Journal of the Taiwan Institute of Chemical Engineers 41 (2010) 475–481

Contents lists available at ScienceDirect

Journal of the Taiwan Institute of Chemical Engineers

journal homepage: www.elsevier.com/locate/jtice

Adaptive process monitoring using efficient recursive PCA and moving window PCA algorithms

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ARTICLE INFO

Article history:
Received 6 January 2010
Received in revised form 9 March 2010
Accepted 11 March 2010

Keywords:
Adaptive process monitoring
Fault detection
Recursive PCA
Moving window PCA
Rank-one matrix update

ABSTRACT

In process monitoring, principal component analysis (PCA) is a very popular method and has found wide applications. Conventionally, a fixed PCA model is used for monitoring. This paper presents the use of both recursive PCA (RPCA) and moving window PCA (MWPCA) to online update the PCA model and its corresponding control limits for monitoring statistics. An efficient algorithm is derived based on rank-one matrix update of the covariance matrix, which is tailored for RPCA and MWPCA computations. By the proposed method, the performance of process monitoring can be improved in two aspects. First, more consistent PCA model and control limits for monitoring statistics are resulted because of the increasing number of normal observations for modeling. Second, for parameter-varying processes, when natural drifting behavior or changing of operation region is acceptable, more reasonable PCA model and control limits for monitoring statistics are obtained in an adaptive manner. Simulation results have shown the effectiveness of the proposed approaches compared to the conventional PCA and RPCA methods.

1. Introduction

Statistical process monitoring (SPM) is a widely used technique for fault diagnosis of chemical processes to improve process quality and productivity. The principal component analysis (PCA) is a most popular method for this purpose (MacGregor and Kourti, 1995; Wise and Gallagher, 1996). The basic strategy of PCA is to discard the noise and collinearity between process variables, while preserving the most important information of the original data set. To use PCA for process monitoring, a PCA model is first established based on collected process data under normal operating. Then, the control limits of monitoring statistics (e.g. T^2, Q) are calculated and thus the process can be online monitored by these statistics (Jackson, 1991).

Many successful applications of PCA for process monitoring have been reported in the literature (MacGregor and Kourti, 1995; Raich and Cinar, 1995). Despite its tremendous success, conventional PCA-based monitoring technique has a few major drawbacks. One is that normal operating data may be insufficient when the process monitoring is started. Since the confidence limits of monitoring statistics are obtained from a statistical manner, the number of normal observations would be the more the better. It is thus desirable that the new observation, once found normal, is augmented into the normal data set to modify the confidence limits, making them more consistent. The other drawback is the inability to deal with processes with time-varying parameters, where it interprets the natural changes in the process as fault. The PCA-based monitoring with fixed-model may lead to numerous false alarms. Thus, updating the PCA model to make it more representative of the current process status is necessary.

Constructing the PCA model requires computation of singular value decomposition (SVD) or eigen-decomposition (Jackson, 1991), so the computational load is usually heavy and not practical for online applications. Therefore, a recursive PCA (RPCA) algorithm is preferred to update the PCA model efficiently. Once a new observation becomes available, it offers efficient computation by updating the PCA model using the previous model rather than completely building it from the whole data set. Wold (1994) proposed the use of exponentially weighted moving average (EWMA) filter for updating of PCA and partial least squares (PLS) models. Li *et al.* (2000) proposed two recursive PCA algorithms for sample-wise and block-wise recursions. Notice that the data on which the PCA model is updated is ever-growing. Such recursive approaches have also been applied in adaptive statistical process control (Choi *et al.*, 2006; He and Yang, 2008; Jin *et al.*, 2006).

However, most industrial processes are time-varying, so that the older samples are not representative of the current process status. Thus, RPCA may be difficult to implement in practice because it leads to a reduction in the speed of model adaptation as the data size increases. Although a forgetting factor can be introduced to down-weight older samples, the selection of this factor is difficult without a priori knowledge of likely conditions

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doi:10.1016/j.jtice.2010.03.015

(Wang *et al.*, 2005). As a result, recursion with a window sliding along the data, i.e. including the newest sample and excluding the oldest one, is more appropriate for time-varying processes. This adaptation approach is so-call as moving window PCA (MWPCA). Wang *et al.* (2005) proposed a fast moving window PCA scheme for process monitoring, where only the recursive update of the correlation matrix was presented but the efficient algorithm for updating PCA model was not addressed. Recently, Liu *et al.* (2009) proposed the moving window kernel PCA for adaptive monitoring of nonlinear process. Although the MWPCA approach can be used for monitoring time-varying processes, it will encounter difficulty in the case of only limited samples available to initialize the monitoring procedure.

Motivated by the difficulties encountered when RPCA or MWPCA is solely implemented for process monitoring, the study reported in this paper focuses on developing a novel adaptive monitoring scheme for time-varying processes by taking advantage of both RPCA and MWPCA. Efficient algorithms for RPCA and MWPCA to online update the PCA model is derived based on rank-one matrix update of the covariance matrix (Erdogus *et al.*, 2004), and these algorithms can be implemented for the sample-wise and moving window recursions. Consequently, a complete system for online adaptive process monitoring, which combines the RPCA and MWPCA algorithms, is proposed.

The paper is organized as follows. In Section 2, the preliminaries about the conventional PCA and its drawbacks are provided. The efficient algorithms to recursively update the PCA model for RPCA and MWPCA are illustrated in Sections 3 and 4, respectively. Section 5 presents the complete adaptive process monitoring procedures. The performance of the proposed monitoring scheme is demonstrated through simulation examples in Section 6. Finally, conclusions are drawn in Section 7.

