{h}_t\mathbf{h}_t^T|\mathbf{o}_{1:T})$, and $E(\mathbf{h}_{t-1}\mathbf{h}_t^T|\mathbf{o}_{1:T})$ are three required statistics for calculation of the expectation value of the log-likelihood function in the M-step. Therefore, in the E-step of the EM algorithm, those three statistics need to be determined, given as follows:

$$E(\mathbf{h}_t|\mathbf{o}_{1:T}) = \mathbf{g}_t = \mathbf{F}_t\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_t\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)^{-1}\left(\mathbf{g}_{t+1} - \mathbf{A}\mathbf{f}_t\right) + \mathbf{f}_t \tag{12}$$

$$E(\mathbf{h}_t\mathbf{h}_t^T|\mathbf{o}_{1:T}) = var(\mathbf{h}_t|\mathbf{o}_{1:N}) + E(\mathbf{h}_t|\mathbf{o}_{1:T})E^T(\mathbf{h}_t|\mathbf{o}_{1:T}) = \mathbf{G}_t + \mathbf{g}_t\mathbf{g}_t^T$$
$$\mathbf{G}_t = \mathbf{F}_t\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_t\mathbf{A}^T + \mathbf{\Sigma}_h\right)^{-1}G_{t+1}\left[\mathbf{F}_t\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_t\mathbf{A}^T + \mathbf{\Sigma}_h\right)^{-1}\right]^T + \mathbf{F}_t - \mathbf{F}_t\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_t\mathbf{A}^T + \mathbf{\Sigma}_h\right)^{-1}\mathbf{A}\mathbf{F}_t \tag{13}$$

$$E(\mathbf{h}_{t-1}\mathbf{h}_t^T|\mathbf{o}_{1:T}) = \mathbf{F}_{t-1}\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_{t-1}\mathbf{A}^T + \mathbf{\Sigma}_h\right)^{-1}\mathbf{G}_t + \mathbf{g}_{t-1}\mathbf{g}_t^T \tag{14}$$

where $t = 2, 3, \ldots, T$, $g_T = f_T$, $G_T = F_T$, and

$$\boldsymbol{f}_t = E(\mathrm{h}_t|\mathrm{o}_{1:t}) = \boldsymbol{A}\boldsymbol{f}_{t-1} + \left(\mathbf{A}\boldsymbol{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\boldsymbol{B}^T\left[\mathrm{B}\left(\mathbf{A}\boldsymbol{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\boldsymbol{B}^T + \boldsymbol{\Sigma}_o\right]^{-1}\left(\mathrm{o}_t - \mathbf{A}\mathbf{B}\boldsymbol{f}_{t-1}\right) \tag{15}$$

$$\boldsymbol{F}_t = var(\boldsymbol{h}_t|\mathrm{o}_{1:t}) = \boldsymbol{A}\boldsymbol{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h - \left(\mathbf{A}\boldsymbol{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\boldsymbol{B}^T\left[\mathrm{B}\left(\mathbf{A}\boldsymbol{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\boldsymbol{B}^T + \boldsymbol{\Sigma}_o\right]^{-1}\mathrm{B}\left(\mathbf{A}\boldsymbol{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right) \tag{16}$$

It can be noticed that all Eqs. (12)–(16) are calculated through the iterative manner. When $t = 1$, the initial value of $\mathbf{f}_1$ and $\mathbf{F}_1$ are given as

$$\mathbf{f}_1 = \boldsymbol{\mu}_\pi + \mathbf{\Sigma}_\pi\mathbf{B}^T\left[\mathbf{B}\mathbf{\Sigma}_\pi\mathbf{B}^T + \mathbf{\Sigma}_o\right]^{-1}(\mathbf{o}_1 - \mathbf{B}\boldsymbol{\mu}_\pi) \tag{17}$$

$$\mathbf{F}_1 = \mathbf{\Sigma}_\pi - \mathbf{\Sigma}_\pi\mathbf{B}^T\left[\mathbf{B}\mathbf{\Sigma}_\pi\mathbf{B}^T + \mathbf{\Sigma}_o\right]^{-1}\mathbf{B}\mathbf{\Sigma}_\pi \tag{18}$$

Based on those three statistics obtained in the E-step, all parameter values of the supervised LDS model can be updated in the M-step of the EM algorithm. More detailed derivations of the EM algorithm for the supervised LDS model are provided in Appendix A. Through iteratively updating and re-calculating the E-step and the M-step of the EM algorithm until convergence, the optimal parameter set can be obtained.

3. Online fault detection based on SLDS model

After the supervised LDS model has been constructed, it can be used for online fault detection. Since the supervised LDS model is driven by the latent variables, fault detection can be carried out through monitoring the status of those latent variables. Therefore, a T^2 monitoring statistic can be constructed for the fault detection purpose. Suppose we have obtained a series of online data samples, denoted as $\mathbf{X}^{\text{new}} = \left[\mathbf{x}_1^{\text{new}}, \boldsymbol{x}_2^{\text{new}}, \ldots, \boldsymbol{x}_{S-1}^{\text{new}}, \boldsymbol{x}_S^{\text{new}}\right]$ and $\boldsymbol{Y}^{\text{new}} = \left[\mathbf{y}_1^{\text{new}}, \boldsymbol{y}_2^{\text{new}}, \ldots, \boldsymbol{y}_{S-1}^{\text{new}}, \boldsymbol{y}_S^{\text{new}}\right]$. After those data samples have been pre-processed, they can be re-arranged as the observed data matrix, given as

