Nonlinear Process Monitoring Based on Improved KPCA and Extended MVU

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Abstract—**Kernel principal component analysis (KPCA) has been recently proven to be a powerful dimensionality reduction tool for monitoring nonlinear processes. However, the KPCA based monitoring method suffers from several drawbacks. First, the KPCA method depends strongly on its kernel function, but its selection of kernel parameters is problematic. Second, the underlying manifold structure of the data is not considered in process modelling. To overcome these deficiencies, this paper proposes a new process monitoring technique named extended maximum variance unfolding (EMVU). Because the global and local structures of process data probably change in some abnormal states, global and local graphs are designed to exploit the underlying geometrical structure. The feasibility and validity of the EMVU based process monitoring scheme are investigated through a simple numerical example simulation process. The experimental results demonstrate that the EMVU based nonlinear process monitoring method is a good alternative method to the KPCA-based monitoring method.**

Keywords—process monitoring; nonlinear; improved kernel principal component analysis; extended maximum variance unfolding; example simulation

I. Introduction

In manufacturing industry, the demands for operation safety have spurred the development of process monitoring methods over the past several decades [1-2]. There are many multivariate statistical approaches, including principal component analysis (PCA), partial least-squares (PLS), and independent component analysis (ICA) [3-7]. These methods have been widely applied in the chemical industry for process monitoring [8]. Many industrial processes are essentially nonlinear, but these methods have a strong linearity assumption; thus, a linear method is inappropriate for extracting nonlinearities when linear monitoring approaches are applied to the nonlinear processes. In recent decades, the kernel method has found use in the chemical industry [9]. Additionally, the nonlinear PCA algorithm was developed by combining principal curves and neural networks [10]. Unfortunately, this algorithm suffers from computational complexity. In another approach, KPCA and kernel partial least-squares (KPLS) address the problem of nonlinear data analysis. Compared to nonlinear PCA, KPCA can handle a wide range of nonlinearities and provides a much simpler computational framework. KPCA has the advantage that the dimension of its reduced space does not need to be specified before training. However, KPCA has two major drawbacks. The first is that the KPCA monitoring method depends strongly on its kernel function, including popular approaches such as Gaussians and Polynomials kernel functions. The underlying manifold structure of the data is not considered explicitly. The second drawback was discussed by [11]. If the parameters of the kernel function are not properly determined, it is difficult to specify an appropriate reduced dimension. When a prompt response is crucial due to dense expansions in terms of the kernel functions, KPCA incurs a high computational cost in the on-line monitoring phase. But Kernel independent component analysis (KICA) can combine the advantages of KPCA and ICA, but it is also difficult to use in nonlinear fault diagnosis [12-13].

The manifold learning method of maximum variance unfolding (MVU) [14], as a special variation of KPCA, has been proposed. The kernel matrix of MVU is automatically learned from the training data and can avoid the deficiencies of KPCA. Compared to the local techniques, MVU is a global technique. However, the direct application of MVU is not as straightforward as it seems. It can provide only a lower dimensional training samples of the kernel matrix, while process monitoring requires a functional mapping of the kernel function. More importantly, the boundary of the distribution region of the training samples is faithfully preserved. As a result, the direct application of MVU to process monitoring is inappropriate. In [11], Hu et al. tried to use a multivariate linear regression model to model the mapping between the input space and the MVU output space. However, this method is questionable since the high-dimensional and low-dimensional outputs are both nonlinear.

In this paper, a new process monitoring technique called EMVU is proposed to model and monitor the nonlinear process data. It can inherit the advantages from both manifold learning and Gaussian process, thereby overcoming the limitations of KPCA. First, a lower dimensional output space is constructed, and the MVU method is applied to the collected training data. Then, Gaussian process is applied for nonlinear mapping, in contrast to conventional MVU method, and the new samples are obtained. Thus, EMVU can be viewed as an online process monitoring method. Using a cross-validation algorithm, T_2 and squared prediction error (SPE) are calculated.

The remainder of this paper is organized as follows:

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Section 2 reviews and analyses the KPCA method. Section 3 presents the algorithm analysis for EMVU, including manifold learning and manifold learning using Gaussian process. EMVU based on process monitoring is presented in Section 4, including offline modelling and online fault detection. The experiments performed using this method are described in Section 5, and finally, this study is summarized in Section 6.

