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Fault detection and identification using a Kullback-Leibler divergence based multi-block principal component analysis and bayesian inference

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Abstract−Considering the huge number of variables in plant-wide process monitoring and complex relationships (linear, nonlinear, partial correlation, or independence) among these variables, multivariate statistical process monitoring (MSPM) performance may be deteriorated especially by the independent variables. Meanwhile, whether related variables keep high concordance during the variation process is still a question. Under this circumstance, a multi-block technology based on mathematical statistics method, Kullback-Leibler Divergence, is proposed to put the variables having similar statistical characteristics into the same block, and then build principal component analysis (PCA) models in each low-dimensional subspace. Bayesian inference is also employed to combine the monitoring results from each sub-block into the final monitoring statistics. Additionally, a novel fault diagnosis approach is developed for fault identification. The superiority of the proposed method is demonstrated by applications on a simple simulated multivariate process and the Tennessee Eastman benchmark process.

Keywords: Multi-block PCA, Kullback-Leibler Divergence, Bayesian Inference, Plant-wide Process Monitoring

INTRODUCTION

In processing and manufacturing industries, people are trying to produce higher quality products with low unqualified rates to meet the rigorous safety and environmental standards. To guarantee that the state parameters satisfy the given performance indexes, both fault detection and diagnosis are necessary parts of the operating process [1,2]. With the improvement of data storage capability, a great number of data have been collected from industrial systems, especially from the plant-wide process. Thus, multivariate statistical process monitoring (MSPM), has gained more and more attention for its ability to handle and analyze data [3-7].

Among these MSPC methods, principal component analysis (PCA) [8-11], as the most popular data-driven technology, is the most widely used in the industrial process. Through projecting data onto the low dimensional space, PCA can characterize the state of the process, simplify the dimension reduction technology and improve the program of process monitoring. PCA is such a dimension reduction technology that it creates the low-dimensional presentation in some way and still retains the relation structure between the variables. This approach is optimal to capture the variability of the data. The applications of PCA are based on the assumptions that the data collected from an industrial process should satisfy the Gaussian distribution and be linearly related, but, usually, it is hard to meet these two requirements in a practical industrial process. Furthermore, in the single model, the relations of the variables are so complex that it is difficult to clarify the influences between the variables, not to speak of those independent variables. So constructing a suitable model is vital for fault detection.

To solve these problems, various improved measures are put forward. First, to handle the data following non-Gaussian distribution, independent component analysis (ICA) is proposed [12-15], and its combination with PCA is also presented by Ge and Song [16] to handle Gaussian and non-Gaussian process. Meanwhile, many different kinds of nonlinear PCA extensions have also been proposed for nonlinear processes, such as Jia et al. [17], Scholz et al. [18] and Ravi et al. [19]. Finally, to address the complex relations between the variables, multi-block PCA was proposed, which divides the variables into conceptually meaningful blocks and models them [20-22]. This approach can handle numerous data generated by plant-wide monitoring process and reduce the complexity of the data. Usually, multi-block methods are the basis of the cognitions or experiences of the data, so the division viewpoints are especially vital for the multi-block. Lee et al. [23] proposed adaptive multi-block MPCA, which updates the covariance structure recursively to overcome the problem of changing process conditions. Another multi-block PCA method, proposed by Cherry [24], combined several contributions to the field through a combined index. Later, Ge and Song [25] proposed a division method that divided the original data according to the different directions of principal components. The linear variables can be assigned into the same block, but there are missing and overlapped variables in the process of dividing. Tong et al. [26] proposed a system dividing knowledge that divides the whole variables based on four-subspace construction and Bayesian inference. The variables' relevance and irrelevance to the PC subspace and the residual subspace are analyzed, respectively, and then the variables are assigned into their corresponding subspaces. However, all the multi-block methods mentioned above are in accordance with prior knowledge. In the plant-wide process monitoring, the relation-

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ships between the numerous data are various and complex, such as linear, nonlinear, partial correlation, and independence. Clarifying the relations between each variable seems impossible. On the other hand, when a fault occurs, it is unknown whether the relevant variables follow the same variation or not, and whether the independent variables are totally all irrelevant. If the relevant variables have the same variation characteristic, it is not certain that the variations of irrelevant variables are independent with the fault variable. Thus, the irrelevant variables may have effects on the monitoring statistics and, finally, influence the monitoring results.

We propose a novel multi-block method based on probability statistics, Kullback-Leibler divergence and Bayesian Inference (KL-MBPCA). KL-MBPCA divides the original data on the basis of a mathematical statistics method, KL divergence, which quantitatively measures the statistical divergence between two variables. After division, the variables in the same block own similar statistic characteristics and, no doubt, enhance the ability of process monitoring. Since it is a totally data-driven method based on probability statistics, complex relationships among variables do not influence division results obviously, and the mathematical division does not need prior knowledge. Thus, the proposed method can be applied to deal with large amounts of data efficiently and even applied to a plant-wide monitoring process, which is an unsupervised and large-scale system. After the blocks have been divided properly, PCA models are built in each subspace and the monitoring statistics are figured out. To combine the results from each space together, Bayesian inference strategy [25,27] is used and the final statistics are generated.

Once the fault is detected successfully, the corresponding diagnosis should be done for the process monitoring. Fault diagnosis is an important part in fault detection and identification, and is even more difficult than fault detection. The traditional contribution plot has been widely used as a valid method for fault diagnosis [28,29]. However, there are still some disadvantages to this method. The analysis of diagnosability is vague and the accuracy of the diagnosis results cannot be guaranteed, especially when the process is complex and the number of variables is huge. To change this situation, a geometric method has been put forward and applied into the analyses of fault detectability and identification [30,31]. Meanwhile, a reconstruction-based contribution plot method (RBC) was proposed [32] and improved by Ge and Song [25], who employed this approach to linear subspace and the monitoring results are combined by Bayesian inference. More recently, a new contribution plot method was developed by Tong et al. [26] through adding Bayesian posterior probability weighted contribution index to each contribution index, but the number of the possible fault variables is not fundamentally decreased. In this paper, an improved contribution plot method is developed. The variables in the process are divided into several sub-blocks, so if the fault is detected in some sub-block, the fault variables are definitely in this block. Thus, only the contribution rates of the variables in fault sub-blocks are calculated and combined to the final contribution plot. In this way, the possible fault variables are cut down and fewer variables are needed to be analyzed to find the root causes.

The rest of this paper is organized as follows. First, both PCA and KL divergence are briefly reviewed in Section 2. Detailed descriptions of the proposed method KL-MBPCA and its monitoring procedure are given in the next two sections. Section 5 analyzes the applications to two cases, which demonstrates the feasibility and efficiency of KL-MBPCA. Then, some conclusions are drawn.

PRELIMINARIES

To introduce the proposed method more completely, the traditional PCA and KL divergence will be reviewed briefly in this section.

1. Principal Component Analysis

PCA reduces the dimensionality of the dataset though generating a new set of coordinates and projecting original data onto them [1,33]. Given a data matrix $\mathbf{X}\in\mathbf{R}^{n\times m}$ with zero mean and unit variance, where n and m are the numbers of observations and variables, respectively, the covariance matrix **S** can be obtained from matrix **X**, and the loading matrix **P** can be calculated through eigenvalue decomposition method as follows [8]:

$$\mathbf{S}=\frac{\mathbf{X}^T\mathbf{X}}{\mathrm{n}-1}=\mathbf{P}\Lambda\mathbf{P}^T \tag{1}$$

where Λ is the diagonal matrix whose values are the eigenvalues arranged in descending order, and **P** is the corresponding eigenvector matrix. To acquire the variation of the data optimally, the first k principal components are selected to build PCA model and the others compose the residual matrix **E**. Adding the score matrix $\mathbf{T}\in\mathbf{R}^{m\times k}$, the matrix **X** can be expressed as [5]:

$$\mathbf{X}=\mathbf{T}\mathbf{P}^T+\mathbf{E} \tag{2}$$

To detect the faults timely, two statistics, T^2 and SPE, are structured to monitor principle component space and residual space, respectively [1]:

$$T^2=\mathbf{x}^T\mathbf{P}\Lambda_k^{-1}\mathbf{P}\mathbf{x} \tag{3}$$

$$\mathrm{SPE}=\mathbf{r}^T\mathbf{r},\ \mathbf{r}=(\mathbf{I}-\mathbf{P}\mathbf{P}^T)\mathbf{x} \tag{4}$$

where Λ_k is the diagonal matrix composed of the first k eigenvalues and **r** is the projection of **X** in the residual space.