$$\boldsymbol{O}^{\text{new}} = \begin{bmatrix}\mathbf{X}^{\text{new}}\\ \boldsymbol{Y}^{\text{new}}\end{bmatrix} = \left[\mathbf{o}_1^{\text{new}}, \boldsymbol{o}_2^{\text{new}}, \ldots, \boldsymbol{o}_{S-1}^{\text{new}}, \boldsymbol{o}_S^{\text{new}}\right] = \{\begin{bmatrix}\mathbf{x}_1^{\text{new}}\\ \boldsymbol{y}_1^{\text{new}}\end{bmatrix}, \begin{bmatrix}\mathbf{x}_2^{\text{new}}\\ \boldsymbol{y}_2^{\text{new}}\end{bmatrix}, \ldots, \begin{bmatrix}\mathbf{x}_{S-1}^{\text{new}}\\ \boldsymbol{y}_{S-1}^{\text{new}}\end{bmatrix}, \begin{bmatrix}\mathbf{x}_S^{\text{new}}\\ \boldsymbol{y}_S^{\text{new}}\end{bmatrix}\} \tag{19}$$

The expected value of the latent variables corresponding to each observed data can be calculated as follows

$$E\left(\mathrm{h}_t^{\text{new}}|\mathrm{o}_{1:S}^{\text{new}}\right) = \boldsymbol{f}_t^{\text{new}} = \boldsymbol{A}\boldsymbol{f}_{t-1} + \left(\mathbf{A}\boldsymbol{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\boldsymbol{B}^T\left[\mathrm{B}\left(\mathbf{A}F_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\boldsymbol{B}^T + \boldsymbol{\Sigma}_o\right]^{-1}\left(\mathrm{o}_t - \mathbf{A}\mathbf{B}\boldsymbol{f}_{t-1}\right) \tag{20}$$

Then, the T^2 monitoring statistic can be constructed as

$$T_{t,\text{new}}^2 = E\left(\mathrm{h}_t^{\text{new}}|\mathrm{o}_{1:S}^{\text{new}}\right)^T var(\mathrm{h})^{-1}E\left(\mathrm{h}_t^{\text{new}}|\mathrm{o}_{1:S}^{\text{new}}\right) \tag{21}$$

where $t = 1, 2, \ldots, S$, $var(\mathbf{h})$ is the variance of latent variables, which can be determined as the expected value of the training data samples in the modeling process, given as

$$var(\mathrm{h}) = E\left((\mathrm{f}_t - E(\mathrm{f}_t))\left(\mathrm{f}_t - E(\mathrm{f}_t)^T\right)\right)$$
$$\boldsymbol{f}_t = E(\mathrm{h}_t|\mathrm{o}_{1:t}) \in R^{H\times 1}, \quad t = 1, 2, \ldots, N \tag{22}$$

Typically, the control limit of the T^2 monitoring statistic can be determined by the χ^2 distribution, thus $T_{\text{lim}}^2 = \chi_\alpha^2(H)$, where H is the freedom index of the distribution, α is the significant level. Here, the value of α needs to be set by the user. Generally, a big α will cause more false alarms while a small α will render more missing alarms. In practice, the selection of α should be made for the tradeoff between false alarms and missing alarms. In this paper, the value of α is set as 0.01, which means the false alarm rate of normal data samples is 0.01. As a result, if $T_{t,\text{new}}^2 \le T_{\text{lim}}^2$, the system is under control; otherwise, if $T_{t,\text{new}}^2 > T_{\text{lim}}^2$, the status of the latent variables is out of control, which means the observed variables may also go to the outside of the normal operating region. In this case, attentions should be paid and the fault needs to be diagnosed and identified for further process maintenance. A flowchart for modeling and online fault detection of the supervised LDS model is shown in Fig. 2.

4. Industrial case study

Derived from a real industry process, the Tennessee Eastman (TE) process has been used as a benchmark for many years [27]. Lots of control, monitoring, fault diagnosis and optimization algorithms have been tested in this process in the past several decades. The flow chart of TE process is shown in Fig. 3, in which the control structure is also shown schematically. Detailed information about the control structure of this process can be found in Lyman and Georgakis [28]. This process contains five major units: a reactor, a condenser, a separator, a stripper and a compressor. 41 measured variables and 12 manipulated variables are involved in this process. A total of 21 programmed faults can be simulated, which include sixteen known faults and five unknown faults. Detailed information of those 21 faults is given in Table 1. In this paper, 16 process variables and two quality variables (components G and H in stream 9) are selected for fault detection, which are tabulated together in Table 2.

It is noted that the sampling rate of the two quality variables is 6 min in this process, while the sampling rate of other process variables is 3 min. In order to keep accordance for all monitoring variables, the process variables have been down-sampled. For model training of

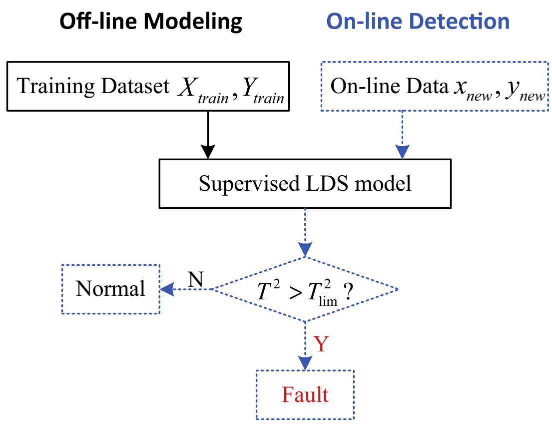


Fig. 2. Flowchart for modeling and online fault detection of the supervised LDS model.