II. Kernel principal component analysis-based process monitoring

A. Improved KPCA method principle

KPCA was originally proposed in [15]. KPCA is an extension of PCA, and it can always be solved as an eigenvalues problem of its kernel matrix. KPCA is an effective technique for dimensionality reduction when the data lie on a non-linear manifold. Unlike other methods, KPCA doesn't need to solve nonlinear optimization problem, it can decrease data noise and eliminate the multiple correlation among the variables. Let the mean-centred training samples $X=[x_1,x_2,\mathrm{L}\ ,x_n]\in\Re^{m\times n}$ denote the original training data set. Then we map these data sets to $\phi(x_1),\phi(x_2),\mathrm{L}\ ,\phi(x_n)\in\Im$, where $x_i\in\Re^m$, m is the number of process variables, and n is the number of observations. That is, $\Re^m\phi(\bullet)\Im^f$, where $\phi(\bullet)$ is an implicit nonlinear mapping function, $\Im$ denotes feature space and *f* is the dimension of the feature space. The covariance matrix in $\Im$ is denoted as follows:

$$\sum\Im=\frac{1}{n}\sum_{i=1}^{n}[\phi(x_i)-\mathrm{c}][\phi(x_i)-\mathrm{c}]^T \tag{1}$$

Here, $\bar{\phi}(x_i)=\phi(x_i)-\mathrm{c}$ describes the centred feature space sample，c denotes the sample mean in the feature space. The eigenvalue problem is solved to obtain the kernel principal component.

$$\begin{aligned}\lambda v=\sum_F v&=\frac{1}{n}\sum_{i=1}^{n}[\bar{\phi}(x_i)^T v]\bar{\phi}(x_i)\\&=\frac{1}{n}\sum_{i=1}^{n}\left\langle\bar{\phi}(x_i),v\right\rangle\bar{\phi}(x_i)\end{aligned} \tag{2}$$

where λ is the eigenvalue and v is the eigenvector of the covariance matrix and $\sum_F\phi(\bullet)$ denotes the inner product. Then, there exist coefficients α_i that satisfy the following equality:

$$v=\sum_{j=1}^{n}\alpha_j\bar{\phi}(x_j) \tag{3}$$

Substituting eq. (3) into eq. (2),

$$\begin{aligned}\lambda\sum_{j=1}^{n}\alpha_j\bar{\phi}(x_j)&=\frac{1}{n}\sum_{i=1}^{n}[\bar{\phi}(x_i)^T]\sum_{j=1}^{n}\alpha_j\bar{\phi}(x_j)\bar{\phi}(x_i)\\\cdots\cdots\cdots\cdots\cdots&=\sum_{i=1}^{n}\left\langle\bar{\phi}(x_i),\sum_{j=1}^{n}\alpha_j\bar{\phi}(x_j)\right\rangle\bar{\phi}(x_i)\end{aligned} \tag{4}$$

Multiplying both sides of eq. (4) by $\bar{\phi}(x_j)^T$ gives

$$\begin{aligned}&\lambda\sum_{j=1}^{n}\alpha_j\left\langle\bar{\phi}(x_k),\bar{\phi}(x_j)\right\rangle\\&=\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_j\left\langle\bar{\phi}(x_i),\bar{\phi}(x_j)\right\rangle\left\langle\bar{\phi}(x_k),\bar{\phi}(x_i)\right\rangle\end{aligned} \tag{5}$$

Define $\bar{K}_{ij}$ as a centred $n\times n$ kernel matrix and $\bar{K}_{ij}=\left\langle\bar{\phi}(x_k),\bar{\phi}(x_j)\right\rangle$, then the eigenvalue problem in eq. (4), which involves only inner products in the feature space, can be transformed into

$$\lambda\alpha=\frac{1}{n}\bar{K}\alpha \tag{6}$$

where $\|\alpha\|=\frac{1}{n\lambda}$. Project $\bar{\phi}(x)$ onto v_k in F can lead to observation x:

$$t_k=\left\langle v_k,\bar{\phi}(x)\right\rangle=\sum_{i=1}^{n}\alpha_i^k\left\langle\bar{\phi}(x_i),\bar{\phi}(x)\right\rangle \tag{7}$$

where k=1, 2, ..., p and p denotes the number of the kernel principal components. We then solve the eigenvalue problem of eq. (5) and project from the input space into the KPCA space using eq. (6). A kernel function of the form $k(x,y)=\left\langle\phi(x),\phi(y)\right\rangle$ is introduced to avoid performing the nonlinear mappings and compute the inner products in the feature space. The Gaussian kernel function $k(x,y)=e^{\frac{-\|x-y\|^2}{c}}$ is also introduced, where c is the width parameter. Empirically, $c=rm\delta^2$, where r is a constant, m is the input space dimension, and δ^2 is the variance of data. In KPCA process monitoring, T^2 and SPE are two commonly used statistics that can reflect the space change[16] in the two subspaces. T^2 can be obtained as follows:

$$T^2=t^T\Lambda^{-1}t \tag{8}$$

where *t* is the p-dimensional score vector obtained by eq. (7), and Λ^{-1} is the diagonal matrix. Use the F-distribution[17] to estimate the upper control limit of T^2.