2. Kullback-Leibler Divergence

The Kullback-Leibler divergence [27,34,35] (also information divergence, relative entropy or I-divergence) measures the difference between two probability distributions, P and Q. Typically, P represents the true distribution and Q represents a model or approximation of P. KL divergence is the additional number of bits between the code data from P and the optimal code based on Q, defined as [35]

$$\mathrm{D}_{KL}(\mathrm{P}\,||\,\mathrm{Q})=\sum_i \mathrm{P(i)}\log\frac{\mathrm{P(i)}}{\mathrm{Q(i)}}\ge 0 \tag{5}$$

with equality if and only if P=Q. A small value of $\mathrm{D}_{KL}(\mathrm{P}||\mathrm{Q})$ means a high similarity. In addition, the probability distribution P can be calculated by kernel density estimation [27] with the formula displayed as follows:

$$\mathrm{P(i)}=\frac{1}{\mathrm{n}_0}\sum_{i=1}^{n_0}\mathrm{K}_h(\mathrm{x}-\mathrm{x}_i) \tag{6}$$

where x_i(i=1, 2, …, n_0) is the samples while n_0 is the corresponding sample number; K_h(g) is a symmetric kernel function and h>0 is a smoothing parameter called the bandwidth. Then the probability distribution Q can be estimated just as the probability distribution P.

For a set of data, the probability distribution of one variable can be regarded as P and any other one is regarded as Q so that the KL divergence between each of them can be calculated. Since KL divergence is a non-symmetric measure, the KL from P to Q is not necessarily the same as the KL from Q to P. Therefore, two divergences, $D_{KL}(P||Q)$ and $D_{KL}(Q||P)$, should be figured out to quantify the relationships between every two variables. This quantification based on KL divergence takes both the linear correlations and nonlinear relations into account.

KL-MBPCA SCHEME

The detailed description of the proposed method KL-MBPCA is presented in this part.

1. Division of the Subspaces

Facing a great quantity of measured data in the plant-wide monitoring, it is difficult for traditional methods to handle the mass data and detect faults, but a multi-block approach can do well by focusing on dividing variables into several sub-blocks to reflect the fluctuation of the variables more distinctly. In such a case, a proper theory is vital to help block and, in this paper, KL divergence is employed because of its statistical characteristics.

Suppose that the collected dataset is $\mathbf{X}\in\mathbf{R}^{n\times m}$, where n is denoted as the sample number and m is denoted as the number of variables. KL method calculates the divergence between two variables x_i and x_j(i=1, 2, …, m; j=1, 2, …, m), and uncovers the similarity among data. Since KL divergence is a non-symmetric measure that both $D_{KL}(p(x_1)||p(x_2))$ and $D_{KL}(p(x_2)||p(x_1))$ should be figured out, where $p(x_i)$, $p(x_j)$ are the probability density functions of x_i, x_j respectively. Then, each variable has to calculate the m−1 KL divergences with the other variables and one KL divergence with itself which equals to zero. To eliminate the influence of asymmetry, the divergence can be defined as

$$D_{KL}(x_i,x_j)=\frac{1}{2}D_{KL}(p(x_i)\,||\,p(x_j))+D_{KL}(p(x_j)\,||\,p(x_i)) \tag{7}$$

So a KL divergence matrix $D_{XL}\in\mathbf{R}^{m\times m}$ is created. The small value of KL represents a high similarity between the two variables while the high value is opposite. To divide the variables more reasonably, a division rule is introduced. First, a value is set as the threshold value. Then, when the KL value between two variables is below the threshold value α, the two variables should be divided into the same block. Otherwise, these two variables should be separated. If the KL values of some variable x_i are all above the threshold value α, the variable x_i should follow the variable x_j, whose KL value is the smallest with the variable x_i, to the same block. On this way we can divide the variables into several blocks as

$$\mathbf{X}=[\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_b] \tag{8}$$

where b is the number of sub-blocks; Set $\mathbf{X}_k\in R^{n\times m_k}$(k=1, 2, …, b) with n samples and m_k variables, and build individual PCA sub-models in each of sub-block as follows [5]

$$\mathbf{X}_k=\mathbf{T}_k\mathbf{P}_k^T+\mathbf{E}_k \tag{9}$$

In each sub-block, the number of principal components is determined by cumulative percentage variance (CPV) rule [1], and thus b PCA sub-models are produced.

2. Bayesian Inference

After constructing the sub-models, the monitored dataset $\mathbf{x}$ is divided into several parts as above, and the monitoring statistics T^2 and SPE in each sub-block are produced. Due to the different number of retained PCs, the corresponding confidence limits from PCA monitoring sub-models are generated as well, but combining these monitoring statistics directly into the final results seems not easy. An intuitionistic and practical strategy is needed to transfer the results in a probabilistic manner. Bayesian inference [25,27] is employed to combine the statistics of each subspace together and give more details for monitoring detection. The fault probability of the T^2 statistic in subspace k can be calculated as follows [27]:

$$P_{T^2}(F|\mathbf{x}_k)=\frac{P_{T^2}(\mathbf{x}_k|F)P_{T^2}(F)}{P_{T^2}(\mathbf{x}_k)} \tag{10}$$

$$P_{T^2}(\mathbf{x}_k)=P_{T^2}(\mathbf{x}_k|N)P_{T^2}(N)+P_{T^2}(\mathbf{x}_k|N)P_{T^2}(F) \tag{11}$$

where N and F are considered as normal and abnormal conditions, respectively. $P_{T^2}(N)$ and $P_{T^2}(F)$, which are the prior probabilities of normal and abnormal process, are set as $1-\beta$ and β, respectively, where β is the significance level. However, to calculate the Eqs. (10), the conditional probabilities $P_{T^2}(\mathbf{x}_k|N)$ and $P_{T^2}(\mathbf{x}_k|F)$ should be figured out first, as follows [25]:

$$P_{T^2}(\mathbf{x}_k|N)=\exp\left\{-\frac{T_k^2(\mathbf{x}_k)}{vT_{k,lim}^2}\right\} \tag{12}$$

$$P_{T^2}(\mathbf{x}_k|F)=\exp\left\{-\frac{T_{k,lim}^2}{vT_k^2(\mathbf{x}_k)}\right\} \tag{13}$$

where v is a tuning parameter and $T_k^2(\mathbf{x}_k)$ is the monitoring statistic T^2 of subspace k. Likewise, the fault probability of the SPE statistic in subspace k can be calculated as follows:

$$P_{SPE}(F|\mathbf{x}_k)=\frac{P_{SPE}(\mathbf{x}_k|F)P_{SPE}(F)}{P_{SPE}(\mathbf{x}_k)} \tag{14}$$

$$P_{SPE}(\mathbf{x}_k)=P_{SPE}(\mathbf{x}_k|N)P_{SPE}(N)+P_{SPE}(\mathbf{x}_k|N)P_{SPE}(F) \tag{15}$$

where the conditional probabilities $P_{SPE}(\mathbf{x}_k|N)$ and $P_{SPE}(\mathbf{x}_k|F)$ are defined as:

$$P_{SPE}(\mathbf{x}_k|N)=\exp\left\{-\frac{SPE_k(\mathbf{x}_k)}{vSPE_{k,lim}}\right\} \tag{16}$$

$$P_{SPE}(\mathbf{x}_k|F)=\exp\left\{-\frac{SPE_{k,lim}}{vSPE_k(\mathbf{x}_k)}\right\} \tag{17}$$

The $SPE_k(\mathbf{x}_k)$ is the monitoring statistic SPE of subspace k. Therefore, according to these two fault probabilities in different subspaces, two final monitoring statistics, $BIC_{T^2}(\mathbf{x})$ and $BIC_{SPE}(\mathbf{x})$, can be given in a weighted form as [25]

$$BIC_{T^2}(\mathbf{x})=\sum_k^b\left\{\frac{P_{T^2}(\mathbf{x}_k|F)P_{T^2}(F|\mathbf{x}_k)}{\sum_k^b P_{T^2}(\mathbf{x}_k|F)}\right\} \tag{18}$$

$$BIC_{SPE}(\mathbf{x})=\sum_k^b\left\{\frac{P_{SPE}(\mathbf{x}_k|F)P_{SPE}(F|\mathbf{x}_k)}{\sum_k^b P_{SPE}(\mathbf{x}_k|F)}\right\} \tag{19}$$

The control limits for $BIC_{T^2}(\mathbf{x})$ and $BIC_{SPE}(\mathbf{x})$ are all set as β, and,

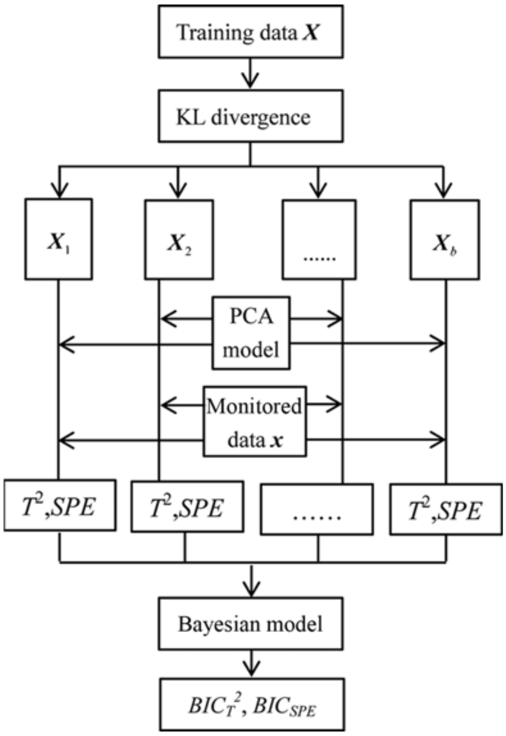

Fig. 1. Illustration of KL-MBPCA for process monitoring.

when any of their values exceeds the level β, some fault is deemed to happen and corresponding detection measures should be done. Otherwise, the monitoring process is considered to be normal.