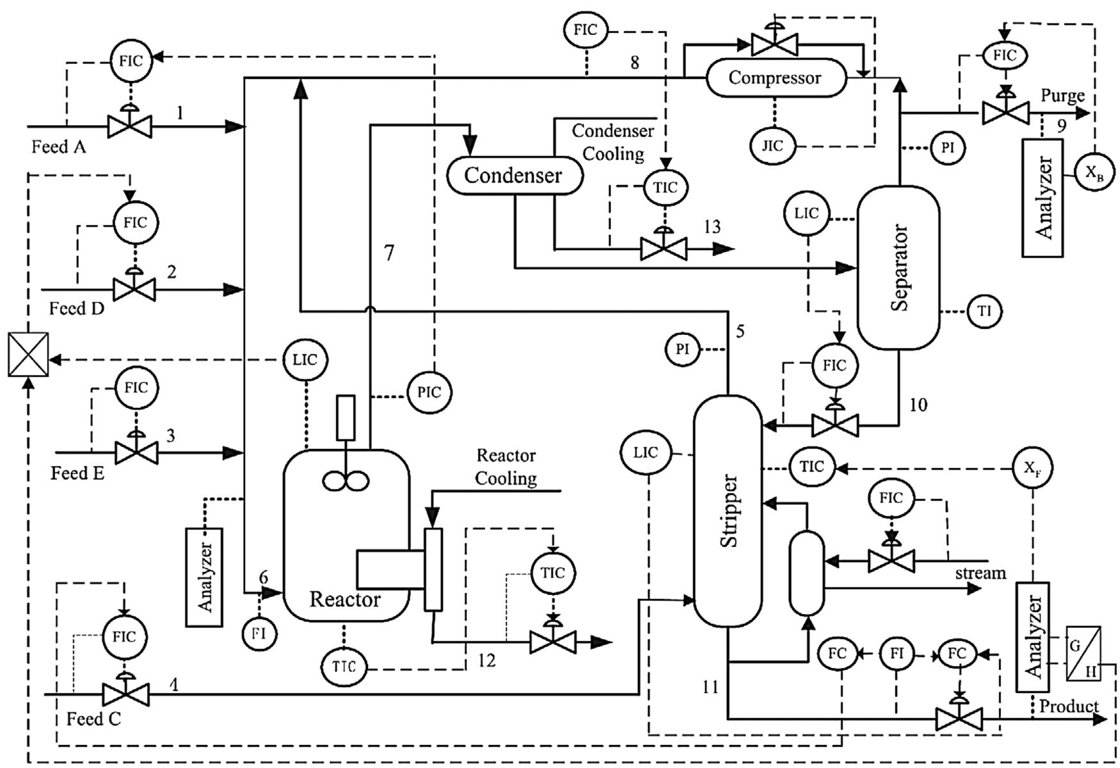


Fig. 3. Flow chart of Tennessee Eastman (TE) process.

supervised LDS, a total of 480 samples have been employed. Both probabilistic PCA model and the traditional LDS model have also been constructed for performance comparison with the new method. All of the 21 programmed faults in this process are used for testing the fault detection performance of the three monitoring approaches. The number of latent variables in the supervised LDS model can be determined through several methods. For example, *H* can be chosen based on the average variance explanation of the latent variable, or it can be determined through automatic relevance determination (ARD) [29]. A more simple way is to predetermine a proper dimensionality via PCA, and then adopt the dimensionality in the supervised LDS model. Fig. 4 illustrates the detailed monitoring results of the LDS and SLDS methods under different numbers of latent variables. Generally, it can be found that the fault detection performance of the supervised LDS model is always better than that of the LDS model.

After all of the three monitoring models have been determined, different fault types are used for performance evaluation. Detailed results of missing detection rates for the three methods are tabulated together in Table 3. In the last row, the average values of the missing detection rates for different methods are calculated. It can be seen that the fault detection performance has been greatly improved by incorporating the dynamic data information into the model, because the missing detection rates of both LDS and SLDS are much lower than that of the PPCA model. Compared to the LDS model based fault detection method, the performance has been further improved by the supervised LDS model. This is due to the incorporation of the quality information into the model. Detailed fault detection results of fault 5, fault 7, and fault 10 by the three methods are shown in Figs. 5–7. It can be seen more clearly that the fault detection performance has been improved by the new method. It should be noted that those faults are active in the rest of the process after they have been detected.

Table 1
Fault descriptions of TE process.

Fault number	Process variable	Type
1	A/C feed ratio, B composition constant (stream 4)	Step
2	B composition, A/C ratio constant (stream 4)	Step
3	D feed temperature (stream 2)	Step
4	Reactor cooling water inlet temperature	step
5	Condenser cooling water inlet temperature	Step
6	A feed loss (stream 1)	Step
7	C header pressure loss-reduced availability (stream 4)	Step
8	A–C feed composition (stream 4)	Random variation
9	D feed temperature (stream 2)	Random variation
10	C feed temperature (stream 4)	Random variation
11	Reactor cooling water inlet temperature	Random variation
12	Condenser cooling water inlet temperature	Random variation
13	Reaction kinetics	Slow drift
14	Reactor cooling water valve	Sticking
15	Condenser cooling water valve	Sticking
16	Unknown	Unknown
17	Unknown	Unknown
18	Unknown	Unknown
19	Unknown	Unknown
20	Unknown	Unknown
21	Valve position constant (stream 4)	Constant position

Table 2
Selected variables in the TE process.