2. Conventional PCA-based process monitoring

PCA involves the decomposition of a data matrix $\mathbf{X} \in \mathbb{R}^{N \times M}$, which contains N regular-sampled observations of M process variables and is typically mean-centered, into a transformed subspace of reduced dimension. This subspace is defined by the span of a chosen subset of the eigenvectors of the covariance or correlation matrix associated with $\mathbf{X}$. Each chosen eigenvector, or principal component (PC), captures the maximum amount of variability in the data in an ordered fashion. In other words, the first PC explains the greatest amount of variation, and the second explains the next largest amount after removal of the first, and so on. In this way, PCA forms the basis of multivariate data analysis (Jackson, 1991). Mathematically, the decomposition is defined as follows:

$$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E} = \hat{\mathbf{X}} + \mathbf{E} \tag{1}$$

The projection of $\mathbf{X}$ onto loadings (PCs), $\mathbf{P}$, generates a set of scores, $\mathbf{T}$, that are linearly independent. Usually, only first few dominant PCs are selected in $\mathbf{P}$ and the residual matrix, $\mathbf{E}$, is thus resulted. In this paper, the covariance matrix, $\mathbf{S}$, defined as the following is used to derive a PCA model.

$$\mathbf{S} = \frac{1}{N-1}\mathbf{X}^T\mathbf{X} \tag{2}$$

The columns of $\mathbf{P}$ are actually eigenvectors of $\mathbf{S}$ associated with the n_{pc} largest eigenvalues $(\lambda_1, \lambda_2, \cdots, \lambda_{n_{pc}})$, converting the calculation of PCA model to an eigen-decomposition problem. Alternatively, matrix $\mathbf{X}$ can also be decomposed using singular value decomposition (SVD) to build the PCA model.

Using PCA to perform process monitoring, an observation vector $\mathbf{x}$ is projected with the help of PCA model to either the predicted or the residual subspace. Two statistics, Hotelling T^2 and squared prediction error (SPE or Q), are developed based on these projections and are often used for monitoring. The T^2 statistic is a scaled 2-norm of a score vector, $\mathbf{t}$, in the principal component (predicted) subspace, and Q statistic is a 2-norm of a residual vector in the residual subspace. They are given by

$$T^2 = \mathbf{t}^T\boldsymbol{\Lambda}^{-1}\mathbf{t} = \mathbf{x}^T\mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{P}^T\mathbf{x} \tag{3}$$

$$Q = \mathbf{e}^T\mathbf{e} = \mathbf{x}^T\left(\mathbf{I}\text{-}\mathbf{P}\mathbf{P}^T\right)\mathbf{x} \tag{4}$$

where $\boldsymbol{\Lambda} = \mathrm{diag}\left[\lambda_1 \quad \lambda_2 \quad \cdots \quad \lambda_{n_{pc}}\right]$. Therefore, this allows scalar thresholds to qualify for process status. The approximated control limits of T^2 and Q statistics, with a confidence level α, can be determined from the normal operating data in several ways by applying the probability distribution assumptions (Jackson and Mudholkar, 1979; Kourti and MacGregor, 1995; Nomikos and MacGregor, 1995). These control limits are given as:

$$T_\alpha^2 = \frac{n_{pc}(N^2-1)}{N(N-n_{pc})}F_\alpha(n_{pc}, N-n_{pc}) \tag{5}$$

$$Q_\alpha = \theta_1\left(\frac{c_\alpha h_0\sqrt{2\theta_2}}{\theta_1} + 1 + \frac{\theta_2 h_0(h_0-1)}{\theta_1^2}\right)^{1/h_0} \tag{6}$$

where $F_\alpha(n_{pc}, N-n_{pc})$ is the upper limit of α percentile of the F-distribution with degree of freedoms n_{pc} and $N-n_{pc}$, c_α is the normal deviate corresponding to the $(1-\alpha)$ percentile, and

$$\begin{aligned} h_0 &= 1 - \frac{2\theta_1\theta_3}{3\theta_2^2} \\ \theta_i &= \sum_{j=n_{pc}+1}^{M}\lambda_j^i; \quad i = 1,2,3 \end{aligned} \tag{7}$$

As a result, the process behavior is considered faulty if the statistic of a new observation exceeds the control limit.

Conventionally, the PCA model and the control limits mentioned above are fixed during online process monitoring. However, the confidence limits are obtained from a statistical manner so that the number of normal observations should be sufficiently large to result in consistent thresholds. For the purpose of process monitoring, abundant normal data may not be available to establish the PCA model in the initial stage. It is thus desirable that the new normal observation is augmented into the normal data set sample by sample in order to modify the control limits recursively. On the other hand, when slow and natural changes occur in the process, a fixed-model monitoring approach will lead to numerous false alarms since the PCA model is no longer representative of current process status. Therefore, the PCA model has to be updated along a moving data window to capture the time-varying behavior of the process. In the next two sections, efficient algorithms to compute the eigen-decomposition of covariance matrix for RPCA and MWPCA are presented, which will in term applied for adaptive process monitoring.

3. Sample-wise recursive PCA algorithm

During the past decades, recursive eigen-decomposition technique has become an interested subject in the field of signal processing. In this study, the recursive eigen-decomposition algorithm based on first-order perturbation (FOP) that first proposed by Champagne (1994) and modified by Erdogus *et al.* (2004) is applied to estimate the corresponding eigenvalues and eigenvectors recursively. The main advantages of this procedure are computationally efficient and easy to be implemented.

FOP-based recursive calculation of eigen-decomposition implicitly updates the covariance matrix, and there are two main tasks in this recursive procedure. In the first step, current covariance matrix should be formulated as the rank-one update of the previous one with an available observation. Secondly, the first-order perturbation method is applied to estimate the eigenvalue and eigenvector matrices for the current covariance structure.

