Two-step Principal Component Analysis for Dynamic Processes*

Zhijiang Lou, Jianyong Tuo, Youqing Wang*

Abstract—A enhanced principal component analysis (PCA), termed as Two-step PCA (TS-PCA), is proposed to handle the dynamic characteristic of industry processes. Differently from the traditional dynamic PCA (DPCA) using the “time lag shift” structure, TS-PCA adopts a new structure to present the dynamic property in the process data. By using this new structure, TS-PCA can extract the time-uncorrelated components from the dynamic data and use it for process monitoring. In addition, it can update the expectation and standard variance of the process data at each step for data normalization.

Keywords: Process monitoring; principal component analysis (PCA); dynamic PCA (DPCA); discrete–time state space model; state space PCA (SS-PCA).

I. INTRODUCTION

As one of the most common statistical process monitoring (SPM) methods, principal component analysis (PCA) [1-3] developed significantly in the last few decades. The basic strategy of PCA is to reduce the data dimension by projecting the correlated variables onto a smaller set of new variables that are uncorrelated and retain most of the original variance. One basic assumption for PCA is that the monitored data should be uncorrelated in time, i.e., Gaussian assumption. However, for most industrial processes, variables remain at a steady state but rather will move around the steady state according to the dynamic characteristics of the process and exhibit some degree of autocorrelation.

Dynamic PCA (DPCA) [4-8], which is proposed by Ku et al. [4], attempts to address the dynamic problem by modeling the auto-correlation structure present in the data using a “time lag shift” method. However, one problem for DPCA is that DPCA cannot normalize the dynamic process data just as PCA does for steady-state process. For steady-state process, the data can be normalized to zero mean and unit variance by subtract the sample mean of the training data and divide the sample standard deviation of the training data. However, normalization is unreasonable for dynamic processes, because the expectation and standard variance of each variable changes with the time and they cannot be replaced by fixed values. As a result, the monitoring performance of DPCA is generally not good enough.

In this paper, a new dynamic structure is proposed to represent the dynamic property in the process data. Differently from the “time lag shift” structure in the traditional DPCA presents the static cross-correlation structure and dynamic auto-correlation structure simultaneously, the new dynamic structure presents them separately. Then a two-step PCA (TS-PCA) is proposed to handle with these two structures: it first identifies the dynamic structure, and then monitors the time-uncorrelated component by using PCA. In addition, this new structure can also be used to update the data’s expectation and standard variance at each step and hence TS-PCA can successfully handle with the dynamic property.

The remainder of this paper is organized as follows. Section II briefly reviewed the PCA and DPCA. Then TS-PCA is proposed and some of its properties are analyzed in Section III. To fully analyze the characteristics of TS-PCA and compare it with DPCA and PCA, simulation tests are carried out on a numerical process and the Tennessee Eastman (TE) process [9] in Section IV. Finally, the contributions of this study are summarized in Section V.

II. METHOD

A. Principal Component Analysis

When applied in process monitoring, the first step of PCA is to adjust the process data \( X = [x_1, x_2, \cdots, x_n] \in \mathbb{R}^{n \times s} \) (where \( n \) is the number of samples and \( s \) is the number of variables) to zero mean and unit variance as follows:

\[
X'(t) = \frac{X(t) - E(X(t))}{\sigma(X(t))}
\]

(1)

where \( t \) denotes the sample time, \( E(X(t)) \) and \( \sigma(X(t)) \) refer to the expectation and standard variance of data \( X(t) \). For a steady-state process, the expectations \( E(X(t)) \) and standard variances \( \sigma(X(t)) \) can be replaced by the training data’s mean \( \bar{X} \) and standard deviation \( D(X) \), respectively. Then (1) can be changed to

\[
X'(t) = \frac{X(t) - \bar{X}}{D(X)}
\]

(2)

Then PCA decomposes the new data matrix \( X'(t) \) into a transformed subspace of reduced dimensions, which is defined by the span of a chosen subset of the eigenvectors of the covariance or correlation matrix associated with \( X'(t) \). Each chosen eigenvector, or principal component (PC), captures the
maximum amount of variability in the data in an ordered fashion. Mathematically, the decomposition is defined as follows:

\[ \mathbf{X}'(t) = \mathbf{T}(t)\mathbf{P}^T + \mathbf{E}(t) = \hat{\mathbf{X}}(t) + \mathbf{E}(t) \]  