No.	Measured variables
1	A feed
2	D feed
3	E feed
4	A and C feed
5	Recycle flow
6	Reactor feed rate
7	Reactor temperature
8	Purge rate
9	Product separator temperature
10	Product separator pressure
11	Product separator underflow
12	Stripper pressure
13	Stripper temperature
14	Stripper steam flow
15	Reactor cooling water outlet temperature
16	Separator cooling water outlet temperature
17	Component G in stream 9
18	Component H in stream 9

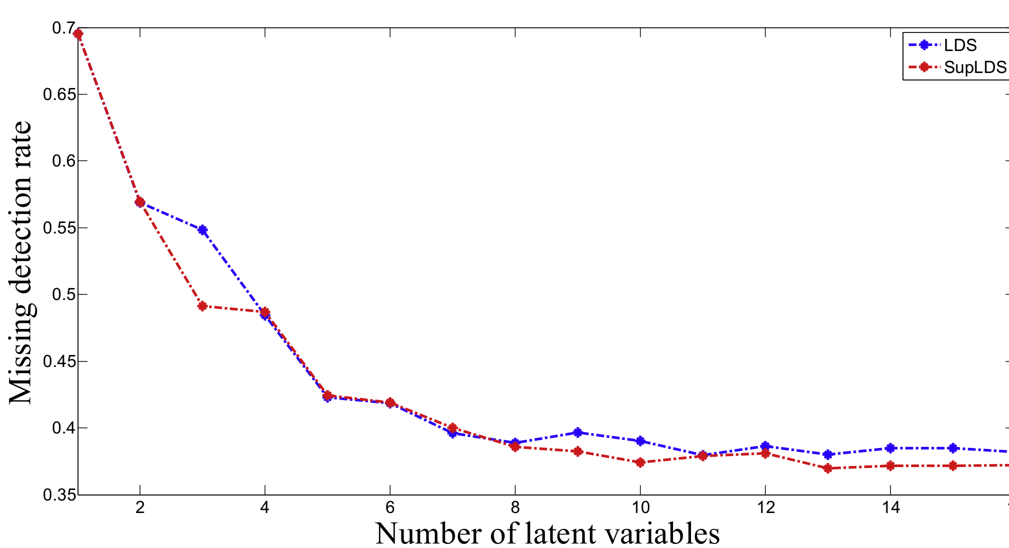


Fig. 4. Monitoring results of the LDS and SLDS methods under different numbers of latent variables.

