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# A model updating approach of multivariate statistical process monitoring

Bo He
*Department of Automation*
*Tsinghua University*
*Beijing, 100084, P.R.China*
heb05@mails.tsinghua.edu.cn

Xianhui Yang
*Department of Automation*
*Tsinghua University*
*Beijing, 100084, P.R.China*
yangxh@mail.tsinghua.edu.cn

***Abstract* –Multivariate statistical process control based on conventional principal component analysis (PCA) has been used widely in practice. The slow and normal changes in the processes often lead to false alarm since the conventional PCA algorithm is static. In this paper, we proposed a model updating approach of multivariate statistical process monitoring. By the proposed approach, the PCA model which presents the norm operation condition has been remodeled every N samples. Those remodeling data are chosen by quality information and engineer experience. Furthermore, the method of calculating the updating interval has been discussed. Finally, this model updating approach has been evaluated by a mathematic example and CSTR process simulation. The results show the effectiveness of this method.**

***Index Terms* –*Adaptive process monitoring; principal component analysis; fault detection; model updating; update interval.***

## I. INTRODUCTION

Multivariate statistical process control (MSPC) has been widely applied to process monitoring and fault detection in manufacturing to improve quality and productivity. Multivariate statistical projection method such as principal component analysis (PCA) is cornerstone of the MPSC since modern industrial process often produce huge amount of data due to the large number of frequently measurement variables [1-3].

As the characters of most industrial processes changed slowly over time, MSPC based on conventional PCA with static model have some drawbacks. The most important drawback is that the PCA model and control limits can't accommodate the variation of the process. The static PCA model interprets the natural slow changes of the process as faults. Therefore, it is necessary to update the PCA model so as to accommodate the natural changes of the process [4].

To address this problem, a large number of adaptive PCA algorithms are recommended during the past decades. Wold proposed a scheme of updating the PCA model by exponentially weighted moving average (EWMA) filter [5]. Li and Yue proposed a recursive PCA algorithm to accommodate the slow changes in the process [6]. More recently, Choi and Martin introduced forgetting factor to recursive PCA to update the mean and standard deviation [7]. Since the speed of adaptation decreased with the increment of the data size, the RPCA can be improved by adding newest samples and discarding the oldest samples to keep the size of training data set. Wang et al. proposed a fast moving window PCA algorithm [8] and He et al. proposed a variable MWPCA algorithm for adaptive process monitoring [9]. Liu et al. proposed the moving window kernel PCA scheme to monitoring the nonlinear processes [10].

Both of the RPCA and moving window PCA (MWPCA) scheme update the model immediately when the new sample or new sample block becomes available. This 1-Step update method can lead to mistakes or false alarms when the statistical models can't tell the differences between the slow ramp faults and the normal changes. Consequently, the fault data are added into the training data set, the ability of the PCA model to detect this type of fault is getting worse and worse. In this paper, we proposed a new model updating approach, which choose the training data by using the prior knowledge and the information from the quality system, to monitor processes adaptively. In other word, only the normal data chosen by the engineers with experiences and the quality information would be used for building the PCA model. As the selection of forgetting factor in RPCA and length of moving window in MWPCA[11]，the selection of the update interval is very important to apply this algorithm in practice. In this paper, we proposed a method of calculating the update interval based on normal historical data set and slow ramp fault data set.

This paper is organized as follows. In Section II, the review of MSPC based on conventional PCA is provided. The model updating approach and the method of calculating the update interval are discussed in Section III. Section IV presents two simulation examples to demonstrate that the proposed algorithms are very effective to adaptive process monitoring. Finally, the conclusions are drawn in Section V.

## II. REVIEW OF MSPC BASED ON PCA

One of the most commonly used MSPC methods is based on principal component analysis (PCA). MSPC based on PCA can monitor all the variables simultaneously and obtain information on the 'directionality' of the process variations by extracting variable correlation from all the process data. PCA is a projection method finds the latent variables which explain the maximal amount of variability of the process data to reduce the dimensionality of the problem. In this section we discuss the main points of MSPC using PCA.