Denote $\mathbf{X}_k = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \cdots \quad \mathbf{x}_k]^T$ as the initial mean-centered data matrix. As a new observation $\mathbf{x}_{k+1}$ becomes available, the recursive calculation of the covariance matrix, assuming the mean value unchanged for simplicity, is given as

$$\mathbf{S}_{k+1} = \frac{1}{k}\sum_{i=1}^{k+1}\mathbf{x}_i\mathbf{x}_i^T = \frac{k-1}{k}\mathbf{S}_k + \frac{1}{k}\mathbf{x}_{k+1}\mathbf{x}_{k+1}^T \tag{8}$$

The recursive calculation of $\mathbf{S}_{k+1}$ by considering the update of mean value will be provided later. Let the eigen-decompositions of the covariance matrix be

$$\begin{aligned}\mathbf{S}_{k+1} &= \mathbf{P}_{k+1}\boldsymbol{\Lambda}_{k+1}\mathbf{P}_{k+1}^T \\ \mathbf{S}_k &= \mathbf{P}_k\boldsymbol{\Lambda}_k\mathbf{P}_k^T\end{aligned} \tag{9}$$

where $\mathbf{P}$ and Λ denote the eigenvector and eigenvalue matrices, respectively. By defining $\boldsymbol{\alpha}_{k+1} = \mathbf{P}_k^T\mathbf{x}_{k+1}$, and substituting this definition and Eq. (9) into Eq. (8), the following recursive formula for matrices $\mathbf{P}$ and Λ are obtained.

$$\mathbf{P}_{k+1}(k\boldsymbol{\Lambda}_{k+1})\mathbf{P}_{k+1}^T = \mathbf{P}_k\left[(k-1)\boldsymbol{\Lambda}_k + \boldsymbol{\alpha}_{k+1}\boldsymbol{\alpha}_{k+1}^T\right]\mathbf{P}_k^T \tag{10}$$

Also, apply eigen-decomposition to the matrix $[(k-1)\boldsymbol{\Lambda}_k + \boldsymbol{\alpha}_{k+1}\boldsymbol{\alpha}_{k+1}^T]$ as

$$\left[(k-1)\boldsymbol{\Lambda}_k + \boldsymbol{\alpha}_{k+1}\boldsymbol{\alpha}_{k+1}^T\right] = \mathbf{V}_{k+1}\mathbf{D}_{k+1}\mathbf{V}_{k+1}^T \tag{11}$$

Substituting Eq. (11) into Eq. (10), the recursive update rules for eigenvectors and eigenvalues, i.e. the PCA model, are determined as

$$\begin{aligned}\mathbf{P}_{k+1} &= \mathbf{P}_k\mathbf{V}_{k+1} \\ \boldsymbol{\Lambda}_{k+1} &= \frac{\mathbf{D}_{k+1}}{k}\end{aligned} \tag{12}$$

Let $\mathbf{D}_{k+1} = \boldsymbol{\Lambda}_k + \mathbf{Q}_{\boldsymbol{\Lambda},k+1}$ and $\mathbf{V}_{k+1} = \mathbf{I} + \mathbf{Q}_{\mathbf{V},k+1}$, where $\mathbf{Q}_{\boldsymbol{\Lambda},k+1}$ and $\mathbf{Q}_{\mathbf{V},k+1}$ are small perturbation matrices, and $\mathbf{Q}_{\boldsymbol{\Lambda},k+1}$ is naturally diagonal. Thus, the recursive algorithm of Eq. (12) is transformed into the problem of finding $\mathbf{Q}_{\boldsymbol{\Lambda},k+1}$ and $\mathbf{Q}_{\mathbf{V},k+1}$. By some derivation (Erdogus *et al.*, 2004), the ith diagonal entry of $\mathbf{Q}_{\boldsymbol{\Lambda},k+1}$ is found as α_i^2, and the (i, j)th entry of $\mathbf{Q}_{\mathbf{V},k+1}$ is given by

$$\mathbf{Q}_{\mathbf{V},k+1}(i,j) = \begin{cases} 0 & \text{for } i = j \\ \dfrac{\alpha_i\alpha_j}{\lambda_j + \alpha_j^2 - \lambda_i - \alpha_i^2} & \text{for } i \neq j \end{cases} \tag{13}$$

where α_i is the ith element of α_{k+1} and λ_i is the (i, i)th element of Λ_k. Sometimes, the algorithm may become unstable when two successive eigenvalues get very close. A stabilization mechanism of the following has been found effective to prevent this undesirable behavior:

$$\begin{aligned}\mathbf{Q}_{\mathbf{V},k+1}(i,j) &= \frac{\alpha_i\alpha_j}{\max\left(\delta\lambda_1, \lambda_j + \alpha_j^2 - \lambda_i - \alpha_i^2\right)} \quad \text{if } i > j \\ \mathbf{Q}_{\mathbf{V},k+1}(i,j) &= \frac{\alpha_i\alpha_j}{\min\left(-\delta\lambda_1, \lambda_j + \alpha_j^2 - \lambda_i - \alpha_i^2\right)} \quad \text{if } i < j\end{aligned} \tag{14}$$

where δ is a small positive number.

Notice that it is assumed the mean values of these variables are constant in Eq. (8). In fact, the mean value of $\mathbf{X}_{k+1}$, i.e. $\mathbf{b}_{k+1}$, can also be updated by the following recursive relation:

$$\mathbf{b}_{k+1} = \frac{k}{k+1}\mathbf{b}_k + \frac{1}{k+1}\mathbf{x}_{k+1}^0 \tag{15}$$

where the superscript "0" denotes the original observation (not mean-centered). The recursive representation of $\mathbf{X}_{k+1}$ is given by

$$\mathbf{X}_{k+1} = \begin{bmatrix}\mathbf{X}_k - \mathbf{1}\,\Delta\mathbf{b}_{k+1}^T \\ \mathbf{x}_{k+1}^T\end{bmatrix} \tag{16}$$

where $\Delta\mathbf{b}_{k+1} = \mathbf{b}_{k+1} - \mathbf{b}_k$, and $\mathbf{1} = [1 \quad 1 \quad \cdots \quad 1]^T \in \mathbb{R}^k$. Substituting Eq. (16) into the definition of covariance matrix (Eq. (2)) yields

$$\begin{aligned}\mathbf{S}_{k+1} &= \frac{1}{k}\mathbf{X}_{k+1}^T\mathbf{X}_{k+1} \\ &= \frac{1}{k}\left(\mathbf{X}_k^T\mathbf{X}_k - 2\Delta\mathbf{b}_{k+1}\mathbf{1}^T\mathbf{X}_k + \Delta\mathbf{b}_{k+1}\mathbf{1}^T\mathbf{1}\Delta\mathbf{b}_{k+1}^T + \mathbf{x}_{k+1}\mathbf{x}_{k+1}^T\right)\end{aligned} \tag{17}$$

