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Process Monitoring Based on Recursive Probabilistic PCA for Multi-mode Process ⋆

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Abstract: A recursive probabilistic principal component analysis (PPCA) based data-driven fault identification method is proposed to handle the missing data samples and the mode transition in multi-mode process. This model is recursively obtained by using the increasing number of normal observations with partly missing data. First, based on the singular value of historic data matrix, the whole process is divided into different steady modes and mode transitions. For steady modes, the conventional PPCA is used to obtain the principal components, and to impute the missing data. When the mode is a mode transition, the proposed recursive PPCA is applied, which can actually reveal the between-mode dynamics for process monitoring and fault detection. After that, in order to identify the faults, a contribution analysis method is developed and used to identify the variables which make the major contributions to the occurrence of faults. The effectiveness of the proposed approach is demonstrated by the Tennessee Eastman chemical process. The results show that the presented approach can accurately detect abnormal events, identify the faults, and it is also robust to mode transitions.

Keywords: Multi-mode, mode transition, missing data, recursive probabilistic PCA, Fault detection and identification.

1. INTRODUCTION

Since 1990s, multivariate statistical methods, such as principal component analysis (PCA), avoid of directly modelling of complex systems, have been successfully applied to the monitoring and fault diagnosis in many industrial processes (Chiang et al. (2001)). However, often caused by a sudden mechanical breakdown, sensor failure or malfunction occurred in data acquisition system, partly missing data or irregularly sampled data is a common phenomenon in industrial practice. Up to now, the missing data sample problem is being a major challenge of most of existing monitoring approaches. The process monitoring and fault detection techniques with partly missing measurements have not been well studied.

Based on a Gaussian latent variable model, probabilistic principal component analysis (PPCA) method, whose parameters can be determined by the eigenvalue decomposition of the measurement sample covariance matrix or the expectation-maximization (EM) algorithm (Kim and Lee (2003)), has been regarded as an efficient method for handling missing data and forming a mixture model. However, PPCA often follows the unimodal distribution assumption of the operating data, which is similar to PCA. In practice, mode transition often takes place in some of industrial processes because of different manufacturing strategies, various product specifications, and so on. Therefore, PPCA is not adaptive to multi-mode process in general, since it can lead to the frequent false alarms in the case of the operation mode is transiting from one mode to another.

Recently, there are many literature reported on the conditional monitoring for multi-mode process which consider the case of changing setting parameters. In (Hwang and Han (1999)), a multi-level clustering PCA method was proposed to solve the multi-mode problem in Tennessee Eastman (TE) process. A Gaussian mixture model and PCA method have been combined together, which can improve the efficiency of modeling the whole process (Xu et al. (2010)). After that, Xu also proposed a mixture PCA model to capture normal distribution of production process (Xu et al. (2011)). These methods did not consider the mode transition in multi-mode process. To solve this problem, Zhao has proposed a PCA-based modeling and monitoring strategy for multi-mode processes with between-mode transitions. A mode-common subspace for all modes data is separated at first. Then, the operating data for each mode is projected to the mode-common subspace and a mode-special remaining subspace. A mode transition identification algorithm was designed to detect the abnormal behaviors (Zhao et al. (2010)). Wang identified the stable modes, mode transitions, and noise at first. Then, according to the data distribution, a proper multivariate statistical algorithm was chosen to detect the fault for each mode (Wang et al. (2012)). Zhang proposed a recursive PCA to separate the multi-modes by taking into account of the cross-mode correlations and extracting the common information between the different modes(Zhang

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et al. (2012)). And then, to improve the monitoring performance of the between-mode, Zhang extracted the common subspace form the different modes and between-mode transition which was been applied to conditional monitoring for the electro-fused magnesia furnace(Zhang and Li (2013)). And then, this method has also been generalized to detect the fault of non-gaussian processes (Zhang et al. (2013)).