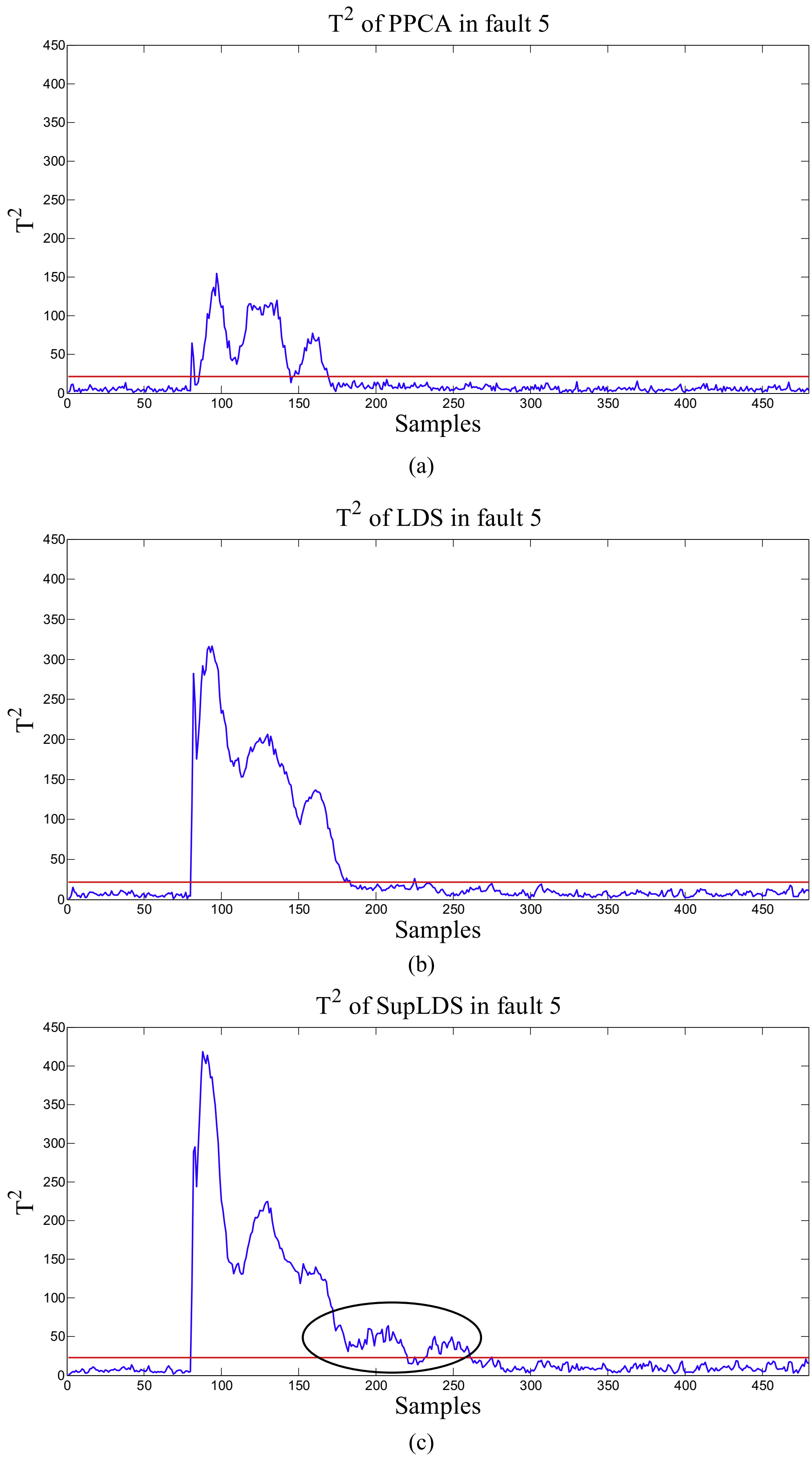


Fig. 5. Fault detection results of fault 5.

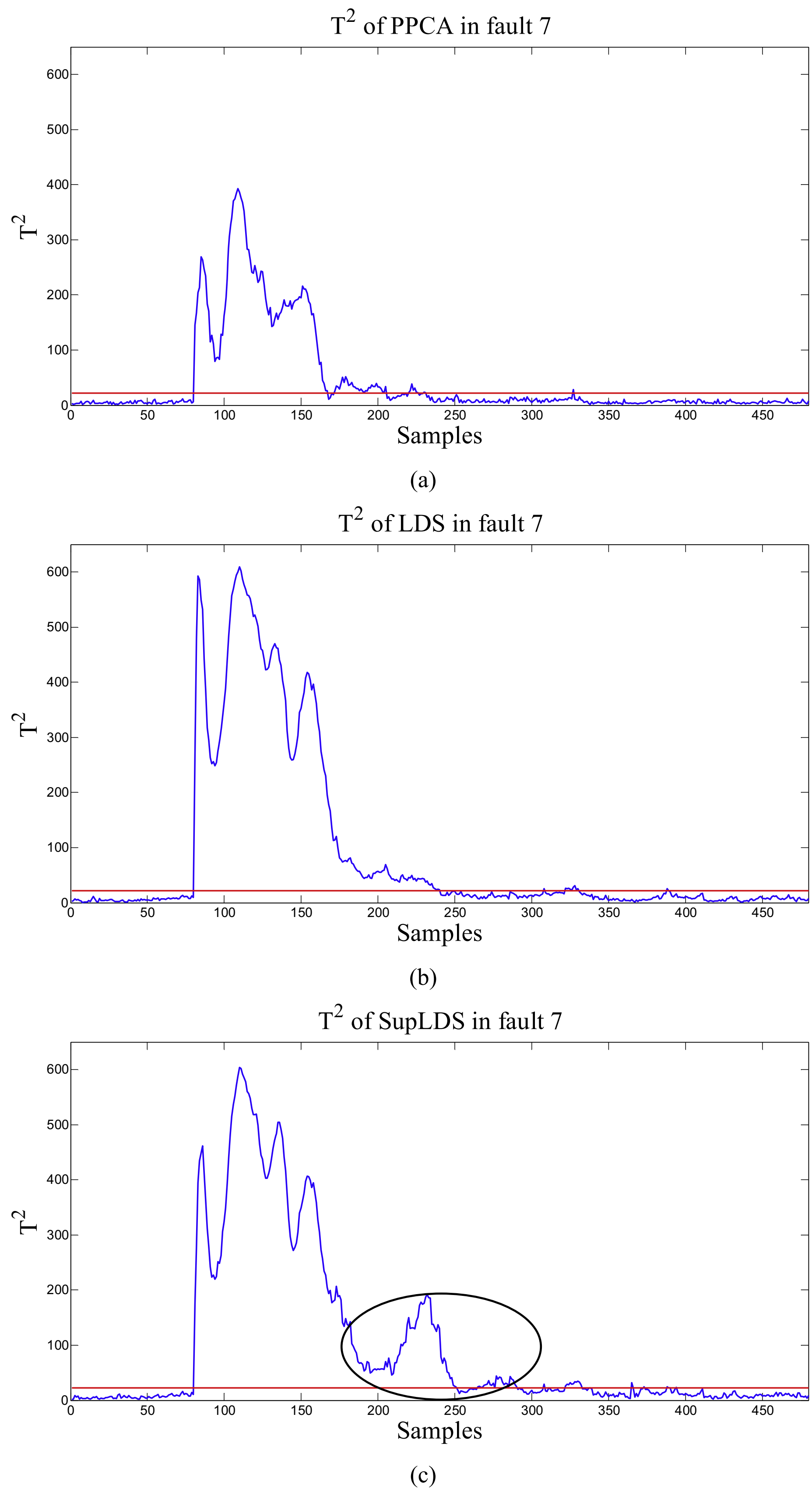


Fig. 6. Fault detection results of fault 7.