PROCESS MONITORING

Based on the proposed method, a detailed procedure in process monitoring is introduced in this section.

1. Fault Detection Based on KL Divergence and Bayesian Inference

A schematic diagram of the proposed multi-block ICA based on KL divergence and Bayesian inference is shown in Fig. 1 and the specific steps are summarized as follows:

1-1. Process Monitoring

Step 1: Collect the training dataset from the Plant-Wide Process under normal condition;

Step 2: Calculate the KL divergences between each two variables;

Step 3: Specify the threshold value and divide the variables based on KL divergences and the proposed division rule;

Step 4: Establish PCA sub-models in each subspace;

Step 5: Collect monitored data **x** from the industrial process and divide the variables into blocks just as the results of Step 3;

Step 6: In each sub-block, the monitoring statistics T^2 and SPE are computed and their corresponding confidence limits are determined;

Step 7: Specify the significance level β and combine the results from all subspaces based on Bayesian inference;

Step 8: New monitoring statistics $BIC_{T^2}(\mathbf{x})$ and $BIC_{SPE}(\mathbf{x})$ are generated and the fault will be detected when $BIC_{T^2}(\mathbf{x})>\beta$ or $BIC_{SPE}(\mathbf{x})>\beta$.

2. Novel Contribution Plots for Fault Diagnosis

Once the fault is detected in the plant-wide process, further research about diagnosing the root cause of the faults should be done. Although various methods have been investigated, contribution plots [28,29] provide an intuitive and efficient solution. For the monitored sample $\mathbf{x}_k$ in the subspace k, the dataset can be expressed as

$$\mathbf{x}_k=[x_k^1, x_k^2, \ldots, x_k^{m_k}]^T \tag{20}$$

where m_k is the number of variables in the subspace k. The contribution rate of the q^{th} variable x_k^q can be defined as

$$\text{cont}_{l,q}=\frac{t_l}{\sigma_l^2}p_{l,q}(x_k^q-\mu_q) \tag{21}$$

where t_l is the PC score rejecting to the l^{th} loading vector. μ_q, σ_l^2, $p_{l,q}$ are the corresponding mean value, eigenvalue, and the element of PC loading. So general contribution rate of the q^{th} variable is formulated as

$$\text{CONT}_q=\sum_{l=1}^{r}(\text{cont}_{l,q}) \tag{22}$$

where r is the number of the PC scores which cause the process out of control. To select the variables for final contribution plot, it is necessary to define the fault block. The monitoring statistics T^2 and SPE in each subspace have been figured out, so the process of each subspace can be monitored and the missed detection rates can be computed. Set a value λ for judging the state of sub-block. If the missed detection rate is greater than λ, this subspace is defined as a fault block. Otherwise, it is normal. Then calculate the contribution rates of the variables in fault block and combine them into the final results. In this way, the contribution rates of several fixed variables are calculated so that the root cause of the faults can be amplified and diagnosis becomes easier.

3. Some Advantages of KL-MBPCA

Compared with the traditional PCA method which only builds the single model, the proposed method constructs multi-block PCA according to the KL divergence. The variables in the same block are similar to each other and the diagnosis of the root cause is simplified. Due to the difficulty of combining the two monitoring statistics from sub-blocks, Bayesian inference is applied to transfer the statistics into fault probabilities. In fault diagnosis, the data obtained in the plant-wide process are so numerous that processing and making contribution plots seem difficult for the conventional PCA. What is worse, the chance of false identification may increase if the detection method is not appropriate. Thus, the proposed method makes a diagnosis based on the subspaces whose monitoring statistics are abnormal. This approach can narrow the number of possible responsible variables and reduce workload to find the real root causes of the faults.

APPLICATION

In this section, the simulations of proposed method in two systems are presented. At the same time, comparison studies with other methods are also provided.

1. Numerical Example

To illustrate the efficiency of the proposed method KL-MBPCA, a simple five-variable system is constructed by the following equation [25]:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 0.95 & 0.82 & 0.94 & 0 & 0 \\ 0.23 & 0 & 0.92 & 0 & 0 \\ 0.61 & 0.62 & 0.41 & 0 & 0 \\ 0 & 0 & 0 & 0.35 & 0 \\ 0 & 0 & 0 & 0.81 & 0.75 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \end{bmatrix} + \text{noise}$$

where $[r_1\ r_2\ r_3\ r_4\ r_5]^T$ follow Gaussian distribution with zero-mean and standard deviations of 1, 0.8, 0.6, 0.9 and 0.7, respectively. The noise in the equation follows zero-mean normal distribution with a standard deviation of 0.1. Under normal conditions, 500 data samples are generated as the training data, and scaled to zero mean and unit variance. To estimate the KL divergence, 200 samples from 101 to 300 are selected to calculate the probability distribution for

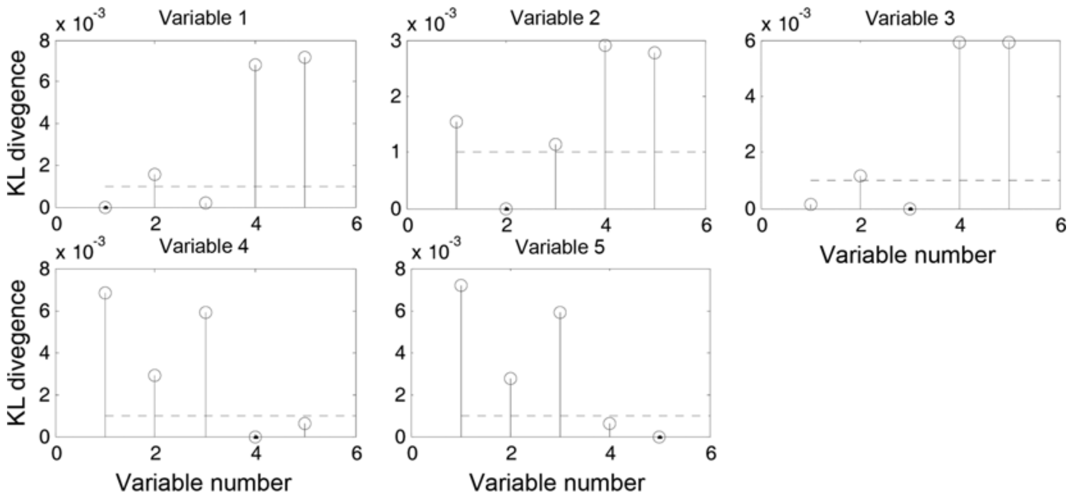

Fig. 2. The KL divergence between each two variables.