It should be noted that all of aforementioned methods are the improvements of PCA approaches, which implies that the performance and efficiency of those approaches are still susceptible to the influence of commonly occurred interference factors such as stochastic noise and missing data (Wang and Li (2012); Xia et al. (2013); Elshenawy et al. (2009)). To overcome monitoring problems both on data missing and mode transition in multi-mode process, this paper proposed a recursive PPCA method within a probabilistic framework. The historical data are divided into serval operation modes and the mode transitions between them based on the singular value recognition. Than, the PPCA method is used to model the steady modes and the recursive PPCA method is used to model the mode transition. The missing data can also be estimated in a probabilistic framework. After that, a Mahalanobis contribution analysis based on the recursive PPCA method is proposed for fault detection and diagnosis. The efficiency of our approach is illustrated through the TE chemical process, and the result shows that the presented approach can accurately detect abnormal events and identify the faults in the multi-mode system.

2. MODELING OF MULTI-MODE SYSTEM

2.1 PPCA and Recursive PPCA Algorithm

Assume that the latent variable model relates a d-dimensional observed variable y to a q-dimensional score vector of latent variable x , which implies:

$$y = Wx + \mu + \epsilon \tag{1}$$

where $W \in R^{d\times q}$ a linear transformation matrix which is composed of the eigenvectors of sample covariance matrix corresponding to the $q(q < d)$ largest eigenvalues, μ is the mean of the data y, and ϵ is the noise term which is assumed to be Gaussian and isotropic, $\epsilon \sim G(0, \sigma^2 I)$. Then, the conditional probability distribution $y|x$ is also Gaussian, which is follow

$$y|x \sim G(Wx + \mu, \sigma^2 I) \tag{2}$$

Furthermore, by adopting a Gaussian prior distribution for the scores variables x, $x \sim G(0, I)$, then, the marginal distribution of y is Gaussian in the form of $y \sim G(\mu, C)$, where the covariance matrix is $C = WW^T + \sigma^2 I$. Therefore, the PPCA method provides a way to constrain the model complexity via the selection of q, and the model parameters can be estimated by the maximum likelihood algorithm (Qu et al. (2009); Li et al. (2013)).

When the process transit from one mode to another, the recursive PPCA method can update the model parameters in a recursive way. Suppose that the historical output data can be denoted as $Y_k = [y_1, y_2, ..., y_k]^T$, where $y_i \in R^d, (i = 1, ..., k)$. If a new observation y_{k+1} is available, then the mean value is changed to

$$\mu_{k+1} = \frac{k}{k+1}\mu_k + \frac{1}{k+1}y_{k+1} \tag{3}$$

Define a variable as

$$\Delta\mu_{k+1} = \mu_{k+1} - \mu_k \tag{4}$$

then, the covariance matrix S_{k+1} can be calculated recursively as

$$S_{k+1} = \frac{1}{k}\sum_{i=1}^{k+1}(y_i - \mu_{k+1})^T(y_i - \mu_{k+1}) \tag{5}$$

Notice that $S_k = \frac{1}{k-1}\sum_{i=1}^{k}(y_i - \mu_k)^T(y_i - \mu_k)$, (5) can be reformulated as

$$\begin{aligned} S_{k+1} = & \frac{k-1}{k}S_k + \Delta\mu_{k+1}\Delta\mu_{k+1}^T \\ & + \frac{1}{k}(y_{k+1} - \mu_k - \Delta\mu_{k+1})(y_{k+1} - \mu_k - \Delta\mu_{k+1})^T \end{aligned} \tag{6}$$

Equation (6) indicates that S_{k+1} is two rank-one modifications from S_k. Consequently, the above update procedure has to be performed twice to estimate the eigenvalues and eigenvectors matrix for the current covariance matrix. After that, the parameters of the proposed PPCA model can be estimated by the observations and the updated values.