Table 3
Missing detection rates of the three methods under different fault cases.

Faults	Missing detection rates		
	PPCA	LDS	SupLDS
1	0.01	0.0025	0.0025
2	0.0325	0.02	0.0225
3	1	0.985	0.9525
4	1	0.9925	0.9925
5	0.7875	0.7425	0.5725
6	0	0	0
7	0.6675	0.5725	0.465
8	0.0525	0.02	0.02
9	0.9975	0.9825	0.975
10	0.83	0.12	0.11
11	0.935	0.6725	0.6225
12	0.03	0.005	0.0025
13	0.065	0.0525	0.0525
14	0.025	0.075	0.01
15	1	0.9375	0.935
16	0.9125	0.4675	0.49
17	0.2325	0.0275	0.0275
18	0.1125	0.1025	0.105
19	0.9775	0.9825	0.975
20	0.885	0.1425	0.105
21	0.7175	0.425	0.4225
Average	0.536667	0.396548	0.374286

Therefore, it means that more T^2 values are above the threshold, the smaller is the missing detection rate. The improved fault detection rates by the new method have been marked in circles.

5. Conclusions

In this paper, a supervised form of the LDS model has been developed and used for fault detection. Compared to the traditional LDS model, additional quality information has been successfully incorporated into the monitoring model. As a result, the fault detection performance has been improved by the new developed supervised LDS model. Although the improvement brought by the supervised LDS model is limited compared to the LDS model in the case provided in this paper, the idea of incorporating the quality information into the dynamic model is quite important for process monitoring. This is because the quality variables can serve as a supervised term in both information extraction and monitoring model construction processes.

It worth to be noticed that the supervised LDS model can be considered as a basic quality related dynamic fault detection model, which means additional improvements can be made upon this model. For example, mixture models can be developed to address those processes which have multiple operating conditions; nonlinear extensions can be made to describe the complicated dynamic relationships among different process variables; a further discriminant model can be formulated for the fault classification purpose; different fault types can be considered, such as process-relevant but quality-irrelevant faults, quality-relevant faults, etc, in which cases more meaningful monitoring statistics need to be developed. Besides, different sampling rates of the quality and process variables can be further considered in the supervised LDS model. In this case, the missing data estimation, Bayesian data inference, or even the semi-supervised learning approaches can be employed for model development and applications.

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Appendix A. Detailed derivation of the EM algorithm for SLDS

Re-write the log-likelihood function as:

$$E\{L\left(\boldsymbol{\theta}\right)\} = E\{\ln p(\mathbf{h}_1) + \sum_{t=2}^{T} \ln p(\mathbf{h}_t|\mathbf{h}_{t-1}) + \sum_{t=1}^{T} \ln p(\mathbf{o}_t|\mathbf{h}_t)\} \tag{23}$$

In order to update the parameter set in the M-step of the EM algorithm, three statistics $E(\mathbf{h}_t|\mathbf{o}_{1:T})$, $E(\mathbf{h}_t\mathbf{h}_t^T|\mathbf{o}_{1:T})$, and $E(\mathbf{h}_{t-1}\mathbf{h}_t^T|\mathbf{o}_{1:T})$ need to be calculated in the E-step. This can be done through the forward and backward algorithm, depicted in Fig. 8. First, initialization of the latent variable distribution is given as $p(\mathbf{h}_1|\mathbf{o}_1) = N(\boldsymbol{\mu}_\pi, \boldsymbol{\Sigma}_\pi)$. The forward recursion for calculation of the $p(\mathbf{h}_t|\mathbf{o}_{1:t})$ is as follows

$$p(\mathbf{h}_t|\mathbf{o}_{1:t}) = \frac{\int_{\mathbf{h}_{t-1}} p(\mathbf{o}_t|\mathbf{h}_t)\, p(\mathbf{h}_t|\mathbf{h}_{t-1})\, p(\mathbf{h}_{t-1}|\mathbf{o}_{1:t-1})}{\int_{\mathbf{h}_{t-1},\mathbf{h}_t} p(\mathbf{o}_t|\mathbf{h}_t)\, p(\mathbf{h}_t|\mathbf{h}_{t-1})\, p(\mathbf{h}_{t-1}|\mathbf{o}_{1:t-1})}, \quad 2 \le t \le T \tag{24}$$