$$T^2_{p,n,\alpha}:\ \frac{p(n-1)}{n-p}F_{p,n-p,\alpha} \tag{9}$$

The SPE can be obtained as follows:

$$SPE=\left\|\bar{\phi}(x)-\bar{\phi}_p(x)\right\|^2=\sum_{i=1}^{n_0}t_i^2-\sum_{i=1}^{p}t_i^2 \tag{10}$$

where n_0 denotes the number of nonzero eigenvalues. The upper control limit of SPE can be estimated as:

$$SPE_\alpha=g\chi_h^2 \tag{11}$$

where $g=\frac{b}{2a}$, and $h=\frac{2a^2}{b}$. Here, g is a weighting parameter, a is the estimated mean, b is the variance of SPE, and h is the number of degrees of freedom.

In many practical nonlinear monitoring processes, a single KPCA model is usually not the most effective approach for all conditions. Different conditions may need different width

parameters to maximize their respective performance. The single Gaussian kernel function cannot satisfy all conditions. To overcome the shortcomings of a single Gaussian kernel function, we use a series of Gaussian kernel functions that have different width parameters:

$$k^{(i)}(x,y) = e^{\frac{-\|x-y\|^2}{c_i}} \tag{12}$$

where $c_i = 2^{i-1} rm\delta$ and i=1, 2,…, n_s. Then

$$\lambda^{(i)}\alpha^{(i)} = \frac{1}{n}k^{(i)}\alpha^{(i)} \tag{13}$$

Therefore, $T^{2(i)}$ (i=1, 2,…, n_s) and $SPE^{2(i)}$ (i=1, 2,…, n_s) can be constructed for each KPCA submodel. We can also estimate their upper control limit T^i_{limit} (i=1, 2,…, n_s) and SPE^i_{limit} (i=1, 2,…, n_s).

B. Determine KPCA method principal component numbers

In the process of nonlinear monitoring feature extraction, a reasonable determination of the principal component number is very important. An estimation of the number of the principal components[18] with large uncertainty is not appropriate. When the principal component number is greater, the model will be accurate. However, the analysis and diagnosis of this model is more complicated. If the principal component number is too small, then it is not too sufficient to extract the feature information of the nonlinear monitoring data. Additionally, the error rate of the analysis and diagnosis will be increased. Therefore, we must determine the KPCA method principal component numbers in the nonlinear monitoring feature extraction[19].

The number of components can be evaluated by two methods. One is the average method: the mean of the characteristic root $\bar{\lambda}$ is calculated first, based on the characteristic roots, principal component numbers that are greater than $\bar{\lambda}$ are chosen. The other is the empirical method. It can determine the principal component numbers by the cumulative contribution rate.

In actual nonlinear monitoring feature extraction, we usually use the empirical method, determining the principal component numbers according to the cumulative contribution rate. In the simulation experiment, when the number of principal component is twenty-five, we can get a cumulative contribution rate of 85%.

III. Extended Maximum Variance Unfolding

A. Maximum variance unfolding and constraints

MVU is a special variation of KPCA also known as semi-definite embedding. It is often used for nonlinear data dimensionality reduction. When we use MVU, its kernel matrix is often semidefinite programming to avoid suffering from local optima. The details of the constraints are as follows: first, the kernel matrix should be positive semidefinite. This can guarantee that the elements can be interpreted as dot products of the training samples. Second, the kernel matrix should store the dot products of mapped training samples to ensure that the eigenvalues of the kernel matrix as measures of variance can be interpreted along the principal components. This means that

$$\begin{aligned}&\sum_{i=1}^{N}\phi(X_i) = 0 \Leftrightarrow \left\|\sum_{i=1}^{N}\phi(X_i)\right\|^2 \\ &= = \sum_{i=1}^{N}\sum_{j=1}^{N}\left\langle\phi(X_i),\phi(X_j)\right\rangle = \sum_{i=1}^{N}\sum_{j=1}^{N}K_{ij} = 0\end{aligned} \tag{14}$$