Following the prior distribution assumptions, we obtain

$$E(x_i) = (W^TW + \sigma^2 I)^{-1}W^T(y_i - \mu) \tag{7}$$

and

$$E(x_i x_i^T) = \sigma^2(W^TW + \sigma^2 I)^{-1} + E(x_i)E(x_i)^T \tag{8}$$

where $E(\cdot)$ is the expectation operator, $i = 1...k$. Then, the corresponding log-likelihood of observed data under this model is defined as

$$l_k = \sum_{i=1}^{k}\log p(y_i, x_i) \tag{9}$$

where the joint probability density $p(y_i, x_i)$ is given by

$$\begin{aligned} p(y_i, x_i) = & (2\pi\sigma^2)^{-d/2} \times \exp\{\frac{-\|x_i\|^2}{2}\} \\ & \times\exp\{\frac{-\|y_i - Wx_i - \mu\|^2}{2\sigma^2}\}(2\pi)^{-q/2} \end{aligned} \tag{10}$$

Take the conditional expectation with respect to the distribution in Equation (10), we obtain

$$\begin{aligned} E(l_k) = & -\sum_{i=1}^{k}\{\frac{d}{2}\log\sigma_k^2 + \frac{1}{2}tr(E(x_i x_i^T)) \\ & + \frac{1}{2\sigma_k^2}\|y_i - \mu_k\|^2 - \frac{1}{\sigma_k^2}E(x_i)^T W_k^T(y_i - \mu_k) \\ & + \frac{1}{2\sigma_k^2}tr(W_k^T W_k E(x_i x_i^T))\} \end{aligned} \tag{11}$$

Maximize the conditional expectation of(11) with respect to W_k and σ_k^2, then the parameters are updated as

$$W_k = \left[\sum_{i=1}^{k}(y_i - \mu_k)E(x_i)^T\right]\left[\sum_{i=1}^{k}E(x_i x_i^T)\right] \tag{12}$$

$$\sigma_k^2 = \frac{1}{kd}\sum_{i=1}^{k}\{\|y_i-\mu_k\|^2 - 2E(x_i)^T W_k^T(y_i-\mu_k) \\ +tr\left(E(x_i x_i^T)W_k^T W_k\right)\} \tag{13}$$

Let the window width of original data is L, namely, the sample y_{k-L+1} will be replaced by the new observation y_{k+1} at $k+1$ instant. Thus, we can update model with new parameters of W and σ^2.

2.2 Missing data Imputation Approach

For an incomplete measurement y_k, it can be divided into the observable part $y_{k,o}$ and the missing part $y_{k,u}$. Therefore, (9) is rewritten as

$$l_k = \sum_{i=1}^{k}\log p(y_{i,o}, y_{i,u}, x_i) \tag{14}$$

Similar to the Maximum Likelihood Estimation in prior subsection, we obtain the estimation of y_k

$$\tilde{y}_k(n) = \theta_k W_k[{N_k}^{-1}{W_k}^T(y_k-\mu_k)] + \mu_k \tag{15}$$

where $N_k = {W_k}^T W_k + \sigma_k^2 I$. The value of θ_k can be obtained by minimizing $\|\tilde{y}_{k,o} - y_{k,o}\|^2$.

Based on above results, at $k+1$ time instant, an EM algorithm for PPCA modeling can be summarized as follows:

Let $\mu_{k+1}(0) = \mu_k$, $W_{k+1}(0) = W_k$,$\sigma_{k+1}(0) = \sigma_k$,$N_{k+1}(0) = W_{k+1}(0)^T W_{k+1}(0) + \sigma_{k+1}^2(0)I$, then repeat the following steps:

$$\begin{aligned}
&\tilde{y}_{k+1}(n+1) = \theta_{k+1}(n+1)W_{k+1}(n)[N_{k+1}(n)^{-1} \\
&\qquad W_{k+1}(n)^T(y_{k+1}(n) - \mu_{k+1}(n))] + \mu_{k+1}(n) \\
&\min_{\theta_{k+1}(n+1)}\{\|\tilde{y}_{k+1,o}(n+1) - y_{k+1,o}\|^2\} \\
&\mu_{k+1}(n+1) = \frac{k}{k+1}\mu_k + \frac{1}{k+1}\tilde{y}_{k+1} \\
&\Delta\mu_{k+1}(n+1) = \mu_{k+1}(n+1) - \mu_k \\
&S_{k+1}(n+1) = \frac{1}{k}\sum_{i=1}^{k}(\tilde{y}_i(n)-\mu)(\tilde{y}_i(n)-\mu)^T \\
&W_{k+1}(n+1) = S_{k+1}(n)W_{k+1}(n)(\sigma_{k+1}(n)^2 I) \\
&\qquad + N_{k+1}(n)^T S_{k+1}(n)W_{k+1}(n))^{-1} \\
&\sigma_{k+1}(n+1)^2 = \frac{1}{p}tr(S_{k+1}(n) \\
&\qquad - S_{k+1}(n)W_{k+1}(n)N_{k+1}(n)^{-1}W_{k+1}(n+1)^T)
\end{aligned} \tag{16}$$

where the n is the number of iterations. Above setps are repeated iteratively until convergence and then the process of parameters learning is finished.

3. ONLINE MONITORING AND FAULT DIAGNOSIS

For simplification of the expression, we assume that the whole process has two stationary modes and a between-mode, which is shown in Fig.1. Than, Mode 1 and Mode 2 are steady modes built with regular PPCA, while the between-mode transition will be modelled by the proposed recursive PPCA method.

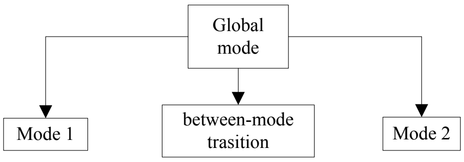

Fig. 1. Global mode structure

3.1 Mode Detection and Process Modeling

It is noted that the singular values of process data can be changed with the increasing samples in between-mode (Wang and Li (2012)). Let $Y = U\Sigma V^H$, where $\Sigma = diag(\tau_1, \tau_2, ..., \tau_p,)$, and define $\tau^2 = \sum_{i=1}^{p}\tau_i^2 = \|Y\|_F$, then the mode detection index at k time instant can be defined as

$$T_k(j) = \frac{1}{L}\sum_{i=k-L+1}^{k}\Sigma_i(j,j) \tag{17}$$

which presents the average of parameter τ at k time instant, where $\Sigma_k(j,j)$ is the jth diagonal values of Σ_k , and Σ_k means the matrix Σ at k time instant as well. Then, at $k+1$ time instant, we have

$$T_{k+1}(j) = \frac{1}{L}\sum_{i=k-L+2}^{k+1}\Sigma_i(j,j) \tag{18}$$

Therefore, mode transition time can be recognized by the range ability of τ^2, as:

$$\frac{T_{k+1}(j) - T_k(j)}{T_k(j)} > \gamma_j \tag{19}$$

where γ_j is a predefined parameter in dynamic process, which is related to mode transitions and determined by human experience (Wang and Li (2012)).

3.2 Confidence Bound and Fault Diagnosis

Based on probability theory, the β% confidence bound can be defined as (Chen and Sun (2009)):

$$\int_{y:p(y)>h} p(y)dy = \beta \tag{20}$$

where $p(y)$ is the probability distribution of y, and the squared Mahalanobis distance based equivalent confidence bound, which can be used for fault detection and diagnosis, is shown as follow:

$$M_k^2 = (y_k-\mu_k)^T S_k^{-1}(y_k-\mu_k) > \chi_d^2(\beta) \tag{21}$$

where β is the fractile of the χ^2 distribution with the degree of freedom d, and the value can be updated as

$$M_{k+1}^2 = (y_{k+1}-\mu_{k+1})^T S_{k+1}^{-1}(y_{k+1}-\mu_{k+1}) > \chi_d^2(\beta) \tag{22}$$