(3)

where \( \mathbf{T} \in \mathbb{R}^{n \times k} \) refers to the score matrix, \( \mathbf{P} \in \mathbb{R}^{k \times m} \) refers to the loading matrix, \( k \) is the number of PCs, and \( \mathbf{E} \in \mathbb{R}^{n \times m} \) is the residual matrix. Then \( \mathbf{T}^2 \) and \( \mathbf{SPE} \) statistics [2] are constructed to monitor the process. Statistic \( \mathbf{T}^2 \) represents the distance between the location of the new data projected onto the subspace and the origin of subspace; statistic \( \mathbf{SPE} \) is a measure of the approximation error of the new data within the PCA subspace.

B. Dynamic Principal Component Analysis

In order to address the dynamic characteristics of the process, DPCA incorporates the description of variable autocorrelation into the standard PCA framework, by introducing time-shifted replicates as additional variables in the \( \mathbf{X} \) matrix:

\[ \tilde{\mathbf{X}} = [\mathbf{x}_1(1), \mathbf{x}_1(1), \ldots, \mathbf{x}_1(1), \mathbf{x}_2(1), \mathbf{x}_2(2), \ldots, \mathbf{x}_2(q), \mathbf{x}_3(q), \ldots, \mathbf{x}_q(q)] \]  

(4)

where \( q \) refers to the time lag. Therefore, in simple terms, DPCA is essentially the same as the original PCA approach, except that the data matrix is now composed of additional time-shifted replicates of the original variables.

For the implementation of the DPCA, one key point is that: for dynamic process, the expectation and standard variance of each variable changes with the time and they cannot just be replaced by the training data’s mean \( \tilde{\mathbf{X}} \) and standard deviation \( \mathbf{D}(\mathbf{X}) \). Without the correct \( \mathbf{E}(\mathbf{X}(t)) \) and \( \sigma(\mathbf{X}(t)) \), the new data matrix \( \mathbf{X}'(t) \) and the loading matrix \( \mathbf{P} \) will be wrong, and as a result, DPCA will have high false alarm rate and low fault detection rate.

III. THE PROPOSED METHOD

For TS-PCA, the following model is adopted to represent a general dynamic process:

\[ \mathbf{X}(t+1)^T = \mathbf{AX}(t)^T + \mathbf{U}(t)^T \]  

(5)

\[ \mathbf{U}(t) = \mathbf{T}_n(t)\mathbf{p}_n^T + \mathbf{E}_n(t) \]  

(6)

According to (5), process data \( \mathbf{X}(t+1) \) is divided into two parts: the autocorrelation component \( \mathbf{AX}(t)^T \) (\( \mathbf{A} \in \mathbb{R}^{m \times m} \)) and the time-uncorrelated component \( \mathbf{U}(t) \in \mathbb{R}^{n \times m} \), which can be decomposed as (6).

Two assumptions are introduced for this dynamic system: first, it is asymptotically stable, i.e. all eigenvalues of \( \mathbf{A} \) are strictly inside the unit circle; second, part \( \mathbf{U}(t) \) follows Gaussian distribution and it is statistically independent of the past process data \( \mathbf{X}(t) \) and \( \mathbf{U}(t-1) \), which means all \( \mathbf{U}(t) \) have the same expectations \( \mathbf{E}(\mathbf{U}(t)) = \mathbf{v} \) and standard variances \( \sigma(\mathbf{U}(t)) = \mathbf{v} \).

Based on (5), one can get

\[ \mathbf{X}(t+1)^T - \mathbf{AX}(t)^T - \mathbf{U}(t)^T = \mathbf{U}(t)^T - \mathbf{U}(t-1)^T \]  

(7)

As \( \mathbf{E}(\mathbf{U}(t)^T - \mathbf{U}(t-1)^T) = 0 \) and \( \mathbf{U}(t)^T \) is statistically independent of \( \mathbf{X}(t) \), one gets

\[ E \left\{ (\mathbf{X}(t+1)^T - \mathbf{AX}(t)^T - \mathbf{U}(t)^T) \mathbf{X}(t) \right\} = E \left\{ (\mathbf{U}(t)^T - \mathbf{U}(t-1)^T) \mathbf{X}(t) \right\} = 0 \]  