By the facts of $\mathbf{X}_k^T\mathbf{X}_k = (k-1)\mathbf{S}_k$, $\mathbf{1}^T\mathbf{X}_k = 0$ and $\mathbf{1}^T\mathbf{1} = k$, Eq. (17) results the following recursive calculation of covariance matrix:

$$\mathbf{S}_{k+1} = \frac{k-1}{k}\mathbf{S}_k + \frac{1}{k}\mathbf{x}_{k+1}\mathbf{x}_{k+1}^T + \Delta\mathbf{b}_{k+1}\Delta\mathbf{b}_{k+1}^T \tag{18}$$

Eq. (18) indicates that $\mathbf{S}_{k+1}$ is two rank-one modifications from $\mathbf{S}_k$. Consequently, the procedure of rank-one update presented above has to be performed twice to estimate the eigenvalue and eigenvector matrices for the current covariance matrix.

4. Moving Window PCA algorithm

When slow and natural process changes occur in the processes, it is suitable to update the PCA model by a moving window because the old data cannot represent the current status of the process. That is, the newest sample is augmented to the data matrix and the oldest sample is discarded, keeping a fixed number of samples in the data matrix (i.e. fixed window size).

Let the kth data matrix with window size N be $\mathbf{X}_k = [\mathbf{x}_{k-N+1} \quad \mathbf{x}_{k-N+2} \quad \cdots \quad \mathbf{x}_k]^T$, and the next data matrix would be $\mathbf{X}_{k+1} = [\mathbf{x}_{k-N+2} \quad \mathbf{x}_{k-N+3} \quad \cdots \quad \mathbf{x}_{k+1}]^T$. These two data matrices share a transient data matrix of $\tilde{\mathbf{X}} = [\mathbf{x}_{k-N+2} \quad \mathbf{x}_{k-N+3} \quad \cdots \quad \mathbf{x}_k]^T$. A two-step adaptation, as shown in Fig. 1, is used to recursively update the covariance matrix. First, with eliminating the oldest sample from $\mathbf{X}_k$, the mean vector and covariance matrix associated with $\tilde{\mathbf{X}}$ can be represented in terms of $\mathbf{b}_k$ and $\mathbf{S}_k$ as:

$$\tilde{\mathbf{b}} = \frac{N}{N-1}\mathbf{b}_k - \frac{1}{N-1}\mathbf{x}_{k-N+1}^0 \tag{19}$$

$$\tilde{\mathbf{S}} = \frac{N-1}{N-2}\left(\mathbf{S}_k - \frac{1}{N-1}\mathbf{x}_{k-N+1}\mathbf{x}_{k-N+1}^T - \Delta\tilde{\mathbf{b}}_k\Delta\tilde{\mathbf{b}}_k^T\right) \tag{20}$$

where $\Delta\tilde{\mathbf{b}}_k = \mathbf{b}_k - \tilde{\mathbf{b}}$. With $\tilde{\mathbf{b}}$ and $\tilde{\mathbf{S}}$, the recursive relations of mean vector and covariance matrix associated with $\mathbf{X}_{k+1}$ are obtained similar to those mentioned in the RPCA algorithm. That is,

$$\mathbf{b}_{k+1} = \frac{N-1}{N}\tilde{\mathbf{b}} + \frac{1}{N}\mathbf{x}_{k+1}^0 \tag{21}$$

$$\mathbf{S}_{k+1} = \frac{N-2}{N-1}\tilde{\mathbf{S}} + \frac{1}{N-1}\mathbf{x}_{k+1}\mathbf{x}_{k+1}^T + \Delta\tilde{\mathbf{b}}_{k+1}\Delta\tilde{\mathbf{b}}_{k+1}^T \tag{22}$$

where $\Delta\tilde{\mathbf{b}}_{k+1} = \mathbf{b}_{k+1} - \tilde{\mathbf{b}}$. Finally, by substituting Eq. (20) into Eq. (22), the recursive calculation of covariance matrix in a moving window scheme is given as

$$\begin{aligned}\mathbf{S}_{k+1} = \mathbf{S}_k &- \frac{1}{N-1}\mathbf{x}_{k-N+1}\mathbf{x}_{k-N+1}^T - \Delta\tilde{\mathbf{b}}_k\Delta\tilde{\mathbf{b}}_k^T + \frac{1}{N-1}\mathbf{x}_{k+1}\mathbf{x}_{k+1}^T \\ &+ \Delta\tilde{\mathbf{b}}_{k+1}\Delta\tilde{\mathbf{b}}_{k+1}^T\end{aligned} \tag{23}$$

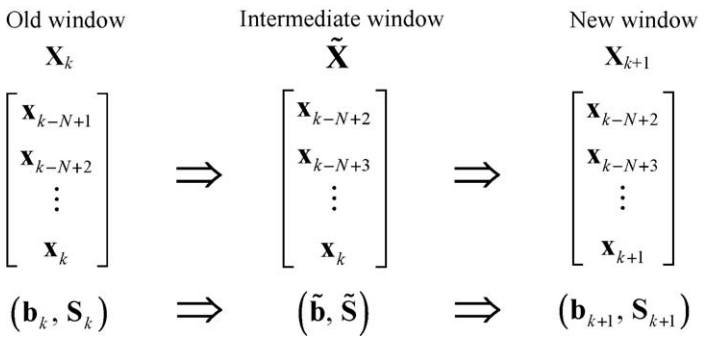

Fig. 1. Two-step adaptation for recursive update data window and covariance matrix.