Therefore, the recalculated monitoring statistic is given by

$$E(M_{k+1}^2) = tr(S_{k+1}^{-1}\{(z-\mu_{k+1})(z-\mu_{k+1})^T + Q\}) \tag{23}$$

where z and Q are related as $y|y_0 \sim N(z, Q)$, whose details can be found in Chen and Sun (2009) and He et al. (22). Finally, we can calculate $\|M_{k+1}^2 - E\left[M_{k+1}^2\right]\|$ for fault diagnosis with 99% confidence bound, and the confidence limit is $M^2_{k+1} - \chi^2_d(\beta)$ (Chen and Sun (2009)). As a result, the process behaviour is considered faulty if the statistic of a new observation exceeds the control limit.

3.3 Modeling and Monitoring for Multi-mode Process

In this part, the step-by-step procedure of recursive PPCA model based multi-mode monitoring approach is given below, and the flowchart of this method on fault detection and diagnosis is shown in Fig. 3. Firstly, the procedure of model development is given, as:

(1) Acquire normal operating data and normalize the data using the mean and standard deviation of each variable.
(2) Calculate parameters of μ, W and σ^2.
(3) Calculate squared Mahalanobis distance M^2 and its confidence limits.
(4) Calculate $E\left[M^2\right]$ and $\|M^2 - E\left[M^2\right]\|$ to estimate contribution of each variable.
(5) Calculate the upper confidence limits for contributions.

In addition, the online fault diagnosis of recursive PPCA approach is also given below:

(1) Obtain new observation data, and then make model detection in multi-mode process.
(2) Recalculate new parameters of μ_{k+1}, W_{k+1} and σ^2_{k+1} .
(3) Recalculate new squared Mahalanobis distance M^2_{k+1} and its confidence limits.
(4) If any statistic exceeds its corresponding confidence limit, calculate the contributions of each variable after fault detection.
(5) Monitor the contribution of each variable and make fault diagnosis.

4. SIMULATION STUDY

In this section, the TE process is used to evaluate the effectiveness of the proposed fault detection and identification approach based on recursive PPCA in multi-mode system. The TE process is an open-lop unstable plant-wide process control problem considered as a benchmark simulation for various process monitoring techniques. This process produces two products (G and H) from four reactants (A, C, D and E), and F is a byproduct. In addition, an inert component B also presents in C stream and in trace amount in the A feed stream. The process consists of five major units, which include an exothermic two-phase reactor, a flash separator, a recycle compressor, a reboiled stripper, and a product condenser(Liu and Chen (2010); Yin et al. (2012)). The TE process has total 11 input variables (without agitator speed) and 41 measurement variables. And the process measurements are sampled with an interval of 3 min. For simplicity, only 22 continuous measurements, listed in Table 1, are selected in this simulation.

Since it is difficult to produce products consistently in industrial scale, the quality control in industry relies significantly on the consistency of process conditions. Because of process changing, the operating conditions have to be adjusted to meet the production specifications, which can cause various operation modes. Some of them are steady state modes, while others are between-mode transitions. In the simulation, we suppose that the whole process is divided into two modes and a between-mode, which are listed on Table 2. Mode transition is introduced