The last constraint is as follows: suppose that training sample x_i is a steel ball. A discrete approximation of the underlying manifold structure is used to form the lattice of steel balls, and the distances and angles between the points and their neighbourhoods should be isometric. Then, we define the binary adjacency matrix $v, v_{ij} = 1$ to indicate the neighbourhood relation, i.e., x_j is the k-nearest neighbour of x_i. Then, the following equation should hold:

$$\begin{aligned}&\left\|\phi(x_i)-\phi(x_j)\right\|^2 = \left\|x_i - x_j\right\|^2 \\ &\Leftrightarrow K_{ii} + K_{jj} - 2K_{ij} = \left\|x_i - x_j\right\|^2\end{aligned} \tag{15}$$

In many nonlinear monitoring processes, the sampled dataset often has complicated distributions, so preserving the local structure is very important. To tackle this problem, the neighbourhood structure of the data is embedded in both local and global information. A specific description is as follows.

B. Local graph minimum

For a local graph minimum, we first calculate the adjacency matrix W. The locality preserving criterion is given as follows[20]:

$$\begin{aligned}&J(p) = \min\sum_{i,j=1}^{n} p^T(x_i - x_j)w_{ij}(x_i - x_j)^T p \\ &= \min p^T x^T(D-W)Xp = \min p^T x^T LXp^T \\ &= \min p^T L^{/} p^T\end{aligned} \tag{16}$$

where L is a Laplacian matrix, $L = D - W$. $L^{/}$ is a local graph matrix, $L^{/} = X^T LX$. D is a diagonal matrix, for which the diagonal elements are the column (or row) sum of W, $D_{ii} = \sum_j w_{ij}$.

C. Global graph maximum

For a global graph minimum, we first obtain an optimal outer shape manifold structure through embedding the neighbourhood information. Consider the local mean centre of each sample x_i, that is more respective than the original mean centre $\bar{x}$. Here, D can reveal the nearby density of the corresponding points. We can obtain the local mean vector[21] x_i by following eq. (15).

$$\bar{x}_i = \frac{1}{n_i}\sum\nolimits_{xj\in N(x_i,j)} X_j \tag{17}$$

where n_i is the number of elements, i=1, 2,..., n, $N(x_i, x_j)$ contains n_i. Therefore, we can obtain the local mean vectors $\bar{X}_i = [\bar{X}_1, \bar{X}_2, \mathrm{L}\ , \bar{X}_n]$. By maximizing the following cost function, we can obtain the projection p:

$$J(p) = \min \sum_{i=1}^{n} p^T (x_i - \bar{x}_i)(x_i - \bar{x}_i)^T p$$
$$= \min p^T (X_i - \bar{X}_i)^T (X_i - \bar{X}_i) p = \min p^T G p \quad (18)$$

where $G = (X_i - \bar{X}_i)^T (X_i - \bar{X}_i)$ is the global graph matrix.

D. Offline modelling strategy and online process monitoring based on EMVU

When applying the EMVU method to process monitoring, the overall procedures of the EMVU-based process monitoring are outlined as follows. Offline modelling: (1) Acquire the historical normal operating data and normalize the data to zero mean and unit variance. (2) Divide the normalized data (i = 1, 2,..., n) into two sets: the training set and the validation set. (3) Using the data, train the EMVU model in the training set. (4) Calculate the monitoring T_2 and SPE statistics of the normal, and record the predictive variances of the calculated EMVU outputs. (5) Determine the control limits for the monitoring indices of the T_2 and SPE. Online monitoring: (1) Record the online measurements, and normalize the new sample data x with the mean and standard deviation calculated in the modelling steps. (2) Obtain the outputs in the reduced space of EMVU. (3) Calculate the monitoring indices T_2 and SPE for the EMVU outputs. (4) Calculate T_2 and SPE, and check to see whether they exceed the corresponding control limits. (5) If the indices are well below the control limits, the process is regarded as normal, and the procedure returns to step (1); otherwise, a potential fault process should be considered. The corresponding steps of the EMVU method for process monitoring are shown in Figure 1.