(8)

In addition, for any \( T \geq 1 \), \( (\mathbf{U}(t+T)^T - \mathbf{U}(t)^T) \) is also statistically independent of \( \mathbf{X}(t) \), so

\[ E \left\{ (\mathbf{X}(t+T+1)^T - \mathbf{AX}(t+T)^T - \mathbf{U}(t+T)^T) \mathbf{X}(t) \right\} = 0 \]  

(9)

Subtracting (8) from (9), one gets

\[ E \left\{ (\mathbf{X}(t+T+1)^T - \mathbf{X}(t+1)^T)^T \mathbf{X}(t) \right\} - A \left\{ (\mathbf{X}(t+T)^T - \mathbf{X}(t)^T) \mathbf{X}(t) \right\} = 0 \]  

(10)

For large summation number \( m \) (\( m \leq n - T - 1 \)), the follow equation can be obtained:

\[ \frac{1}{m} \sum_{i=1}^{m} (\mathbf{X}(i+T+1)^T - \mathbf{X}(i+1)^T) \mathbf{X}(i) - A \left\{ (\mathbf{X}(t+T)^T - \mathbf{X}(t)^T) \mathbf{X}(i) \right\} \approx 0 \]  

(11)

Define

\[ \bar{\mathbf{X}}(t) = \begin{bmatrix} \mathbf{X}(t) \\ \mathbf{X}(t+1) \\ \vdots \\ \mathbf{X}(t+m-1) \end{bmatrix} \]

Then (11) can be changed as follows:

\[ \frac{1}{m} \left\{ (\bar{\mathbf{X}}(T+2)^T - \bar{\mathbf{X}}(2)^T) \bar{\mathbf{X}}(1) \right\} - A \left\{ (\bar{\mathbf{X}}(T+1)^T - \bar{\mathbf{X}}(1)^T) \bar{\mathbf{X}}(1) \right\} \approx 0 \]  

(12)

So matrix \( \mathbf{A} \) can be estimated as

\[ \hat{\mathbf{A}} = \left( \bar{\mathbf{X}}(T+2)^T - \bar{\mathbf{X}}(2)^T \right) \bar{\mathbf{X}}(1) \left\{ (\bar{\mathbf{X}}(T+1)^T - \bar{\mathbf{X}}(1)^T) \bar{\mathbf{X}}(1) \right\}^{-1} \]  

(13)

As a result, the time-uncorrelated component \( \mathbf{U}(t) \) can be estimated as

\[ \hat{\mathbf{U}}(t) = \mathbf{X}(t+1) - \mathbf{X}(t) \hat{\mathbf{A}}^T \]  

(14)

The next step is to use PCA to monitor \( \hat{\mathbf{U}}(t) \) and then to detect process faults. This step is just the same as that for a traditional PCA process. Other steps such as the contribution analysis [10] can also be operated as in PCA.
In TS-PCA, there are two key parameters, i.e. parameter $T$ and the summation number $m$. A large summation number $m$ can make the left of (11) more close to 0 while a large $T$ can make the estimated $\hat{A}$ more robust to disturbance. For simplicity, these two parameters can be chosen as follow rules: when $n$ is large, set $m = T = \frac{n-1}{2}$; otherwise, set $m = \frac{2}{3}(n-1)$ and $T = \frac{1}{3}(n-1)$.

**Remark.** Equation (13) is just one sample method to estimate matrix $A$, which can also be estimated by other algorithms such as least squares estimation (LSE) [11].

IV. SIMULATION RESULTS

A. Test on a simulated dynamic process

To fully analyze the characteristics of TS-PCA and compare it with DPCA and PCA, a simple simulated process is employed to illustrate the monitoring performance of these methods:

$$
\begin{align*}
&x_1(t) = 3x_1(t) + 0.01w_1(t) + 1 \\
&x_2(t) = 0.8x_2(t-1) + 5x_1(t) + 0.01w_2(t) + 2 \\
&x_3(t) = 0.7x_3(t-1) + 0.3x_1(t) + 0.01w_3(t) + 3 \\
&x_4(t) = 2x_2(t) + 0.6x_3(t-1) + 0.01w_4(t) + 4
\end{align*}
$$