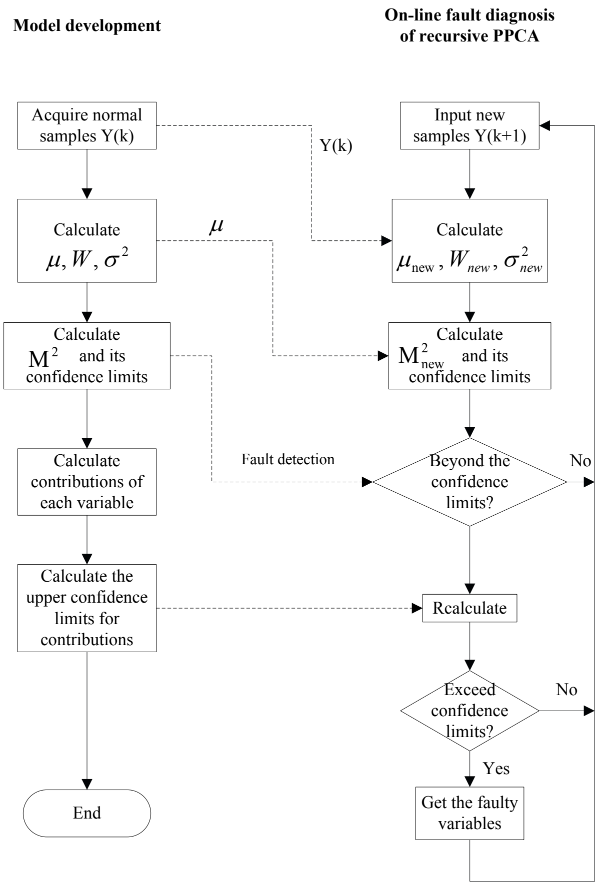

Fig. 2. Procedures of recursive PPCA method

Table 1. Continuously Measured Variables

Variable's ID	Description
1	A feed (stream 1)
2	D feed (stream 2)
3	E feed (stream 3)
4	A and C feed (stream 4)
5	Recycle flow (stream 8)
6	Reactor feed rate (stream 6)
7	Reactor pressure
8	Reactor level
9	Reactor temperature
10	Purge rate (stream 9)
11	Product separator temperature
12	Product separator level
13	Product separator pressure
14	Product separator underflow (stream 10)
15	Stripper level
16	Stripper pressure
17	Stripper underflow (stream 11)
18	Stripper temperature
19	Stripper stream flow
20	Compressor work
21	Reactor cooling water outlet temperature
22	Condenser cooling water outlet temperature

by decreasing the value of reactor temperature from 120 to 110. To test the ability of proposed method, we define mode 1, mode 2 and the mode transition between as normal operating modes, and let failures occur in mode 2. Both methods are performed on the 10% randomly missing data and the number of principal components is set to 5 based on the results of a 10-fold cross validation.

Table 2. Operating Modes of Simulated Te Process

Modes	Samples
Normal Operating Mode 1	1st 300th
Between-mode transition	301st 600th
Normal Operating Mode 2	601st 700th
Faulty Operating Mode	701st 900th

The fault detection result with missing data of the proposed method is shown in Fig. 3. The M^2 calculated from the recursively updated PPCA model as well as the 99% confidence. This figure shows the values of statistics is sharply increasing from 702*th* time instant,and it is outside the M^2 limit at 703*th* time instant, which implies that fault has been detected in mode 2 for the time of the 703*th* sample. For all other time instants from 1 to 700, statistics are within their confidence limits, which means the false alarm rate is significantly eliminated.

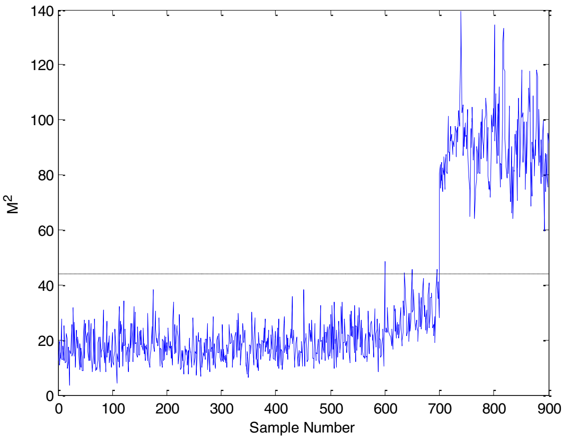

Fig. 3. Monitoring results by recursive PPCA

Based on the measurements of mode 1, the simulation results of PPCA with a 10% randomly missing rate is shown in Fig. 4. In the plot, the regular PPCA based calculated M^2 frequently exceed their respective confidence limits in the mode transition and the steady part of mode 2 where the process is operating normally. The similar results can be obtained if only the measurements of mode 2 are used for regular PPCA. Clearly, both regular PPCA and recursive PPCA can detect the fault correctly at the 703th sample. This may be explained by the fact that mode 2 is a stationary process which is modeling by regular PPCA method in multi-mode system, and only transition process is modeling by recursive PPCA. However, the false alarm rate of conventional PPCA is much higher than the false alarm rate of the proposed method, which means the recursive PPCA method is more effective to multi-mode system.