Eq. (23) indicates that $\mathbf{S}_{k+1}$ is four rank-one modifications from $\mathbf{S}_k$. Consequently, the procedure of rank-one update presented previously can be performed four times to estimate the eigenvalue and eigenvector matrices for the current covariance matrix.

5. Adaptive process monitoring procedures

With the presented recursive RPCA and MWPCA algorithms, an adaptive process monitoring scheme can be implemented in real-time. A sufficient large number of normal observations necessary to obtain consistent thresholds for monitoring statistics, denoted as N_t, has to be prescribed preliminarily. The selection of N_t can depend on the number of process variable and the range of operation region. When the initial size of normal observations is less than N_t, RPCA is applied for process monitoring. Once the data size grows up to N_t, the adaptation mechanism is shifted to MWPCA in order to capture the time-varying behavior of process. A complete implementation of RPCA or MWPCA also requires recursive determination of the number of significant principal components. There are many approaches of determining the number of PCs, but not all the approaches are suitable for recursive implementation (Li *et al.*, 2000). In this study, the cumulative percent variance (CPV) method (Malinowski, 1991), which has been usually applied in literature (e.g. Choi *et al.*, 2006) for the determination of the number of PCs, is used. The CPV is a measure of the percent variance explained by the first n_{pc} PCs:

$$\mathrm{CPV}(n_{pc}) = \frac{\sum_{i=1}^{n_{pc}} \lambda_i}{\sum_{i=1}^{M} \lambda_i} \times 100\% \tag{24}$$

The number of PCs is chosen such that CPV reaches a predetermined value, e.g. 95%.

The complete adaptive monitoring procedures are summarized as follows.

1. Set a value of N_t.
2. For an initial data matrix $\mathbf{X}_k$ with N observations, calculate $\mathbf{P}_k$, $n_{pc,k}$, $\boldsymbol{\Lambda}_k$, $T^2_{\alpha,k}$, and $Q_{\alpha,k}$.
3. Collect new data sample $\mathbf{x}_{k+1}$ and calculate T^2_{k+1} and Q_{k+1} by:

$$T^2_{k+1} = \mathbf{x}^T_{k+1}\mathbf{P}_k\boldsymbol{\Lambda}_k^{-1}\mathbf{P}_k^T\mathbf{x}_{k+1} \tag{25}$$

$$Q_{k+1} = \mathbf{x}^T_{k+1}\left(\mathbf{I}-\mathbf{P}_k\mathbf{P}_k^T\right)\mathbf{x}_{k+1} \tag{26}$$

4. If $T^2_{k+1} > T^2_{\alpha,k}$ or $Q_{k+1} > Q_{\alpha,k}$ for the last samples (i.e., three consecutive out of control samples), the model updating is terminated and an alarm is triggered. Further fault isolation may be conducted.
5. When no process alarms have occurred, update the PCA model based on the new sample $\mathbf{x}_{k+1}$ as follows. If $N < N_t$, calculate $\mathbf{P}_{k+1}$, $n_{pc,k+1}$, and $\boldsymbol{\Lambda}_{k+1}$ using RPCA algorithm, and set $N = N + 1$. Otherwise, if $N \geq N_t$, calculate $\mathbf{P}_{k+1}$, n_{pc}, and $\boldsymbol{\Lambda}_{k+1}$ using MWPCA algorithm. Then, calculate the updated control limits, $T^2_{\alpha,k+1}$ and $Q_{\alpha,k+1}$ using Eqs. (5) and (6), respectively. Set $k = k + 1$ and go to step 3.

6. Simulation examples

The proposed adaptive process monitoring schemes is now applied to simulation examples to demonstrate its effectiveness.

6.1. Mathematical example

Consider a 4×2 linear dynamic process as follows:

$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \mathbf{B}\mathbf{u}_k = \begin{bmatrix} 0.67 & 0.67 & 0 & 0 \\ -0.67 & -0.67 & 0.67 & 0 \\ -0.67 & 0.67 & 0.67 & -0.67 \\ 0.67 & -0.67 & 0 & -0.67 \end{bmatrix}\mathbf{x}_k + \begin{bmatrix} 0.66 & 1.55 \\ 1.97 & 2.38 \\ 4.32 & -0.73 \\ -2.64 & 3.26 \end{bmatrix}\mathbf{u}_k$$

$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{e}_k + \boldsymbol{\mu}_k = \begin{bmatrix} -0.67 & -2.66 & 0.61 & 1.74 \\ 2.51 & -1.28 & 0.25 & -1.40 \\ -0.39 & 3.27 & -1.50 & 0.76 \\ -1.33 & 1.43 & 1.26 & -0.93 \end{bmatrix}\mathbf{x}_k + \mathbf{e}_k + \boldsymbol{\mu}_k \tag{27}$$

where $\mathbf{x}_k \in \mathbb{R}^4$ and $\mathbf{y}_k \in \mathbb{R}^4$ are state and process output, respectively. The process input $\mathbf{u}_k \in \mathbb{R}^2$ and noise $\mathbf{e}_k \in \mathbb{R}^4$ are assumed as Gaussian distribution with $\mathbf{u}_k \sim (0, 0.2^2)$ and $\mathbf{e}_k \sim (0, 0.1^2)$. Six process variables (two inputs and four outputs) are measured. The vector $\boldsymbol{\mu}_k \in \mathbb{R}^4$ is used to represent the operating center of the process output, and it is assumed as $\boldsymbol{\mu}_k = \mathbf{1}$ for normal process operation.

In the first simulation case, with an initial data size of 50, the RPCA algorithm is applied to recursively calculate the control limits of $Q_{0.95,k}$ and $Q_{0.99,k}$ until a data size of 500 is reached. The number of significant PCs is selected by using CPV method, such that the variance explained is approximately 98% of the total variance. After 100 runs of simulation, the variances of $Q_{0.95,k}$ and $Q_{0.99,k}$ for different data size k are plotted in Fig. 2. It can be seen that a more consistent control limit (smaller variance) could be resulted when the data size becomes larger.