Random variables $N_i$ and $\omega_i$ follow the standard Gaussian distribution and $\omega_i$ indicates the process noise. For this process

$$
A = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0.8 & 0 & 0 \\
0.7 & 0 & 0 & 0 \\
0 & 1.6 & 0 & 0.6
\end{bmatrix}.
$$

The first step of TS-PCA is to estimate matrix $A$ using the normal process data. About 2000 normal observations are adopted for estimation, and parameters $m$ and $T$ are set as 1000 and 999. The estimated result is

$$
\hat{A} = \begin{bmatrix}
0.067 & 0.035 & -0.023 & -0.006 \\
-0.056 & 0.811 & 0.055 & 0.007 \\
0.695 & 0.012 & -0.077 & -0.015 \\
-0.072 & 1.621 & 0.013 & 0.614
\end{bmatrix},
$$

which is very close to $A$. This result indicates that (13) can successfully estimate matrix $A$.

Then these 2000 normal observations used for offline modelling. Furthermore, another 3000 samples are generated for online monitoring, where a fault occurs at the 1001th sample point. The occurred fault might be the following three types: Fault 1, a step change with amplitude of 10 in $x_1(t)$; Fault 2, coefficient 0.7 in $x_2(t)$ is changed to 0.6; Fault 3: coefficient 2 in $x_3(t)$ is changed to 2.1.

Table I and Table II list the false alarm rates and fault detection rates of three faults for three methods, TS-PCA, DPCA, and PCA. The best result in these experiments is marked in bold and underline. For DPCA, the lag order $q$ was selected as one for each measurement. In this study, all control limits are based on the confidence limit of 99%.

As shown in Table I, three methods have almost the same false alarm rates. However, in Table II, TS-PCA can successfully detect Fault 2 and Fault 3 while the other two methods cannot. The reason for this result is that TS-PCA has more precise normalization process than DPCA and PCA, and hence it is more sensitive to the abnormal conditions. For Fault 1, PCA and DPCA have much higher $SPE$ statistics than TS-PCA, which seems TS-PCA achieves worsen than them. Indeed, the step change in $x_1(t)$ only affects the distance between the location of the new data projected onto the subspace and the origin of subspace but it will not affects the $SPE$ statistic. As a result, the $SPE$ statistic in Fault 1 should be the same as in normal data. However, as PCA and DPCA falsely normalizes the process and uses the wrong result for process monitoring, both their $T^2$ and $SPE$ statistics beyond the normal values. Different from them, TS-PCA can successfully handle the dynamic problem and hence its $SPE$ statistic is very small.

| TABLE I. | FALSE ALARM RATE COMPARISON OF THREE METHODS ON THE DYNAMIC PROCESS, (%) |
| Methods | PCA | DPCA | TS-PCA |
| Indices | $T^2$ | SPE | $T^2$ | SPE | $T^2$ | SPE |
| False alarm rates | 0.75 | **0.60** | 1.10 | 0.85 | 1.00 | 0.70 |

| TABLE II. | FAULT DETECTION RATE COMPARISON FOR THE 3 FAULTS ON THE DYNAMIC PROCESS, (%) |
| Methods | PCA | DPCA | TS-PCA |
| Indices | $T^2$ | SPE | $T^2$ | SPE | $T^2$ | SPE |
| Fault 1 | **100.00** | 8.51 | **100.00** | 57.52 | 94.60 | 0.65 |
| Fault 2 | 1.30 | 0.25 | 0.70 | 1.55 | 1.00 | **93.85** |
| Fault 3 | 0.45 | 0.90 | 0.85 | 0.96 | 1.10 | **89.19** |

B. Test on Tennessee Eastman process

The Tennessee Eastman (TE) process [9] is a benchmark test bed that has been widely used to test the performance of various monitoring approaches. There are 22 continuous process measurements, 19 composition measurements, and 12 manipulated variables in the entire process, and 21 predefined faults are introduced in this process. The TE process is adopted in this paper to demonstrate the superiority of TS-PCA. In this study, only 33 variables will be monitored.
since the 19 composition measurements are difficult to measure in real time and one manipulated variable, the agitation speed, is not manipulated. The training and testing data sets for each fault are consisted of 480 and 960 observations, respectively. All faults in the test data set were introduced from sample 161. In addition, another 960 normal data are adopted to calculate the false alarm rate.