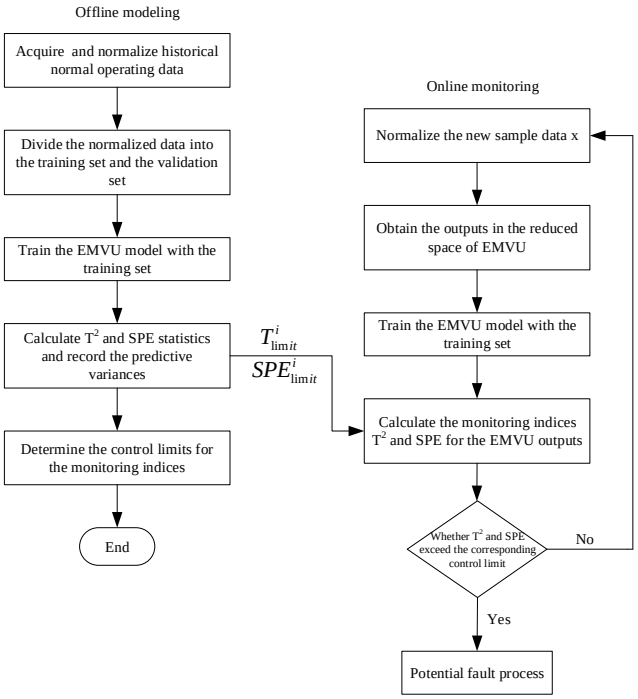

Fig. 1. Flowchart of EMVU method for process monitoring

IV. Case Studies

In this section, we apply the EMVU method described in this paper to fault detection in a simple numerical example to verify the effectiveness. Here, we compare the results obtained using PCA, KPCA and EMVU. This process is shown as follows:

$$y_1 = 10a^3 + 1.5a^2 - 1.5a + 0.1 + c_1 \quad (19)$$

$$y_2 = 30b + c_2 \quad (20)$$

$$y_3 = a + c_3 \quad (21)$$

where $a = b^2 - 1$, and $b \in (0,1)$. c_1, c_2 and c_3 are random noise variables with small magnitudes. Using the above equations, we can obtain 500 normal sample data. 100 faulty samples are generated using the below equations:

$$y_1 = 0.5a^2 - 2a + 0.5 + c_1 \quad (22)$$

$$y_2 = a^2 + a + \sin(\pi \times a) + c_2 \quad (23)$$

$$y_3 = a^2 - a - \cos(\pi \times a) + c_3 \quad (24)$$

All data are shown in Fig. 2, where black represents normal samples and red represents faulty samples. We can see from Fig. 2 that there are many faulty samples close to the normal samples, but they are not significant. Therefore, we must use a method that can recognize them quickly.

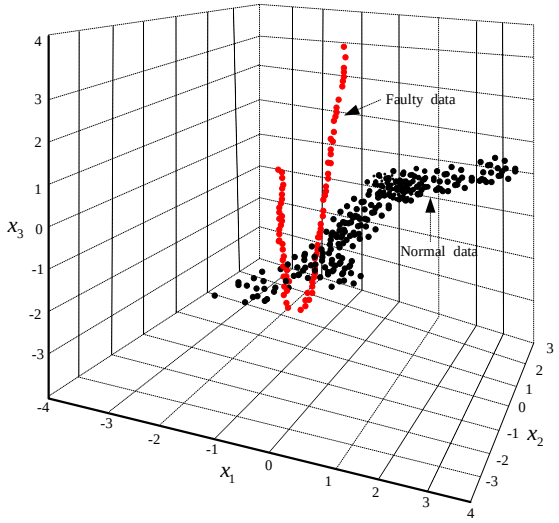

Fig. 2. Normal and faulty data in the original input space

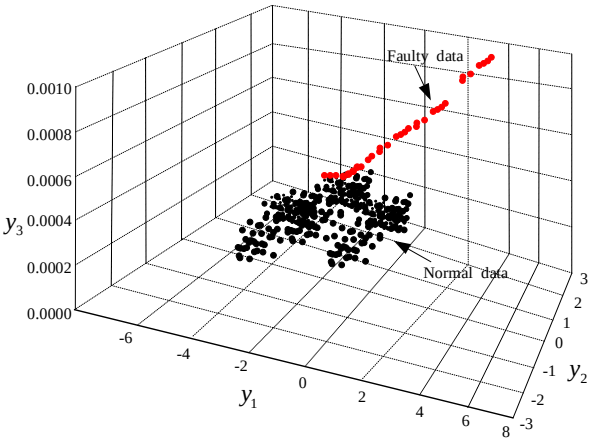

Fig. 3 Normal and faulty data in the output space

During the process monitoring, we first build an EMVU model based on the normal data. Here, we select the number of nearest neighbours as 5, and the dimensionality of the

EMVU output space is 2. A Gaussian process regression model is utilized to approximate the nonlinear mapping between the inputs and the outputs. We use a simple second-order polynomial covariance function defined as $k(x_i, x_j) = (b + \sum_{k=1}^{D} x_{ik} y_{ik})^2$ to implement the Gaussian process regression model. From [22-23], the first two outputs of the eigenvalue spectrum can capture more than 99% variation information. In the KPCA model, we use the same kernel function form as in EMVU, and select 6 principal components. For the PCA model, from [24], the first two principal component can capture more than 90% variation information of the original data.