### *A. Principal Component Analysis*

Let $x_i \in R^M$ denotes a sample vector of the i-th measured variables, a data matrix $X=[x_1, x_2 \cdots\cdots x_N] \in R^{M\times N}$ is composed with N measured variables. PCA depends critically upon the scales of the measured variables. The matrix X is scaled to

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zero mean and unit variance for covariance matrix based PCA. The matrix X can be decomposed into a score matrix $T=[t_1,t_2,\cdots t_N]$ and a loading matrix $P=[p_1,p_2,\cdots p_N]$:

$$X=T\times P^T=\sum_{i=1}^{N} t_i p_i^T \tag{1}$$

where $t_i \in R^M$ is i-th score vector, $p_i \in R^N$ is i-th loading vector.

If the process variables are collinear, most variability of the data matrix is explained by the first K (K<N) components, the loading space can divide into two subspaces: $P=[P_K,P_E]$ .The $P_K$ is predictive subspace and $P_E$ is residual subspace. In most process, the residual matrix E contains measurement noise rather than process information, so we have:

$$X=T_K\times P_K^T+T_E\times P_E^T=\sum_{i=1}^{K} t_i p_i^T+E\approx T_K\times P_K^T \tag{2}$$

B. *MSPC based on PCA*

The method of MSPC based on PCA is to project the observation vectors x to both the predictive subspace and residual space through PCA model. Two statistics, Hotelling $T^2$and squared predictive error (SPE or Q), are developed based on this projection and often used for monitoring.

They are given by:

$$T^2=t\Lambda^{-1}t^T=XP_K\Lambda^{-1}P_K^TX^T \tag{3}$$

$$Q=ee^T=X(I-P_KP_K^T)X^T \tag{4}$$

Usually, we use upper control limits with a confidence level $\alpha$ for $T^2$and Q**,** respectively. Jackson and Mudholkar [12] developed an control limit for Q:

$$Q_\alpha=\theta_1\left(\frac{c_\alpha\sqrt{2\theta_2h_0^2}}{\theta_1}+1+\frac{\theta_2h_0(h_0-1)}{\theta_1^2}\right)^{\frac{1}{h_0}} \tag{5}$$

where

$$\theta_i=\sum_{j=k+1}^{n}\lambda_j^i \quad i=1,2,3,\quad h_0=1-\frac{2\theta_1\theta_3}{3\theta_2^2}$$

k is the number of principal components and $c_\alpha$ is the normal deviate corresponding to the $(1-\alpha)$ percentile.

The control limit for $T^2$is Hotelling's $T^2$ statistic:

$$T_\alpha^2=\frac{K(M-1)}{M-K}F_{K,M-1,\alpha} \tag{6}$$

where M is the number of samples for PCA modelling, K is the number of principal components, $\alpha$ is the confidence level, and $F_{K,M-1,\alpha}$ is the $\alpha$ percentile of the F-distribution with degree of freedoms K and M-1.

The process is considered abnormal if either $T^2$ or Q statistics of the new observation exceed the control limit. Further fault isolation may be conducted.

## III. The Model Updating Approach

The MSPC based on conventional PCA discussed in section II is not suitable for monitoring slow time varying process. The processes are regarded as stationary and time invariant Gaussian processes. When slow and nature changes occur in the processes, it is necessary to update the PCA model so as to reduce false alarm rate.