In the second simulation case, the proposed adaptive monitoring procedures will be demonstrated. The value of N_t is set as 300. The first 100 samples were utilized to build the initial PCA model, and the adaptive monitoring is started. The following three scenarios are considered.

- S1: The input variable u_1 slowly drifts away from the normal operating condition ($u^*_{1,k}$) from time, $k = 351$ to $k = 700$ by the

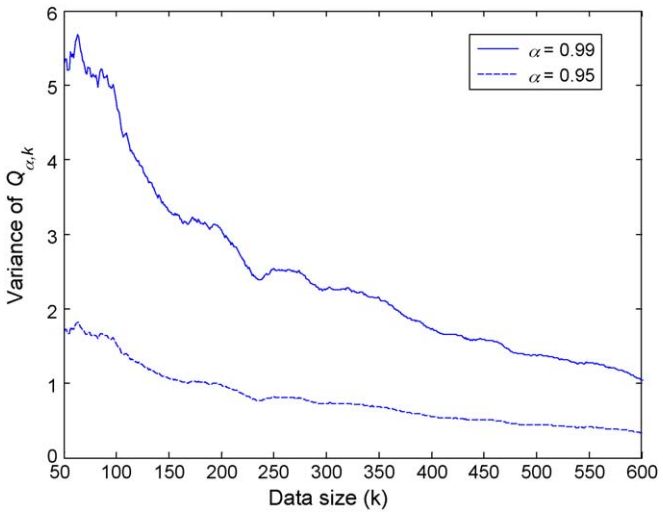

Fig. 2. Variances of confidence limits for Q statistic under different data size.

following relation:

$$u_{1,k} = u^*_{1,k} + 0.008(t - 350) \quad (28)$$

- S2: The operating center also drifts from time, k = 501 to k = 700 by a first-order autoregressive model of the following form:

$$\boldsymbol{\mu}_{k+1} = 1.004\,\boldsymbol{\mu}_k + \boldsymbol{\varepsilon}_k \quad (29)$$

where $\boldsymbol{\varepsilon}_k \sim (0, 0.001^2)$.

- S3: From time k = 801, a process fault is introduced such that the system matrix **C** changes to –**C**.

The drifting behaviors in scenarios S1 and S2 are reflective of normal process changes such as catalyst deactivation or equipment fouling, while scenario S3 represents a fault.

The monitoring statistics obtained by the proposed monitoring method are shown in Fig. 3. The PCA model is updated by RPCA algorithm until the data size grows up to 300, so that the number of false alarms is reduced at time interval [201,300] in Fig. 3, compared to that at time interval [1,100]. From time k = 301, the PCA model is updated by MWPCA algorithm and the monitoring charts show that the process remains in control after the drifting has been introduced. After time point k = 801, it is found that the monitoring indices continuously exceed their thresholds, which

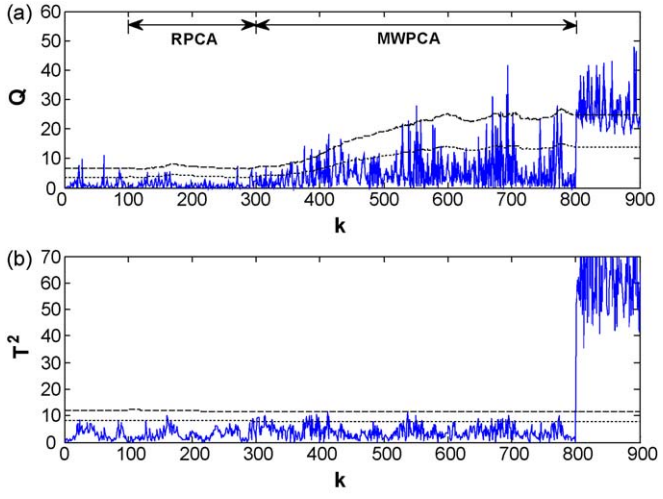

Fig. 3. Monitoring charts for proposed method (RPCA + MWPCA). (a) Q statistic and (b) T^2 statistic (dashed-line: 99% confidence limit; dotted-line: 95% confidence limit).

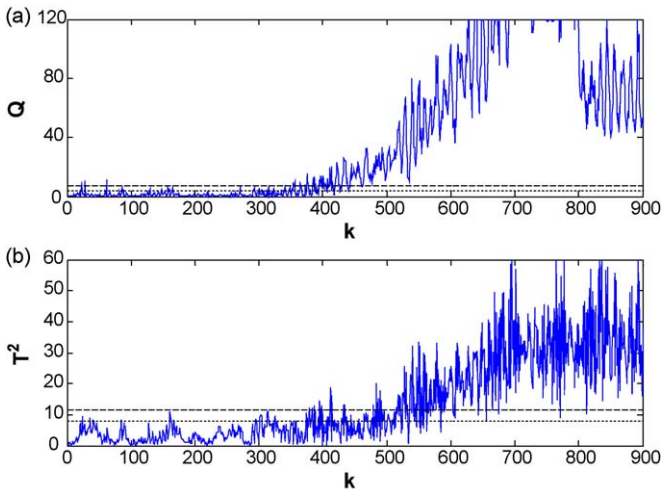

Fig. 4. Monitoring charts for conventional PCA. (a) Q statistic and (b) T^2 statistic (dashed-line: 99% confidence limit; dotted-line: 95% confidence limit).

indicates a fault has been successfully detected. Consequently, the model updating is terminated. Although the adaptation of the PCA model accommodates to the slow process changes, the proposed monitoring system is still able to detect abnormal behavior of the process.