Then, we use the three models to monitor the fault samples. The control indices T^2 and SPE of EMVU are shown in Fig. 4, the KPCA output is shown in Fig. 5 and the PCA results are shown in Fig. 6. By considering EMVU's output space in Fig. 3, we can see that there are many faulty samples located outside the normal sample. According to Fig. 4, for a large number of points, the SPE exhibits model fitness, but in this case, T^2 statistic is not very sensitive. Therefore, SPE control performs better than T^2. However, in Fig. 4, the T^2 and SPE of EMVU statistics are calculated in the output space. The bottom plot shows the monitoring result based on the predictive variance: the predictive variance contains similar information between the training data and the test data in the input space, and the T^2 and SPE of EMVU statistics show better detection ability, as verified in Fig. 3. From all the three figures, we can see that the control limits adopt the corresponding confidence level at 99%. The missing alarm rates of EMVU reach 24%. The detailed monitoring results can be seen in Fig. 4, which shows that KPCA is better than PCA but worse than EMVU. In addition, KPCA requires 6 PCs to obtain these characteristics but the EMVU only need 2 outputs. Therefore, the EMVU method is better than KPCA and PCA for use in a nonlinear monitoring system.

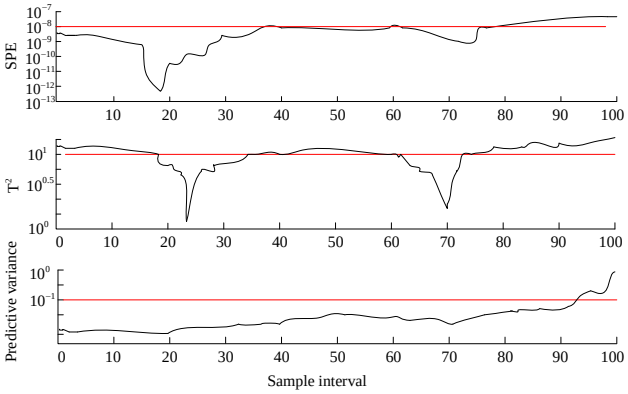

Fig. 4 Monitoring results of EMVU model monitoring

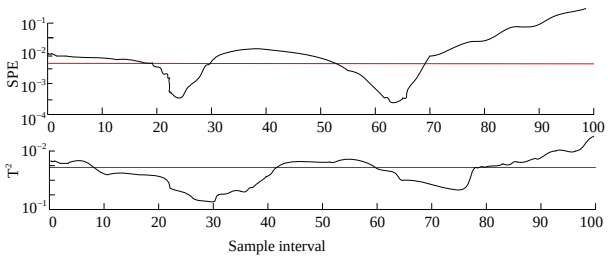

Fig. 5 Monitoring results of KPCA model monitoring

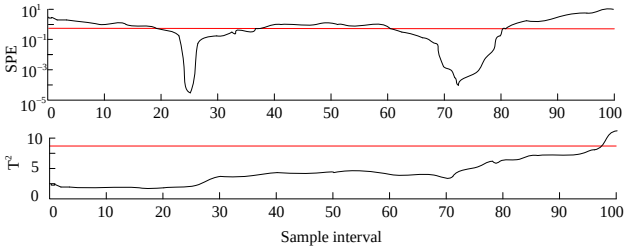

Fig. 6 Monitoring results of PCA model monitoring

V. Conclusion

This paper proposes a new nonlinear process monitoring technique based on improved KPCA and extended MVU method to perform fault detection and identification. Compared to PCA, by using KPCA and extended MVU monitoring method, we can obtain the following attractive advantages. (1) EMVU considers the manifold structure of data and leads to lower-order models. The dimensions of the model space can be set effectively determined. (2) We can determine the parameters in the EMVU model easily. By learning its implicit mapping, the parameters in an EMVU model can be determined automatically through a supervised procedure. (3) In on-line nonlinear monitoring, dimensionality reduction was performed for a new observed process sample, making this method more powerful in fault detection. Then, case studies on a simple numerical example demonstrated the effectiveness of the proposed method.

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