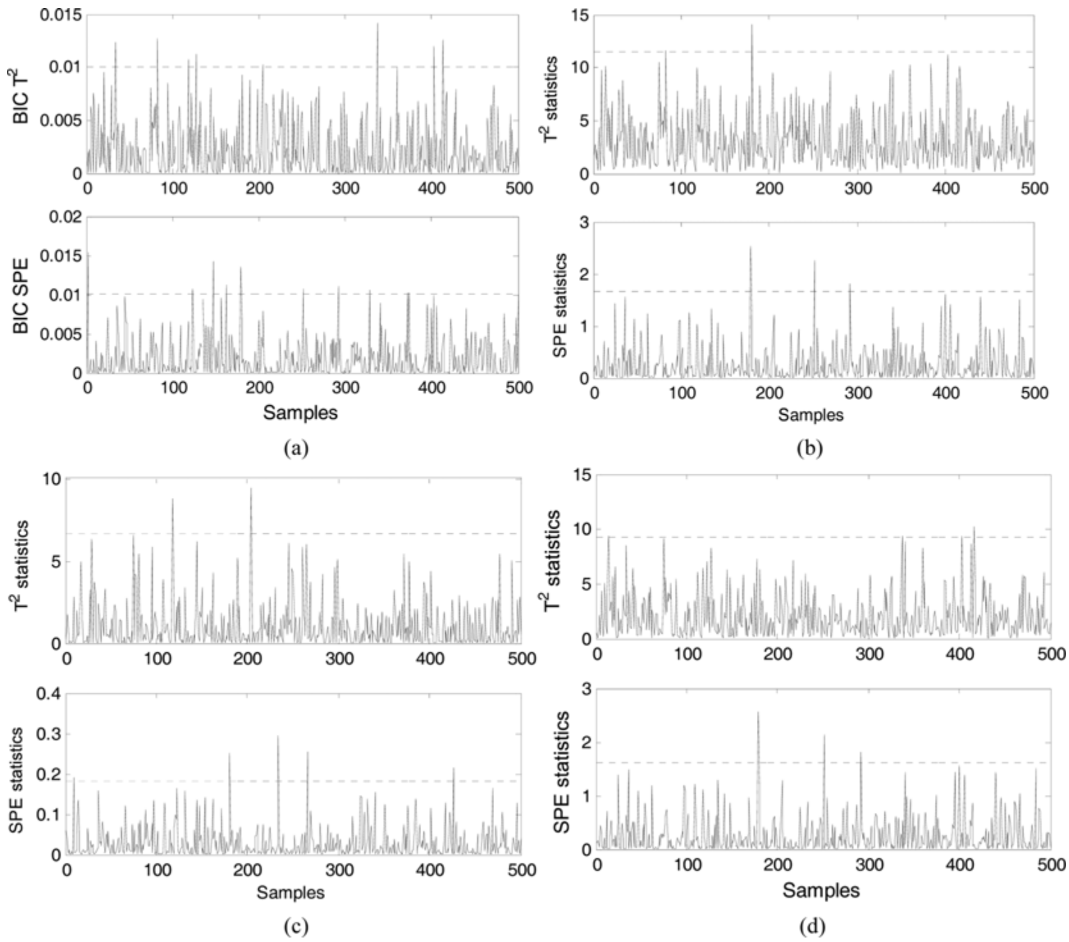

Fig. 3. Monitoring results of normal condition (a) KL-MBPCA; (b) PCA; (c) subspace 1; (d) subspace 2.

each variable. The KL values between each two variables are figured out and shown in Fig. 2. For better judgment, the threshold value α is set as 0.001. Then, the variable division can be done reasonably. From the chart, it is not difficult to find that the KL values are obviously smaller between x_1 and x_3, and between x_4 and x_5, so two sub-blocks are produced. For the rest variable x_2, place it into the block which its closest variable x_3 belongs to. Thus, two sub-blocks are developed based on KL divergence. The first sub-block contains x_1, x_2 and x_3, and the second contains x_4 and x_5.

To prove the superiority of the proposed method, the following two cases are generated with 500 samples.

Case 1: introduce a step change of x_3 by 1 from sample 151;

Case 2: add a step change of 3 to r_5 from sample 151 to the end.

First, training data under normal operation are collected for simulation. The comparison charts between the traditional method PCA and the proposed method KL-MBPCA are in Fig. 3(a) and (b). All the confidence limits of the monitoring statistics are set as 99%. As can be seen from the charts, few points exceed the confidence limits both in traditional method PCA and the proposed method KL-MBPCA, even in the two subspaces showed in Fig. 3(c) and (d). This means that the proposed method behaves well when the plant-wide monitoring process is running without any fault.

Then, the first fault case is tested by the two methods and their corresponding results are shown in Fig. 4(a) and (b) which illustrate the validity of KL-MBPCA and the infeasibility of the traditional PCA. The missed detection rate has decreased from 0.69 to 0.16. Compared with the subspace 2 presented in Fig. 4(c), the subspace 1, showed in Fig. 4(d), can detect the fault accurately because the fault case (variable x_3) and its similar variables, x_1 and x_2, belong to the same block. Similarly, the monitoring results of case 2 are displayed in Fig. 5(a) and (b), and their missed detection rates are 0.12 and 0.68, respectively, which show good performance of the proposed method as well. The results can be explained by the charts Fig. 5(c) and (d). Subspace 2 can detect the fault because there is a step change added to r_5 which is relevant with variable 5. Therefore, the sub-block can detect the fault without the disturbance of other nonsensical variables, while the traditional PCA cannot do so.

After the fault has been detected, the contribution plot should be utilized for fault diagnosis. As shown in Fig. 6, the novel contribution plots based on the proposed method are given. Keeping in touch with the introduction above, for case 1, there is a variation in subspace 1 and the monitoring result of subspace 2 indicates it is normal, so only the variables in subspace 1 are selected to make the contribution plot. As known from case 1, variable 3 indeed has changed and the other two variables are affected. This diagnosis result is in accord with the fact. The same explanation to case 2. The contribution rates of the variables in subspace 2 are picked out to reflect the result of fault diagnosis. The result is consistent with the fact

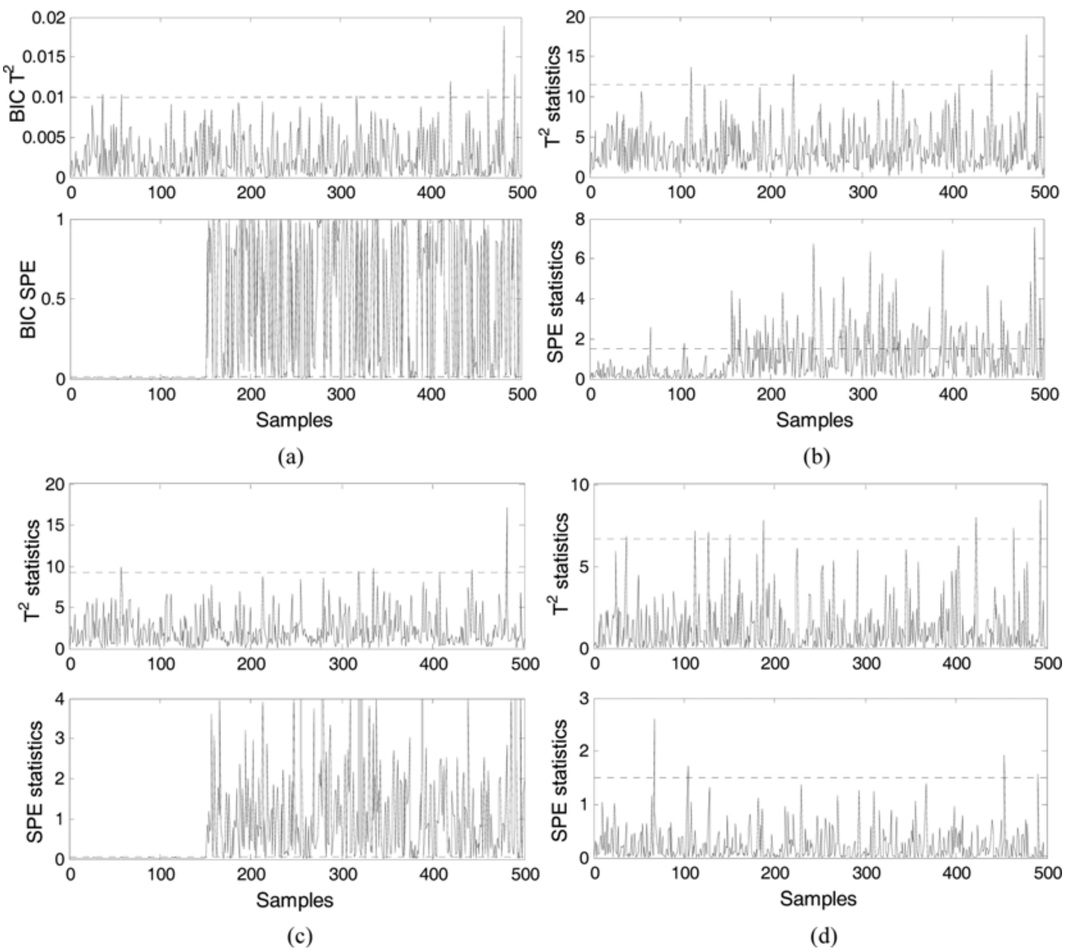

Fig. 4. Monitoring results of fault case 1 (a) KL-MBPCA; (b) PCA; (c) subspace 1; (d) subspace 2.