A. *Adaptive Multivariate Statistical Process Monitoring*

To address this limitation, a large number of adaptive PCA algorithms are recommended during past decades. Most of these algorithms calculate the PCA models adaptively by using the original data more recently rather than the older ones. The method of recursive PCA algorithm is to recursively update the mean, standard deviation, and covariance matrix when a new sample or a new sample block $x_{k+1}$ becomes available. They equations of updating models are given by:

$$m_{k+1}=\alpha m_k+(1-\alpha)x_{k+1} \tag{7}$$

$$(X^TX)_{k+1}=\gamma(X^TX)_k+(1-\gamma)x_{k+1}^Tx_{k+1} \tag{8}$$

where $m_k$ is the mean vector of the variables at time k , $\alpha$ and $\gamma$ are both forgetting factors.

The moving window PCA (MWPCA) algorithm is another major adaptive monitor method used in practice. MWPCA's adaptation is achieved efficiently by add the newest sample to the data matrix and discard the oldest sample. Consequently, the length of the moving window is invariant.

Let the K-th data matrix with window length N be $X_K=[x_{K-N+1},x_{K-N+2},\cdots,x_k]$ .The fast MWPCA algorithm proposed by Wang and Kruger follows these steps:

i) Downdating: $X_K^{'}=[x_{K-N+2},x_{K-N+3},\cdots,x_k]$ ,calculate the intermediates $m_k^{'}$ and $(X^TX)_K^{'}$ from $m_k$ and $(X^TX)_k$;

ii) Updating: $X_{K+1}=[x_{K-N+2},x_{K-N+3},\cdots,x_K,x_{K+1}]$ , calculate the $m_{k+1}$ and $(X^TX)_{k+1}$ from $m_k^{'}$ and $(X^TX)_K^{'}$ .

Both of the adaptive monitor methods discussed above update the model immediately when the new sample or new sample block becomes available. By using this 1-Step update method, the data contaminated by the slow ramp faults will be added into the data matrix to build the PCA model. It is because that sometimes the statistics of the fault data don't violate the control limit at once, such that the adaptive algorithm continued to regard the new fault data as normal data. Consequently, the PCA model gradually accommodates the faults, and the ability of the PCA model to detect this type of faults is getting worse and worse. In other word, sometimes the PCA models can't tell the difference between slow time varying and slow ramp faults, so the data with faults' information are also added into the training set. We need some other information provided by the quality systems which often have seriously time delay for online monitoring.

Moreover, it is very difficult to find a suitable length of the moving window or the value of forgetting factor in practice. The length of the moving window (for recursive PCA is forgetting factor) is a key parameter to guarantee the ability of PCA model to accommodate the slow time variant of the process, so it is usually small in order to reduce the false alarm rate. Obviously, if the length of moving window (for recursive PCA is forgetting factor) is not large enough, the ability of the PCA model to detect the slow ramp faults or disturbances would worse than conventional PCA.

In this paper, we propose an alternative adaptive monitor method based on a new model updating approach called N-steps remodeling PCA algorithm. This method follows these procedures:

i) Modeling: Build the PCA model from the normal historic data. The normal data are chosen by process quality variables, observation records or any other information which can guarantee their validity.
ii) Monitoring: Use the PCA model built in procedure i) to monitor the process with N samples. Either Q control limit or $T^2$ control limit is violated during this procedure, the model updating is terminated and an alarm is triggered. Further fault isolation may be conducted.
iii) Remodeling: After N samples, choose the nearest normal data from the last N samples to rebuild the PCA model. The normal data are selected by using information from quality system to guarantee their validity. Back to ii).

In N-steps remodeling PCA, we used some knowledge from quality system while build the PCA model. It is a way to guarantee the process data collected to build the model represent normal condition. Compare with the Moving window PCA and the recursive PCA, the PCA model built by this model updating approach is more suitable for slow time varying process with slow ramp fault which is very common in the process industry.

Moreover, the update interval N is also a key parameter for the PCA model to accommodate the slow time varying process. If the update interval N is not large enough, the ability to detect the hidden slow ramp faults is worse than conventional PCA just like the window length is too short in moving window PCA. Meanwhile, N can't be too large because of the slow variant of process. The method of calculating the update interval N is another topic discussed in this paper.