For comparison, the monitoring statistics obtained by the conventional PCA and the RPCA methods are shown in Figs. 4 and 5, respectively. The conventional PCA method without model updating, where the first 300 samples are used to build the PCA model, is no longer valid after the process begins to change at time point k = 351. On the other hand, the performance of RPCA method is better than that of conventional PCA method. However, Fig. 5 shows that, after the process drifting introduced, the number of false alarms begins to increase as the data size becomes larger, because RPCA leads to a slower speed of model adaptation than MWPCA. It is evident that the proposed approach, which combines the RPCA and MWPCA algorithms, is very effective for adaptive process monitoring.

6.2. Simulated CSTR process

A nonisothermal CSTR process (Yoon and MacGregor, 2001; Choi *et al.*, 2006) is considered for the application of the proposed

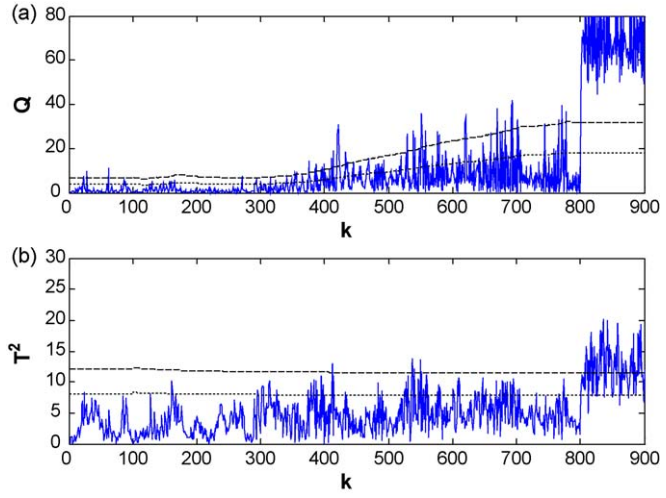

Fig. 5. Monitoring charts for RPCA. (a) Q statistic and (b) T^2 statistic (dashed-line: 99% confidence limit; dotted-line: 95% confidence limit).

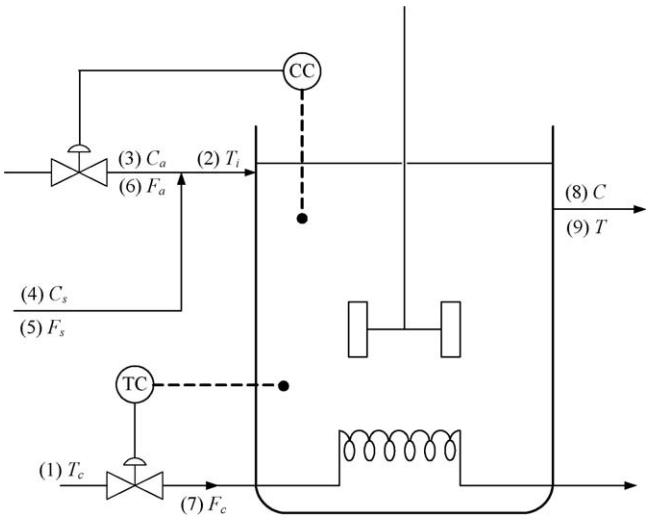

Fig. 6. Nonisothermal CSTR process and nine measured variables: (1) coolant temperature, (2) reactant mixture temperature, (3) reactant A concentration, (4) solvent concentration, (5) solvent flow rate, (6) solute flow rate, (7) coolant flow rate, (8) outlet concentration, and (9) outlet temperature.

adaptive process monitoring method. The schematic diagram of the process is given in Fig. 6. In the CSTR, reactant A is premixed with a solvent, and then it was converted into product B with a first-order reaction rate

$$r = \beta_r k_0 e^{-E/RT} C \tag{30}$$

The dynamics of the process is described as follows:

$$V\frac{dC}{dt} = F(C_i - C) - V r \tag{31}$$

$$V\rho c_p \frac{dT}{dt} = \rho c_p F(T_i - T) - \frac{\mathrm{UA}}{1 + 0.5\mathrm{UA}F_c\rho_c c_{pc}}(T - T_c) + (-\Delta H_r)Vr \tag{32}$$

The concentration of the reactant mixture is calculated by

$$C_i = \frac{F_a C_a + F_s C_s}{F_a + F_s} \tag{33}$$

The outlet temperature (T) and concentration (C) are controlled with PI controllers by manipulating the inlet coolant flow rate (F_c) and the inlet reactant flow rate (F_a), respectively. The model and controller parameters are given in Table 1. All process inputs and disturbances are generated using normally distributed random signal. In addition, all measured variables are contaminated with white noise (see Table 2).

Table 1
Model parameters used in the CSTR modeling and the PI controller parameters.

Notation	Parameters and constants	Value
V	Volume of reaction mixture in the tank	$1\,m^3$
ρ	Density of reaction mixture	$10^6\,g/m^3$
ρ_c	Density of coolant	$10^6\,g/m^3$
c_p	Specific heat capacity of the reaction mixture	$1\,cal/(g\,K)$
c_{pc}	Specific heat capacity of the coolant	$1\,cal/(g\,K)$
ΔH_r	Heat of reaction	$-1.3\times10^7\,cal/kmol$
k_0	Preexponential kinetic constant	$10^{10}\,min^{-1}$
E/R	Activation energy/ideal gas constant	8330 K
UA	Heat transfer coefficient	6.5×10^6
$K_c(T)$	Temperature controller gain	−1.5
$\tau_I(T)$	Integral time	5
$K_c(T)$	Concentration controller gain	0.4825
$\tau_I(C)$	Integral time	2

Table 2
Mean and variance of process inputs, disturbance, and measurement noise.