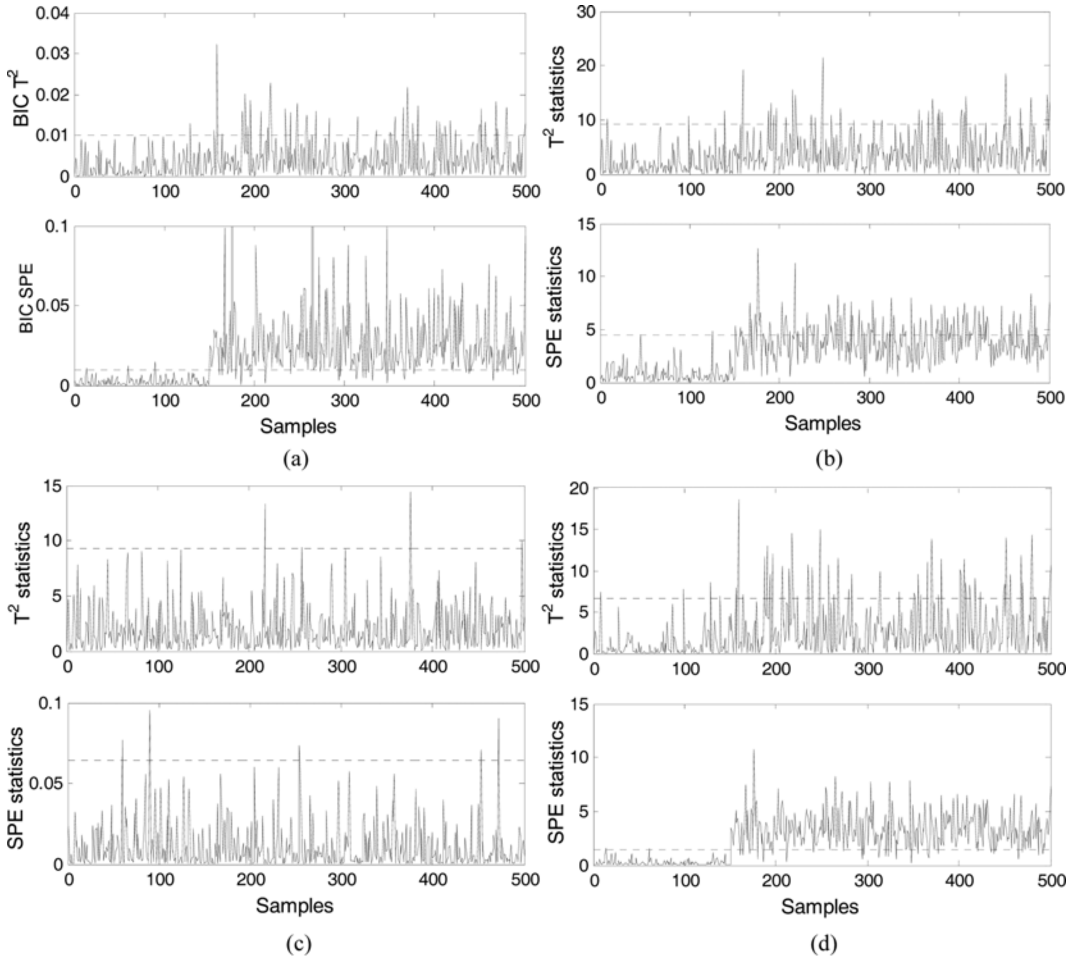

Fig. 5. Monitoring results of fault case 2 (a) KL-MBPCA; (b) PCA; (c) subspace 1; (d) subspace 2.

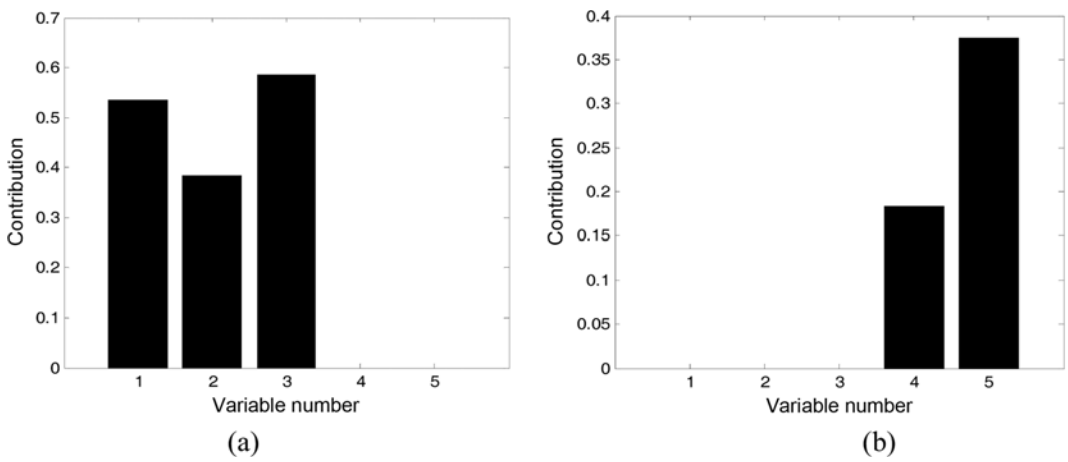

Fig. 6. Contribution plots for (a) case 1; (b) case 2.

that there is a step change added to variable 5. Although the precise diagnosis results cannot be found from the charts, the number of responsible variables for the faults has fallen. This progressive measure helps exclude some variables and finally find the root causes.

2. Application to TE Process

To simulate a realistic industrial process, the Tennessee Eastman process, shown in Fig. 7, was created by Downs and Vogel [36] and widely used to test the utility of various monitoring methods. The simulator is composed of five major unit operations: a reactor, a product condenser, a vapor-liquid separator, a recycle compressor and a product stripper. There are 41 measured variables and 12 manipulated variables in this system, but only 33 main variables, listed in Table 1, are used for monitoring, suggested by Lee et al. [15]. Since any change of the system may affect the variables, 21 different prepro-

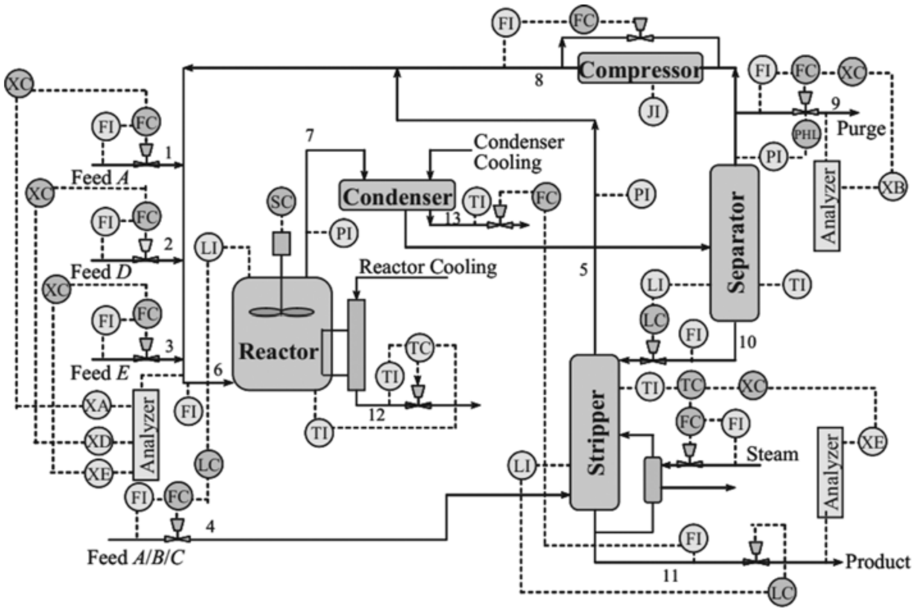

Fig. 7. Control system of the tennessee eastman process.

Table 1. Orocess faults for the 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, B, 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

grammed faults, shown in Table 1, are generated in the process by introducing faults from sample 161. Each monitored variable, shown in Table 2, contains 960 observations. At the same time, a normal dataset, composed of 500 observations, is also generated as training data. The simulation code can be downloaded from http://brahms.scs.uiuc.edu.

2-1. Monitoring Results

First, normal data from sample 101 to 250 are selected to calculate the probability distributions of the 33 variables, respectively. Then, according to the KL formula, the KL divergences between each two variables are figured out and KL divergence matrix $D_{KL} \in R^{m\times m}$(m=33) is created. The variable division can be done just as the proposed division rule. The threshold value α is set as 0.001. So 33 variables are divided into seven sub-blocks and the variables in each sub-block are given in Table 3. The training data is used to check the false alarm rates of each fault, and then the missed detection rates for all 21 faults are calculated and tabulated in Table 4. To prove the superiority of KL-MBPCA, the traditional method

Table 2. Process monitoring variables in the TE process

No.	Process measurements	No.	Process measurements
1	A feed (stream 1)	18	Stripper temperature
2	D feed (stream 2)	19	Stripper steam flow
3	E feed (stream 3)	20	Compressor work
4	Recycle flow (stream 8)	21	Reactor cooling water outlet temperature
5	Reactor feed rate (stream 6)	22	Separator cooling water outlet temperature
6	Reactor pressure	23	D feed flow valve (stream 2)
7	Reactor level	24	E feed flow valve (stream 3)
8	Reactor temperature	25	A feed flow valve (stream 1)
9	Reactor temperature	26	Total feed flow valve (stream4)
10	Purge rate (stream 9)	27	Compressor recycle valve
11	Product separator temperature	28	Purge valve (stream 9)
12	Product separator level	29	Separator pot liquid flow valve (stream10)
13	Product separator pressure	30	Stripper liquid product flow valve (stream 11)
14	Product separator underflow (stream10)	31	Stripper steam valve
15	Stripper level	32	Reactor cooling water flow
16	Stripper pressure	33	Condenser cooling water flow
17	Stripper underflow (stream 11)		