*B. The Method of calculating the update interval*

As discussed in previous segment, the update interval N is very important for the PCA model to adapt to the varying process. The value of N depends on two factors, one is the time-variation of the process, and the other is the slope of ramp faults and disturbances. In most process, the normal time variation is very slow compare with the variation caused by ramp faults. Consequently, we can calculate upper limit of N by finding how slowly the time varying process changes and determine the lower limit by calculating the measure of all known ramp faults' time variability.

This method follows these procedures:

a) Upper limit:

i) Select S normal process samples from the historic database and rearrange them by time;
ii) Build a PCA model from the first k samples of the rearranged S samples;
iii) Calculate all the S samples' Q and $T^2$ statistics by using the PCA model built in step ii), denote the results: $Q(i), T^2(i),\ \forall i \in [1,2,\cdots,S]$.
iv) The upper limit of N is given by :

$$N_{upper} = \min\{\frac{Q_\alpha}{\sum_{i=1}^{M}\frac{Q(i)}{i\cdot S}}, \frac{T_\alpha^2}{\sum_{i=1}^{M}\frac{T^2(i)}{i\cdot S}}\} \tag{9}$$

where the $Q_\alpha$ and $T_\alpha^2$ is the Q and $T^2$ statistics' limits, respectively.

b) Lower limit:

i) Determine the number of slow ramp faults in the process by historical data, denote the faults f(1), f(2),…f(n).
ii) Select M process samples contaminate by f(1) from the historical data and rearrange them by time;
iii) Build a PCA model from the first k samples of the rearranged S samples;
iv) Calculate all the S samples' Q and $T^2$ statistics by using the PCA model built in step iii), denote the results: $Q(i), T^2(i),\ \forall i \in [1,2,\cdots,S]$.
v) The lower limit of N with f(1) is given by :

$$N_{lower}(1) = \max\{\frac{Q_\alpha}{\sum_{i=1}^{M}\frac{Q(i)}{i\cdot S}}, \frac{T_\alpha^2}{\sum_{i=1}^{M}\frac{T^2(i)}{i\cdot S}}\} \tag{10}$$

vi) Calculate all the lower limit of N with f(1),f(2),…,f(n),and select the maximum of them.

$$N_{lower} = \max\{N_{lower}(1), N_{lower}(2), \cdots, N_{lower}(n)\} \tag{11}$$

c) Result :

Since the value of the N is between the upper limit and the lower limit, we have:

$$N = \mathrm{fix}(\alpha(N_{upper} - N_{lower}) + N_{lower}) \tag{12}$$

where the $\alpha \in [0,1]$, and the function fix(x) give the nearest integer smaller than or equal to x.

In addition, the information about quality is often time-delayed in practice. Consequently, the N should be large enough to get the information from quality system such as off-line experiment, measurements from instrument with time-delay, et al.

## IV. Simulation Examples

The model update approach discussed in previous sections is now applied to simulation examples to demonstrate its effectiveness.

*A. Simple mathematical example*

There are 4 variables in this simple stochastic process, with an underlying dimensionality of two. Denotes the original data matrix $\bar{X} = [\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4]$ .The $\bar{x}_1$ and $\bar{x}_2$ are represented as uncorrelated Gaussian measurement of zero mean and unit variance. The remaining two variables are formed by adding and subtracting $\bar{x}_1$ and $\bar{x}_2$, respectively.

The original data were contaminated by Gaussian measure noises of zero mean and standard deviation of 0.1. A slow ramp signal with an increment of 0.002 was added to $\bar{x}_3$ and a slow ramp signal with a decrement of 0.002 was added to $\bar{x}_4$, respectively.

In this study, 3000 samples are generated. The first 500 samples are used to form the training data set which represents the normal operation condition. The remaining 2500 samples are used to form the test data set.

This simulation is augmented to represent a slow drift of the variables which are common in practice. For instance, a leak, pipe blockage, catalyst degradation, or performance deterioration in individual process units can lead to slow time varying changes in process.