Input and disturbance			Measurements		
Variable	Mean	Variance	Variable		Variance
F_s	$0.9\,m^3/min$	1.90×10^{-1}	(1)	T_c	2.5×10^{-2}
T_i	370 K	4.75×10^{-1}	(2)	T_i	2.5×10^{-2}
T_c	365 K	4.75×10^{-1}	(3)	C_a	1.0×10^{-1}
C_a	$17.3\,kmol/m^3$	4.75×10^{-1}	(4)	C_s	2.5×10^{-4}
C_s	$0.3\,kmol/m^3$	1.875×10^{-2}	(5)	F_s	4.0×10^{-5}
β_r	1	1.90×10^{-3}	(6)	F_a	4.0×10^{-5}
			(7)	F_c	1.0×10^{-1}
			(8)	C	2.5×10^{-4}
			(9)	T	4.0×10^{-3}

To demonstrate the performance of the proposed method, a slow drifting behavior in parameter β_r is considered to represent the slow process change. The simulation was run for 500 min, and the change of β_r is introduced with a slope of $-0.001\,min^{-1}$ at time $k = 301$. The value of N_t is set as 200. The first 100 samples were utilized to build the initial PCA model, and the adaptive monitoring

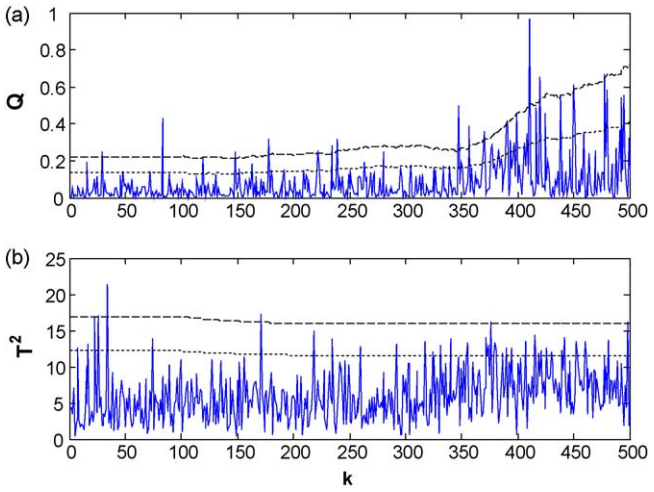

Fig. 7. Monitoring charts using proposed method (RPCA + MWPCA) for CSTR process. (a) Q statistic (b) T^2 statistic (dashed-line: 99% confidence limit; dotted-line: 95% confidence limit).

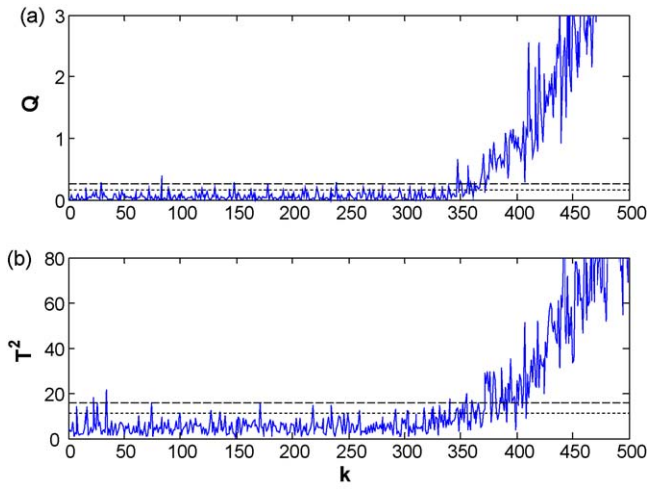

Fig. 8. Monitoring charts using conventional PCA for CSTR process. (a) Q statistic (b) T^2 statistic (dashed-line: 99% confidence limit; dotted-line: 95% confidence limit).

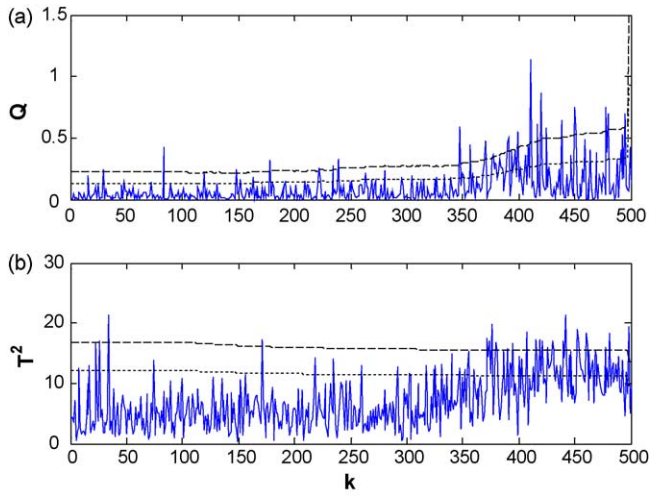

Fig. 9. Monitoring charts using RPCA for CSTR process. (a) Q statistic (b) T^2 statistic (dashed-line: 99% confidence limit; dotted-line: 95% confidence limit).

is then applied. During the simulation, the number of principal component for the adaptive model is five. The monitoring statistics obtained by the proposed monitoring method are shown in Fig. 7. For comparison, the monitoring statistics obtained by the conventional PCA and the RPCA methods are given in Figs. 8 and 9, respectively. These results clearly indicate that the proposed monitoring method outperforms the conventional PCA and the RPCA methods.

7. Conclusions

A new adaptive process monitoring method which combines the recursive PCA and moving window PCA has been proposed. The RPCA is used for collecting more normal operating data to obtain a consistent PCA model. On the other hand, the MWPCA can update the PCA model to adapt for normal process changes such as drifting. The number of PCs and the confidence limits for process monitoring are also calculated recursively. Efficient recursive algorithms for both RPCA and MWPCA, which significantly reduce the online computation cost, have been derived based on rank-one matrix update of the covariance matrix. The complete monitoring system is demonstrated through simulation examples and the results have shown the effectiveness of the proposed method. As most industrial processes experience slow and normal changes such as equipment aging, catalyst deactivation, and sensor drifting, the adaptive monitoring scheme is expected to have broad applicability in industry.

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