Table 3. The detailed division in the TE process

Sub-block	1	2	3	4	5	6	7
Variables	x_1, x_8, x_{25}	x_4, x_{10}, x_{21}, x_{26}	x_7, x_{13}, x_{20}, x_{27}	x_{11}, x_{22}, x_{28}	x_{17}, x_{33}	x_{18}, x_{19}, x_{31}	x_2, x_3, x_5, x_6, x_9, x_{12}, x_{14}, x_{15}, x_{16}, x_{23}, x_{24}, x_{29}, x_{30}, x_{32}

Table 4. Missed detection rates of each method in TE

Fault number	PCA T^2	PCA SPE	DPCA T^2	DPCA SPE	CVA T_s^2	CVA SPE	BSPCA BIC_T^2	BSPCA BIC_SPE	KL-MBPCA BIC_T^2	KL-MBPCA BIC_SPE
1	0.008	0.003	0.006	0.005	0.001	0.003	0.008	0.001	0.003	0.007
2	0.020	0.014	0.019	0.015	0.011	0.026	0.015	0.015	0.014	0.029
3	0.998	0.991	0.991	0.990	0.981	0.985	0.988	0.905	0.964	0.917
4	0.956	0	0.939	0	0.688	0.975	0.849	0	0.669	0.003
5	0.775	0.746	0.758	0.748	0	0	0.769	0.728	0.718	0.003
6	0.011	0	0.013	0	0	0	0	0	0.006	0
7	0.085	0	0.159	0	0.386	0.486	0	0	0	0.001
8	0.034	0.024	0.028	0.025	0.021	0.486	0.029	0.026	0.023	0.029
9	0.994	0.981	0.995	0.994	0.986	0.993	0.980	0.916	0.995	0.930
10	0.666	0.659	0.580	0.665	0.166	0.599	0.659	0.433	0.564	0.203
11	0.794	0.356	0.801	0.193	0.515	0.669	0.570	0.470	0.509	0.386
12	0.029	0.025	0.010	0.024	0	0.021	0.011	0.026	0.014	0.001
13	0.060	0.045	0.049	0.249	0.047	0.055	0.058	0.046	0.053	0.050
14	0.158	0	0.061	0	0	0.122	0	0	0	0.009
15	0.988	0.973	0.964	0.976	0.928	0.979	0.970	0.901	0.915	0.891
16	0.834	0.755	0.783	0.708	0.166	0.429	0.750	0.674	0.758	0.164
17	0.259	0.108	0.240	0.053	0.104	0.138	0.110	0.031	0.100	0.086
18	0.113	0.101	0.111	0.100	0.094	0.102	0.106	0.088	0.101	0.088
19	0.996	0.873	0.993	0.735	0.849	0.923	0.850	0.880	0.895	0.293
20	0.701	0.550	0.644	0.490	0.248	0.354	0.728	0.509	0.493	0.159
21	0.736	0.570	0.644	0.558	0.440	0.547	0.611	0.409	0.555	0.396

PCA, DPCA, CVA [1] and the study of Ge et al. [25] (BSPCA) are listed for further comparison.

The current work about the 21 faults is as follows: Faults 3, 9 and 15 are small process faults which are hard to be detected by all methods, so they are ignored in this discussion. For faults 1, 2, 4, 6, 7, 8, 12, 13, 14, 17 and 18, most methods can detect them easily with nearly zero missed detect rates. Among the rest of the faults, it is difficult for PCA and BSPCA to detect faults for faults 5, 10, 16, 19 and 20, but the proposed method KL-MBPCA shows a good performance and cuts the missed detection rates nearly in half. KL-MBPCA has high efficiency because it is a probability and statistics based method which can deal with linear or nonlinear problem without losing any information. In each sub-block, the corresponding statistics and control limits are calculated as well. As long as

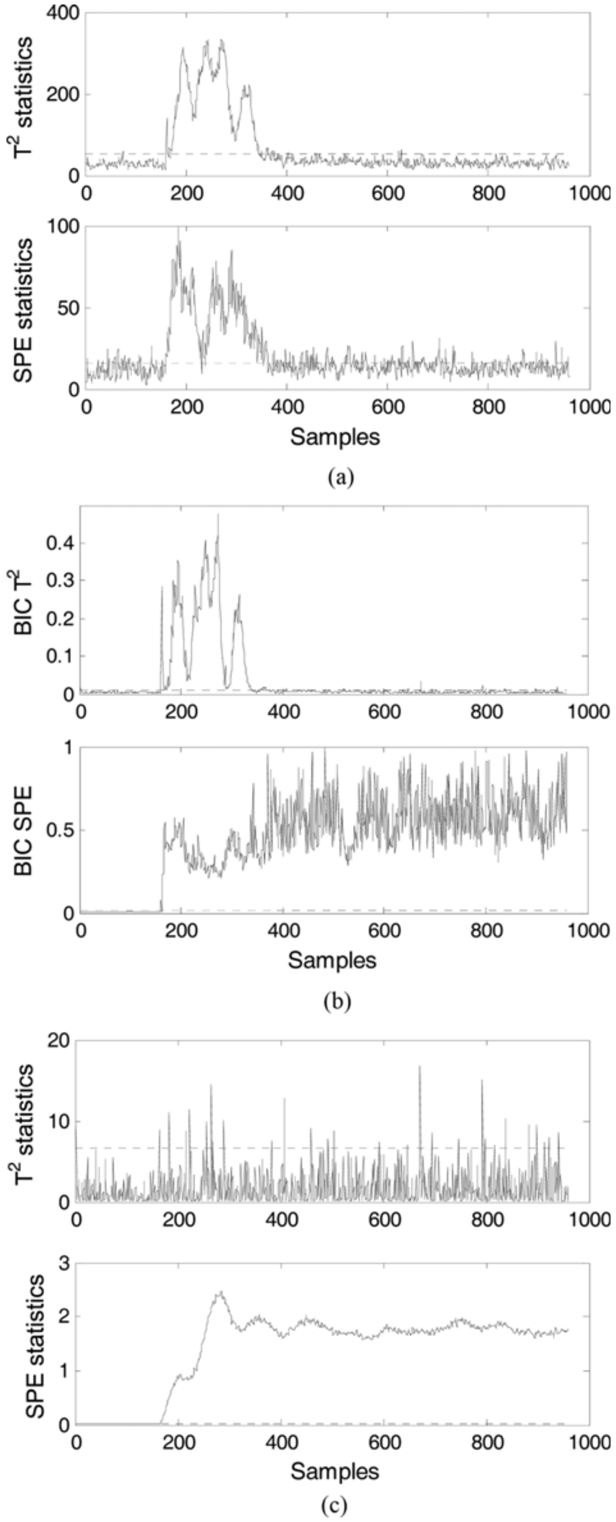

Fig. 8. Monitoring performance for fault 5 (a) PCA; (b) KL-MBPCA; (c) subspace 5.

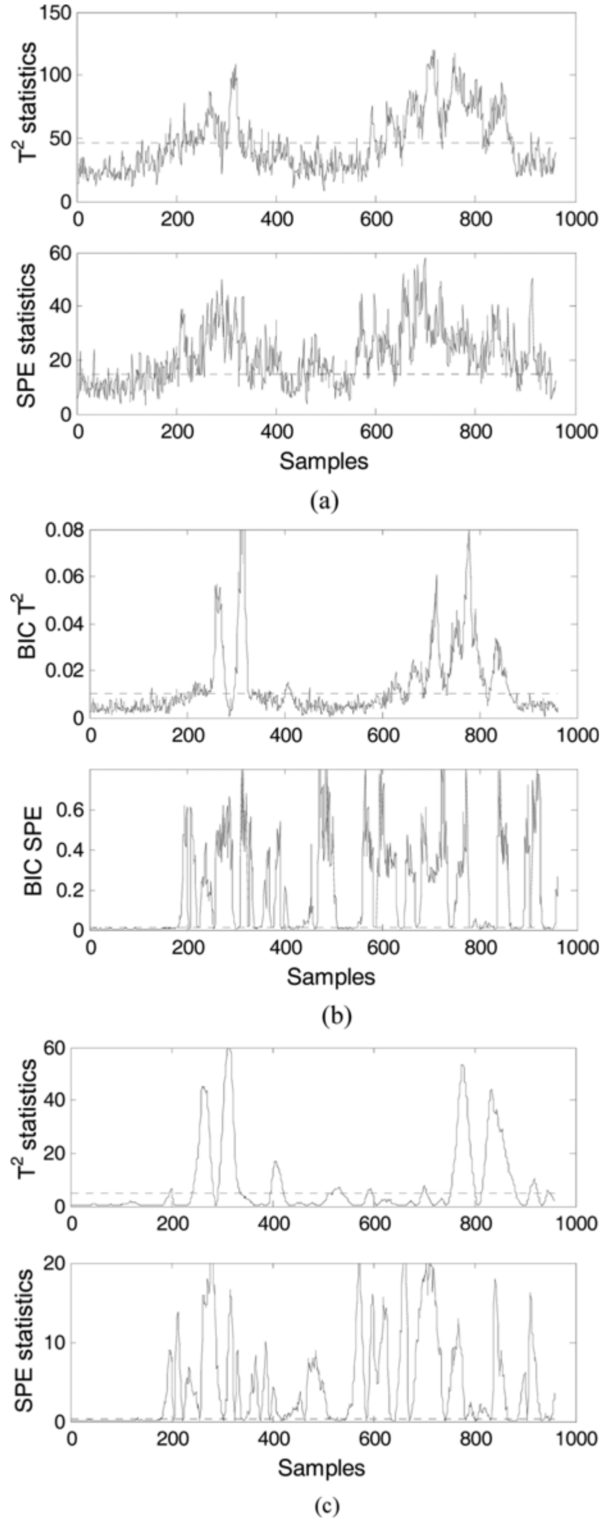

Fig. 9. Monitoring performance for fault 10 (a) PCA; (b) KL-MBPCA; (c) subspace 6.

any statistic in one sub-block exceeds the control limit, the fault is considered to have occurred. For further analysis, detailed detection results of faults 5, 10, 16 and 19 are displayed to verify the superiority of the proposed method compared with original PCA. For fair comparison, 97.5% control limits are set in each simulation.