Furthermore, a slow ramp fault and a step fault are added to the process. A slow ramp fault is added to $x_2(t)$ after 1500 samples with an increment of 0.01 and the step fault is added to $x_1(t)$, $x_2(t)$, $x_3(t)$, $x_4(t)$ with amplitude 1 after 2000 samples.

In the first simulation case, the conventional PCA is adopted to monitor the process. The cumulative percent variance (CPV) method [13], which has been usually used in literature for determining the number of PCs, is used. In this study, the threshold of cumulative variance value is 90%.

The Q statistics obtained by conventional PCA are shown in Figure 1 and the $T^2$statistics are shown in Figure 2.

Obviously, the Q control limit is violated from about 600 samples to 1500 samples although it is normal operation condition. This result agrees with the underlying nature of the process data. As the slow drift exists all the time, the normal operation condition of this process shows significant changes with time. The conventional PCA model can't adapt these changes such that the false alarm rate is too high.

In the second simulation case, the N-steps remodeling PCA algorithm discussed in the previous section is used to monitor the process.

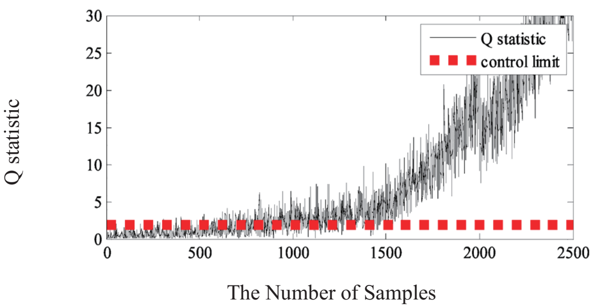


Fig. 1 The Q statistics obtained by conventional PCA for mathematical example

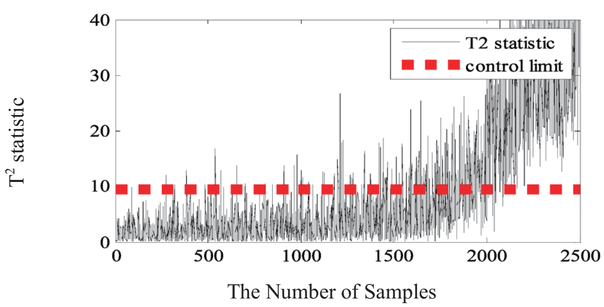


Fig. 2 The $T^2$ statistics obtained by conventional PCA for mathematical example

According to the scheme of the algorithm:

i) Calculate the parameter N. For this purpose, another training data formed by 500 samples which contaminated by the known slow ramp fault is generated. We choose the first 100 samples to build the model. Let $\alpha = 0.9$ , the results are: $N = 276$ .

ii) Monitoring the process with the parameter N calculated in step i)

For comparison, the Q statistics obtained by N-steps remodeling PCA are shown in Figure 3 and the $T^2$statistics are shown in Figure 4.

The performance of the N-Steps remodeling PCA algorithm is much better than the conventional PCA, and the value of N calculated by the proposed method is suitable for this process. Both of the Q control limit and $T^2$ control limit are not violated until the slow ramp fault was added to the process after 1500 samples. This adaptive monitoring scheme can reduce the false alarm rate significantly compare with the conventional PCA.

*B. Simulated CSTR process*

A nonisothermal continuous stirred tank reactor (CSTR) process [14] is adopted to illustrate the proposed method for adaptive process monitoring. In the CSTR, the reactant A is premixed with a solvent, and then converted to product B. Suppose that the volume and the physic properties are constant. The schematic diagram of the process is given in Figure 5.