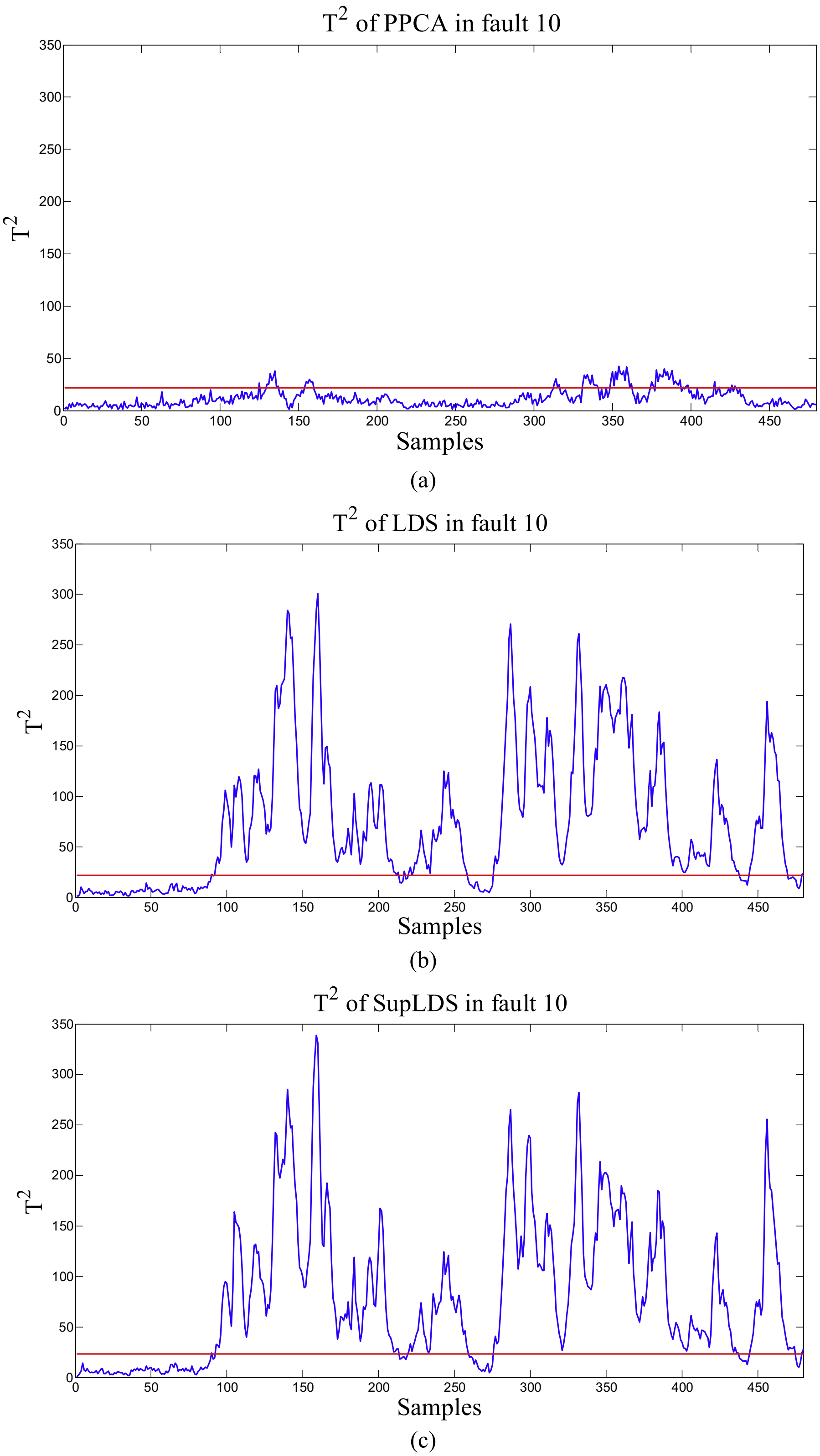
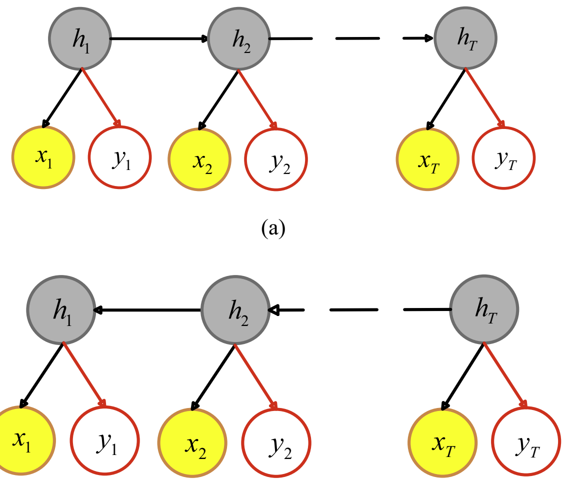


Fig. 7. Fault detection results of fault 10.

Since it is a Gaussian distribution, the mean and variance value can be obtained as

$$\mathbf{f}_t = \mathbf{A}\mathbf{f}_{t-1} + \left(\mathbf{A}\mathbf{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\mathbf{B}^T\left[\mathbf{B}\left(\mathbf{A}\mathbf{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\mathbf{B}^T + \boldsymbol{\Sigma}_o\right]^{-1}\left(\mathbf{o}_t - \mathbf{A}B\mathbf{f}_{t-1}\right) \tag{25}$$

$$\mathbf{F}_t = \mathbf{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h - \left(\mathbf{A}\mathbf{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\mathbf{B}^T\left[\mathbf{B}\left(\mathbf{A}\mathbf{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)\mathbf{B}^T + \boldsymbol{\Sigma}_o\right]^{-1}\mathbf{B}\left(\mathbf{A}\mathbf{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right) \tag{26}$$



(a)

(b)

Fig. 8. Flowchart of forward and backward iteration process.