In the case of fault 5, a step change in the condenser cooling water inlet temperature leads to the step change of its flow rate. Since the control system can compensate this fault it cannot be detected obviously by PCA, which can be seen from Fig. 8(a). However, as shown in Fig. 8(b), KL-MBPCA presents a different monitoring result with monitoring statistics going far away from control limit as soon as the fault occurs. The statistics in subspace 5, shown in Fig. 8(c),

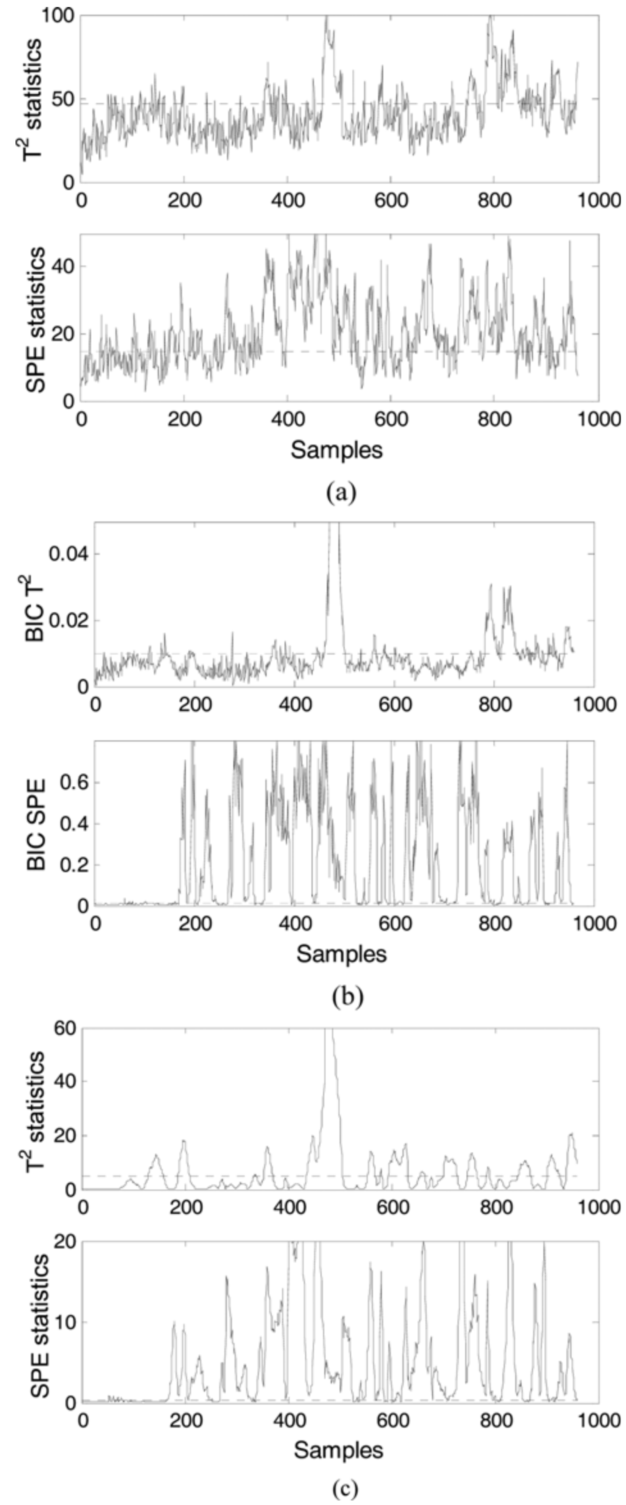

Fig. 10. Monitoring performance for fault 16 (a) PCA; (b) KL-MBPCA; (c) subspace 6.

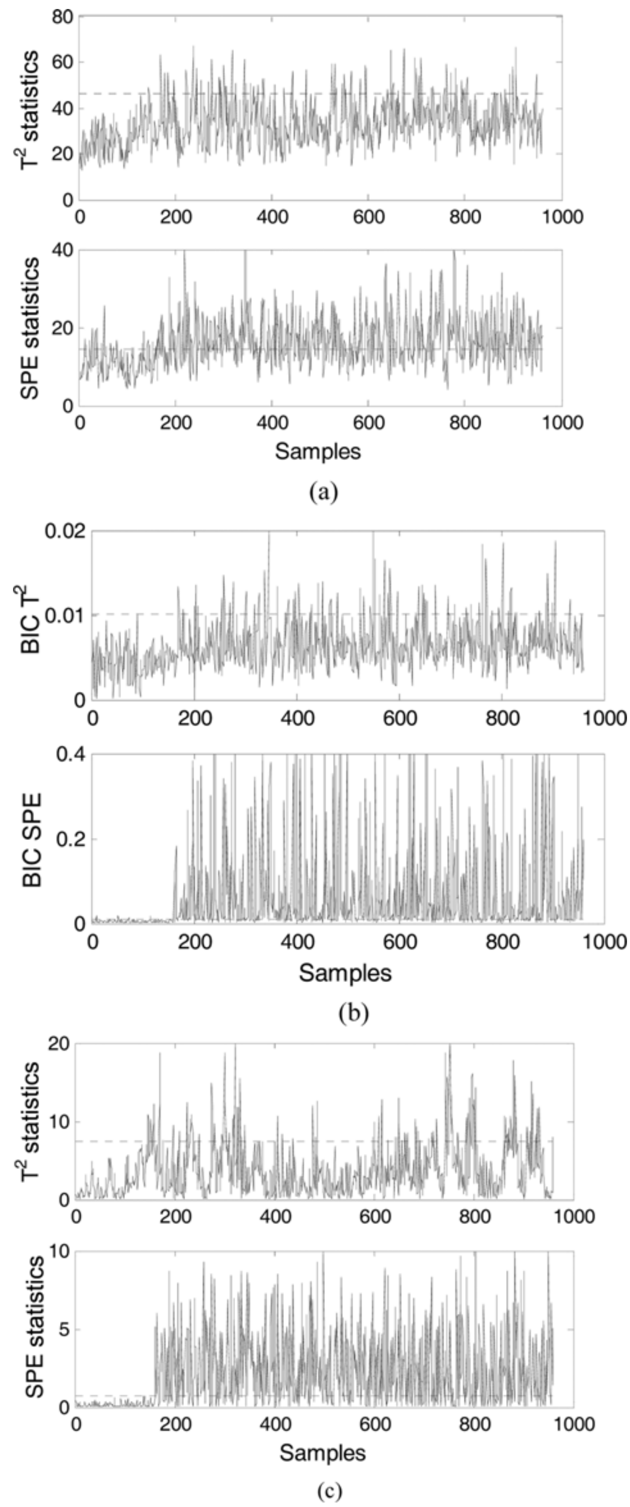

Fig. 11. Monitoring performance for fault 19 (a) PCA; (b) KL-MBPCA; (c) subspace 3.

reflect the variation correctly and timely, but the rest of the subspaces can hardly detect the fault.

Fault 10 is a random change in C feed temperature, which results in a variation in stripper pressure. The comparison charts of PCA and the proposed method are present in Fig. 9(a) and (b), respectively. The BIC_{SPE} of KL-MBPCA performs well with most statistics above the control limit after sample 161. The fluctuation of the statistics produced by the proposed method makes the fault easy to find, but, oppositely, the statistics in PCA stay around the control limit, which is not good for detection. The key subspace for fault detection is also given in Fig. 9(c).

Faults 16 and 19 are two unknown faults in the TE process which are not easy to detect by traditional PCA, shown in Fig. 10(a) and Fig. 11(a), respectively. However, the monitoring results in KL-MBPCA improved visibly, presented in Fig. 10(b) and Fig. 11(b). Their corresponding significant subspaces capture the deviations properly and more details are in Fig. 10(c) and Fig. 11(c).