The reaction is the first order ( $A \rightarrow B$ ) and the reaction rate is:

$$r = \beta_r k_0 e^{-E/RT} C \tag{13}$$

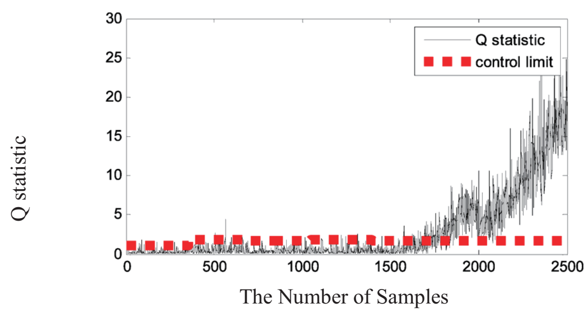


Fig. 3 The Q statistics obtained by N-steps remodeling PCA for mathematical example

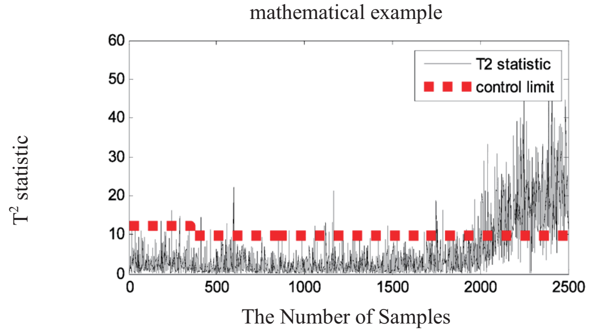


Fig. 4 The $T^2$ statistics obtained by N-steps remodeling PCA for mathematical example

A mathematic model of the process consists of the component material balance and the energy balance is given by:

$$V\frac{dC}{dt} = F(C_i - C) - Vr \tag{14}$$

$$V\rho c_p \frac{dT}{dt} = \rho c_p F(T_i - T) - \frac{UA}{1+0.5UAF_c\rho_c c_{pc}}(T - T_c) + (-\Delta H_r)Vr \tag{15}$$

where the concentration of the reactant mixture ($C_i$) is :

$$C_i = \frac{F_a C_a + F_s C_s}{F_a + F_s} \tag{16}$$

the flow rate of the reactant mixture is $F=F_a+F_s$, the heat transfer coefficient is $UA=aF_c^{\ b}$.

The outlet temperature (T) and concentration (C) are controlled with PI controller by manipulating the inlet coolant flow rate ($F_c$) and the inlet reactant flow rate ($F_a$), respectively.

The parameters used to modelling and the controller parameters are given in Table 1.The process inputs, disturbances, and measurement noise are given in Table 2.

All the disturbances are constructed as first order autoregressive models, that is:

$$\begin{aligned} X(t) &= X_{set} + \Delta X(t) \\ \Delta X(t) &= \Delta X(t-1) + \sigma_e^2 e(t) \end{aligned} \tag{17}$$

where the e(t) is white noise and the $X_{set}$ indicates the set values. All of the measure variables are contaminated by white noise with different variances.

The initial conditions are: $T_i$=370.0K, $T_c$=365.0K, $F_c$=15($m^3$/min), T=368.25K, Fs= 0.9($m^3$/min),Fa=0.1($m^3$/min), C=0.8(kmol/$m^3$), $C_a$=19.1(kmol/$m^3$),$C_s$=0.3(kmol/$m^3$), $\beta_r$=1.0.

The simulation is run for 3000 min and the sampling frequency is 1sample/min. The samples of first 500 min are used to build the PCA model and the remaining 2500 samples are used to reform the test date set. The change of $\beta_r$ with a slope of 0.000002/min is added to the CSTR model. It represents a decrement of the reaction rate caused by slowdown of the stirring device which is common in practice.

A slow ramp fault with a slope of 0.01/min of the inlet concentration of solvent (Cs) is added after 2500min and a step change of Ca with amplitude 1 is added after 2750min.