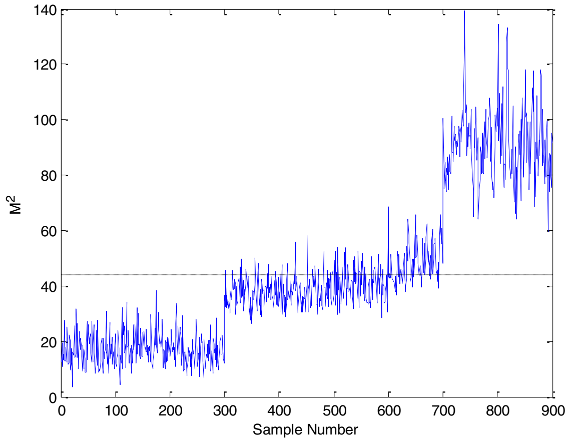

Fig. 4. Monitoring results by conventional PPCA

Furthermore, the diagnosis results are shown in Fig. 5 and Fig. 6, which indicate that the recursive PPCA based and the conventional PPCA based multi-mode monitoring and fault diagnosis have different contribution results. It can be seen that the contributions of the 2nd and 3rd variable are much higher than those of other variables in Fig. 5, which means that the proposed method can isolate fault variables efficiently. However, it is very difficult to determine which variables are the dominant sources of fault in Fig. 6, since 7 variables have exceeded control limits. As a result, the contribution plots shows that the proposed method is capable of isolating variables as few as possible, but not essential, faulty variables to further fault diagnosis.

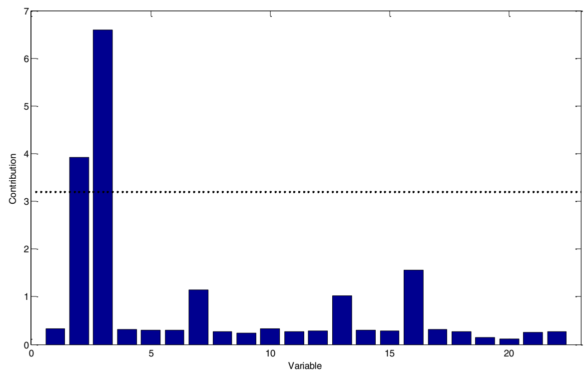

Fig. 5. Recursive PPCA based contribution plots

5. CONCLUSION

In this study, a recursive PPCA model based process monitoring and fault identification approach is developed for the multi-mode processes with randomly missing data. Different from the conventional PPCA, the proposed method recursively obtain the estimation of the missing measurement data and update model parameters. Based on the model detection index, a global mode with steady-state modes and between-mode transitions is thus developed. The illustration results demonstrate that the proposed approach can effectively detect and identify fault with missing data for multi-mode process, and it will not trigger false alarms in between-mode transition.

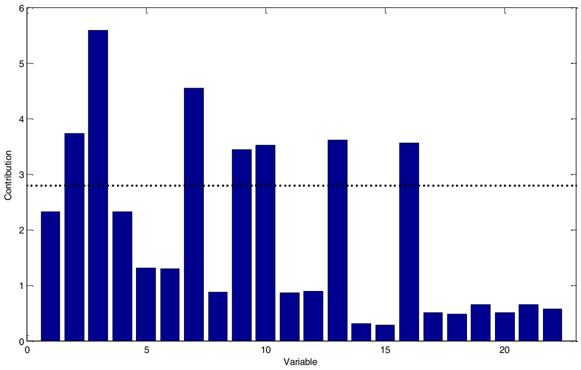

Fig. 6. Conventional PPCA based contribution plots

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