2-2. Fault Diagnosis

Once the fault is detected, it is necessary to identify the variables which are highly correlated with the fault. According to the principle of proposed contribution plot method, the abnormal sub-blocks should be selected to make contribution plots for fault identification. As mentioned above, the assumed faults are all introduced from sample 161 to 960, so there are 800 samples after the fault occurs. In some sub-block, if the number of the T^2 or SPE statistics, which stays above the corresponding confidence limits, is greater than 500 (equal to $\lambda \geq 500/800$), this block is termed as the fault block (see Table 5). Meanwhile, the total number of the possible responsible variables for each fault can be computed by adding up the variable numbers of each fault block (listed in Table 5). For fair comparison,

Table 5. Results of the fault identification for all assumed faults

Fault no.	Traditional method	Improved method		
	Possible responsible variables	Possible responsible variables	Fault block	Number of variables
1	x_1, x_{25}, x_4	x_1, x_{25}, x_4	Block1,2,6	10
2	x_{10}, x_{28}, x_{19}	x_{10}, x_{28}, x_{19}	Block2-7	30
4	x_{32}, x_5, x_{22}	x_{32}, x_5, x_6	Block7	14
5	x_{33}, x_{20}, x_{31}	x_{33}, x_{17}	Block5	2
6	x_{32}, x_{16}, x_7	x_{32}, x_{16}, x_7	Block1-7	33
7	x_{26}, x_{20}, x_{19}	x_{26}, x_4, x_{21}	Block2	14
8	x_{16}, x_7, x_{13}	x_{16}, x_7, x_{13}	Block1-7	33
10	x_{18}, x_{31}, x_{19}	x_{18}, x_{31}, x_{19}	Block6	3
11	x_{32}, x_3, x_8	x_{32}, x_2, x_3	Block7	14
12	x_{22}, x_{11}, x_{19}	x_{22}, x_{11}, x_{19}	Block1-7	33
13	x_{19}, x_{31}, x_{18}	x_{19}, x_{31}, x_{18}	Block1-7	33
14	x_9, x_{32}, x_{21}	x_9, x_{32}, x_{21}	Block2,7	18
16	x_3, x_{31}, x_{20}	x_{31}, x_{19}, x_{18}	Block6	3
17	x_{21}, x_{32}, x_9	x_{21}, x_{32}, x_9	Block2,7	18
18	x_{13}, x_8, x_{16}	x_{13}, x_8, x_{16}	Block1-7	33
19	x_5, x_8, x_6	x_{27}, x_7, x_{13}	Block3	4
20	x_{27}, x_{20}, x_{13}	x_{27}, x_{20}, x_{13}	Block3,5	6
21	x_{23}, x_{19}, x_{22}	x_{19}, x_{31}, x_{18}	Block6	3

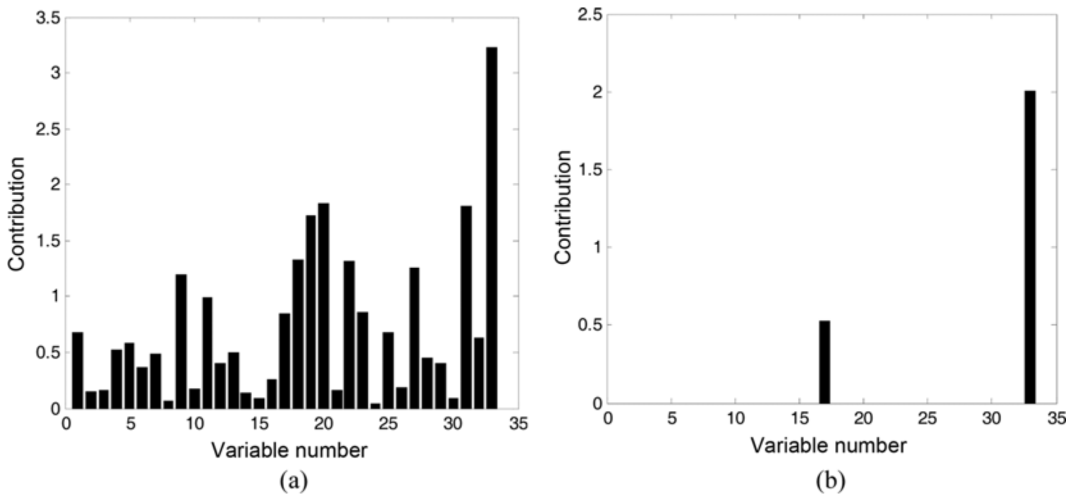

Fig. 12. Contribution plots for fault 5 (a) PCA; (b) KL-MBPCA.

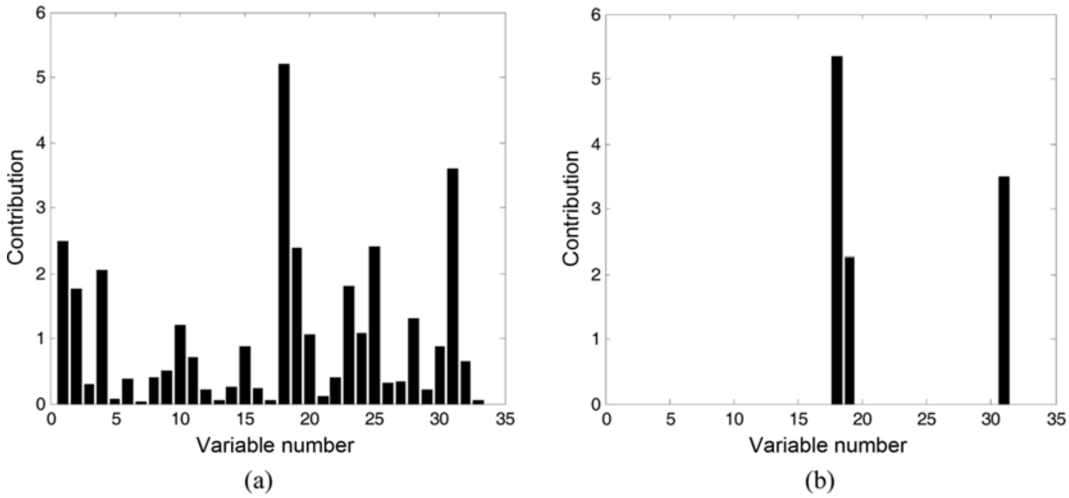

Fig. 13. Contribution plots for fault 10 (a) PCA; (b) KL-MBPCA.

the traditional [28,29] contribution plot method is also employed for fault diagnosis. The three main possible responsible variables of each fault measured by two methods are also displayed and arranged in descending order, which means that the variable having the biggest contribution rate is always first displayed and the smallest is the last. From the table, the main fault variables of the two methods are almost the same, but the number of the fault variables for diagnosis in present method is fewer than that in traditional contribution plot method. This result indicates the superiority of the proposed method for fault identification.

In particular, the contribution plots of PCA and the proposed method KL-MBPCA for fault 5 are shown in Fig. 12(a) and (b). By observing the fault behavior in the TE process, the step change in the condenser cooling water inlet temperature leads to a step change in flow rate. When a fault occurs, the flow rate from the outlet of the condenser to the vapor/liquid separator also changes, which results in the change of stripper underflow. So it is reasonable to identify the stripper underflow (variable 17) and condenser cooling water flow (variable 33) as the root causes for this fault, just like what Fig. 12(b) provides for us. The monitoring result of subspace 5, which is composed of variables 17 and 33, demonstrates good monitoring of fault 5, seen from Fig. 8(c).

Fault 10 is a random change of C feed temperature (stream 4). The contribution plot of PCA, shown in Fig. 13(a), indicates that many variables make contributions, especially variables 18 and 31. However, the contribution plot of KL-MBPCA, shown in Fig. 13(b), only displays three variables that make most contributions. Correlating the knowledge of the TE process, the tripper temperature (variable 18), stripper steam flow (variable 19) and stripper steam valve (variable 31) are in close association with C feed temperature (stream 4). Compared with traditional PCA contribution plots, the contribution plots of the multi-block method provide a positive and efficient diagnosis.

CONCLUSIONS

We have proposed a totally data-driven multi-block PCA method for plant-wide process monitoring. The KL divergence is employed to produce sub-blocks automatically, which would consider both linear and nonlinear relations without prior process knowledge. The PCA is performed in each subspace and Bayesian inference is also used to combine the results. The division of the variables not only reduces the dimensionality of the measured data, but also helps identify the root cause of the fault. Both the application to the cases and the comparison with other methods show the superiority of the proposed method.

This study does not merely aim at this single method; it also can combine probability statistics with many other MSPC methods, which is more suitable for handling numerous data generated from a plant-wide monitoring process. Further researches could be focused on nonlinear, non-Gaussian, batch plant-wide process monitoring with totally data-driven multi-block methods.

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