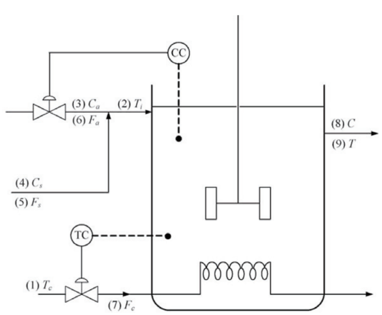


Fig. 5 CSTR process and 9 measured variables (1) coolant temperature (2)reactant mixture temperature (3) reactant A concentration(4)solvent concentration(5)solvent flow rate(6)solute flow rate(7)coolant flow rate(8)outlet concentration(9)outlet temperature

For simplicity, only the outlet concentration control is active in this simulation. For monitoring the process concerned with the control of outlet concentration, we choose 5 variables to build the PCA model which include outlet concentration C, reactant A flow rate Fa, solvent flow rate Fs, reactant A concentration Ca, solvent concentration Cs.

TABLE 1
THE PARAMETERS OF THE CSTR MODEL AND CONTROLLERS

| Notation | Parameters and constants | Value |
|---|---|---|
| V | Volume of reaction mixture in the tank | $1m^3$ |
| $\rho$ | Density of reaction mixture | $10^6 g/m^3$ |
| $\rho_c$ | Density of coolant | $10^6 g/m^3$ |
| $c_p$ | Specific heat capacity of reaction mixture | 1cal/(gK) |
| $c_{pc}$ | Specific heat capacity of coolant | 1cal/(gK) |
| $-\Delta H_r$ | Heat of reaction | $1.3\times10^7$cal/km |
| $k_0$ | Preexponential kinetic constant | ol |
| E/R | Activation energy/ideal gas constant | $10^{10} min^{-1}$ |
| a | Factor of the heat transfer coefficient | 8330K |
| b | Factor of the heat transfer coefficient | $1.681\times10^6$ |
| $P_c$ | The gain of the concentration controller | 0.5 |
| $\tau_c$ | The integral time of the concentration controller | 0.4825<br>2 |
| $P_T$ | The gain of the temperature controller | |
| $\tau_T$ | The integral time of the temperature controller | -1.5<br>5 |

TABLE 2
THE INPUTS, DISTURBANCES AND MEASUREMENTS

| Notation | Measurement noise $\sigma_m^2$ | Disturbance noise $\sigma_e^2$ | Autoregressive coefficient |
|---|---|---|---|
| T | $4\times10^{-4}$ | | |
| C | $2.5\times10^{-5}$ | | |
| $F_c$ | $1\times10^{-2}$ | | |
| $T_c$ | $2.5\times10^{-3}$ | $0.475\times10^{-1}$ | 0.2 |
| $T_i$ | $2.5\times10^{-3}$ | $0.475\times10^{-1}$ | 0.1 |
| $C_a$ | $1\times10^{-2}$ | $0.475\times10^{-1}$ | 0.2 |
| $F_a$ | $4\times10^{-6}$ | | |
| $C_s$ | $2.5\times10^{-5}$ | $1.875\times10^{-3}$ | 0.2 |
| $F_s$ | $4\times10^{-6}$ | $0.19\times10^{-2}$ | 0.1 |
| $\beta_r$ | | $0.0975\times10^{-2}$ | 0.05 |

Conventional PCA is applied first to CSTR model. The CPV method is adopted to choose the PCs with a threshold value 80%.The Q statistics obtained by conventional PCA are shown in Figure 6 and the $T^2$ statistics are shown in Figure 7. Obviously, the Q limit is violated between 1000-1500 samples although it is normal operation condition. The conventional PCA model isn't suitable for this simulation.

The N-steps remodeling PCA is applied to the CSTR process by 2 steps.

i) Calculate N with original training data and a fault date set formed by 500 samples which contaminated by the known slow ramp fault. In this simulation, the N is chosen as 265.
ii) Monitoring the process with N=265.