Then, in the backward step, we try to smooth the estimation results. The initial value of the latent variable distribution in the backward step $p(\mathbf{h}_T|\mathbf{o}_{1:T})$ can be obtained from the forward step. Similarly, The backward recursion of $p(\mathbf{h}_t|\mathbf{o}_{1:T})$ can be derived as follows

$$p(\mathbf{h}_t|\mathbf{o}_{1:T}) = \int_{\mathbf{h}_{t+1}} p(\mathbf{h}_t|\mathbf{o}_{1:t}, \mathbf{h}_{t+1})p(\mathbf{h}_{t+1}|\mathbf{o}_{1:T}), \quad 1 \le t \le T-1 \tag{27}$$

It is also a Gaussian distribution, the mean and variance of which are given as

$$\mathbf{g}_t = \mathbf{F}_t\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_t\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)^{-1}\left(\mathbf{g}_{t+1} - \mathbf{A}\mathbf{f}_t\right) + \mathbf{f}_t \tag{28}$$

$$\mathbf{G}_t = \mathbf{F}_t\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_t\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)^{-1}G_{t+1}\left[\mathbf{F}_t\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_t\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)^{-1}\right]^T + \mathbf{F}_t - \mathbf{F}_t\mathbf{A}^T\left(\mathbf{A}\mathbf{F}_t\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)^{-1}\mathbf{A}\mathbf{F}_t \tag{29}$$

The conditional joint probability of $\mathbf{h}_t$ and $\mathbf{h}_{t-1}$ can be determined as

$$p(\mathbf{h}_t, \mathbf{h}_{t-1}|\mathbf{o}_{1:T}) = p(\mathbf{h}_t, |\mathbf{h}_{t-1}, \mathbf{o}_{1:T})p(\mathbf{h}_{t-1}|\mathbf{o}_{1:T}) = p(\mathbf{h}_t, |\mathbf{h}_{t-1})p(\mathbf{h}_{t-1}|\mathbf{o}_{1:T}) \tag{30}$$

Therefore, the statistic $E(\mathbf{h}_{t-1}\mathbf{h}_t^T|\mathbf{o}_{1:T})$ can be obtained as

$$E(\mathbf{h}_{t-1}\mathbf{h}_t^T|\mathbf{o}_{1:T}) = \boldsymbol{F}_{t-1}\mathbf{A}^T\left(\mathbf{A}\boldsymbol{F}_{t-1}\mathbf{A}^T + \boldsymbol{\Sigma}_h\right)^{-1}\mathbf{G}_t + \boldsymbol{g}_{t-1}\mathbf{g}_t^T \tag{31}$$

Based on the E-step, all parameters in the supervised LDS model can be updated in the M-step, through maximizing of the log-likelihood function. By setting the derivative of $E\{L\left(\boldsymbol{\theta}\right)\}$ with respect to $\boldsymbol{\mu}_\pi$ to zero, the updated value $\boldsymbol{\mu}_\pi^{\text{new}}$ can be calculated as

$$\frac{\partial E\{L\left(\theta\right)\}}{\partial \mu_\pi} = 0 \Rightarrow \boldsymbol{\mu}_\pi^{\text{new}} = E(\mathbf{h}_1|\mathbf{o}_{1:T}) \tag{32}$$

Similarly, by setting the derivative of $E\{L\left(\boldsymbol{\theta}\right)\}$ with respect to other parameters to zero, their updated values can be calculated as follows:

$$\frac{\partial E\{L\left(\theta\right)\}}{\partial \Sigma_\pi} = 0 \Rightarrow \boldsymbol{\Sigma}_\pi^{\text{new}} = E\left(\mathbf{h}_1\boldsymbol{h}_1^T|\mathbf{o}_{1:T}\right) - E(\mathbf{h}_1|\mathbf{o}_{1:T})E\left(\mathbf{h}_1^T|\mathbf{o}_{1:T}\right) \tag{33}$$

$$\frac{\partial E\{L\left(\theta\right)\}}{\partial \mathbf{A}} = 0 \Rightarrow \boldsymbol{A}^{\text{new}} = \sum_{t=1}^{N-1}E\left(\mathbf{h}_{t+1}\mathbf{h}_t^T|\mathbf{o}_{1:T}\right)\left(\sum_{t=1}^{N-1}E\left(\mathbf{h}_t\boldsymbol{h}_t^T|\mathbf{o}_{1:T}\right)\right)^{-1} \tag{34}$$

$$\frac{\partial E\{L\left(\theta\right)\}}{\partial \mathbf{B}} = 0 \Rightarrow \boldsymbol{B}^{\text{new}} = \sum_{t=1}^{N}\mathbf{o}_tE\left(\mathbf{h}_t^T|\mathbf{o}_{1:T}\right)\left(\sum_{t=1}^{N}E\left(\mathbf{h}_t\boldsymbol{h}_t^T|\mathbf{o}_{1:T}\right)\right)^{-1} \tag{35}$$

$$\frac{\partial E\{L\left(\theta\right)\}}{\partial \Sigma_o} = 0 \Rightarrow \Sigma_o^{\text{new}} = \frac{1}{N}\sum_{t=1}^{N}\left(\mathbf{o}_t\mathbf{o}_t^T - \mathbf{o}_tE\left(\mathbf{h}_t^T|\mathbf{o}_{1:T}\right)\mathbf{B}^{\text{new}T}\right) \tag{36}$$

$$\frac{\partial E\{L\left(\theta\right)\}}{\partial \Sigma_h} = 0 \Rightarrow \boldsymbol{\Sigma}_h^{\text{new}} = \frac{1}{N-1}\sum_{t=1}^{T-1}\left(E\left(\mathbf{h}_{t+1}\mathbf{h}_{t+1}^T|\mathbf{o}_{1:T}\right) - \boldsymbol{A}^{\text{new}}E\left(\mathbf{h}_t\boldsymbol{h}_{t+1}^T|\mathbf{o}_{1:T}\right)\right) \tag{37}$$

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