The results obtained by N-steps remodeling PCA are shown in Figure 8 and Figure 9. The performance of the N-Steps remodeling PCA algorithm is much better than the conventional PCA, and the value of N calculated by the proposed method is suitable for this process.

This simulation shows that the N-Step updating PCA algorithm can accommodate the slow change of the process to reduce the false alarm rate caused by the time variation.

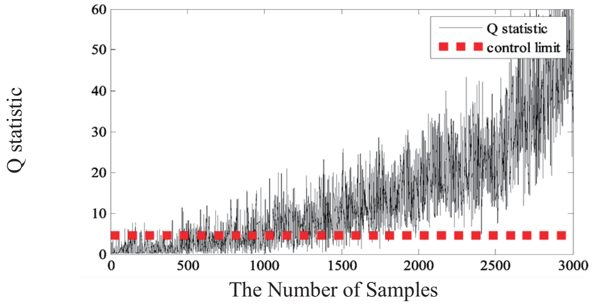


Fig. 6 The Q statistics obtained by conventional PCA for CSTR process

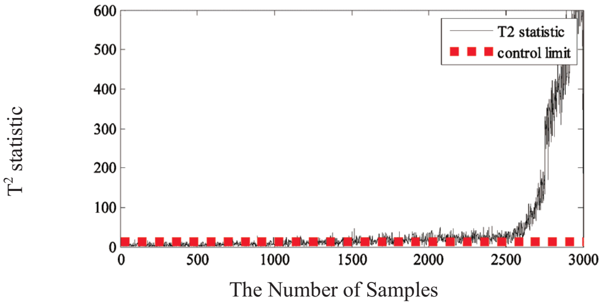


Fig. 7 The $T^2$ statistics obtained by conventional PCA for CSTR process

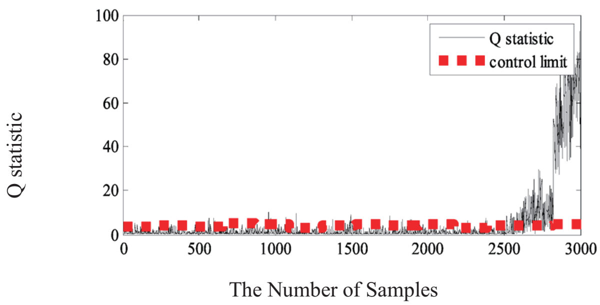


Fig. 8 The Q statistics obtained by N-steps updating PCA for CSTR process

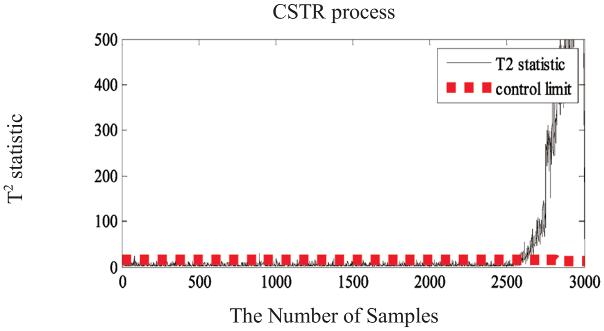


Fig. 9 The $T^2$ statistics obtained by N-steps updating PCA for CSTR process

Meanwhile, it can detect both of the slow ramp fault and step fault efficiently.

In summary, these simulations demonstrate that the proposed model update approach, N-Steps updating PCA, is very effective to adaptive process monitoring.

## V. Conclusion

This paper brought forward a model updating approach for multivariate statistical process monitoring.. It is a new method of adaptive multivariate statistical process control. Furthermore, the method of calculating updating interval N has also been discussed. The upper limit for N is determined by the time variability of the process and the lower limit is determined by the known slow ramp faults. The complete monitoring scheme is demonstrated by both of the mathematic example and the CSTR process. The results of the simulations show that the N-steps updating approach can accommodate the slow change of the process and detect both of the slow ramp fault and step fault efficiently.

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