Table III and Table IV list the false alarm rates and fault detection rates of twenty-one faults for three methods, TS-PCA, DPCA, and PCA. The best result in these experiments is marked in bold and underline. For TS-PCA, parameters \( m \) and \( T \) are set as 320 and 159 because the training data number \( n \) is small. For DPCA, the lag order \( q \) was selected by using a method described in [4]: two lagged variables of each measurement.

As shown in Table III, both PCA and DPCA have false alarm rates larger than 8%, which are much worse than those of TS-PCA. The reason for this phenomenon is that PCA and DPCA just normalize the process data with the mean and standard deviation of the training data, but the expectation and standard variance of the testing data may be quite different from them and hence the normal data will be diagnosed as fault data. Different from the other two methods, TS-PCA monitors the time-uncorrelated \( U \) rather than the autocorrelated \( X \) and hence its false alarm rate is very small.

According to Table IV, TS-PCA achieves the best in 15 faults and it has the best average detection rates among these three methods. Especially for Faults 5, whose detection rates of other methods are generally below 50%, whereas its detection rates under TS-PCA is 100%, which indicates the superiority of TS-PCA. In Table IV, for some faults such as Fault 9, DPCA may achieve better than TS-PCA. However, it gets the high detection rates at the cost of high false alarm rates, so TS-PCA is a more reliable method than DPCA.

### Table III. False Alarm Rate Comparison of Three Methods On the Te Process. (%)

<table>
<thead>
<tr>
<th>Methods</th>
<th>PCA</th>
<th>DPCA</th>
<th>TS-PCA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indices</td>
<td>( T^2 )</td>
<td>SPE</td>
<td>( T^2 )</td>
</tr>
<tr>
<td>False alarm rates</td>
<td>8.55</td>
<td>3.01</td>
<td>3.34</td>
</tr>
</tbody>
</table>

Fig. 1. Monitoring chart for fault 5: (a) PCA; (b) DPCA; (c) TS-PCA;

### Table IV. Fault Detection Rate Comparison for the 3 Faults On the Te Process. (%)

<table>
<thead>
<tr>
<th>Methods</th>
<th>PCA</th>
<th>DPCA</th>
<th>TS-PCA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indices</td>
<td>( T^2 )</td>
<td>SPE</td>
<td>( T^2 )</td>
</tr>
<tr>
<td>Fault 1</td>
<td>99.25</td>
<td>99.75</td>
<td>99.13</td>
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<tr>
<td>Fault 2</td>
<td>98.38</td>
<td>97.25</td>
<td>98.50</td>
</tr>
<tr>
<td>Fault 3</td>
<td>3.63</td>
<td>3.63</td>
<td>0.75</td>
</tr>
<tr>
<td>Fault 4</td>
<td>20.63</td>
<td><strong>100.00</strong></td>
<td>5.50</td>
</tr>
<tr>
<td>Fault 5</td>
<td>26.63</td>
<td>27.75</td>
<td>24.88</td>
</tr>
<tr>
<td>Fault 6</td>
<td>99.13</td>
<td><strong>100.00</strong></td>
<td>98.88</td>
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<td>Fault 7</td>
<td><strong>100.00</strong></td>
<td><strong>100.00</strong></td>
<td><strong>100.00</strong></td>
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<tr>
<td>Fault 8</td>
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<td>97.50</td>
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<tr>
<td>Fault 9</td>
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<td>3.13</td>
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<td>Fault 10</td>
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<td>51.88</td>
<td>38.75</td>
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<tr>
<td>Fault 11</td>
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<td>27.00</td>
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<td>Fault 12</td>
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<td>99.13</td>
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<td>Fault 13</td>
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<td>95.25</td>
<td>94.13</td>
</tr>
<tr>
<td>Fault 14</td>
<td>98.63</td>
<td><strong>100.00</strong></td>
<td>99.63</td>
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<td>Fault 17</td>
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<td>78.25</td>
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<td>Fault 18</td>
<td>89.63</td>
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<td>Fault 19</td>
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<td>Fault 21</td>
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<tr>
<td>Average</td>
<td>57.61</td>
<td>68.37</td>
<td>55.27</td>
</tr>
</tbody>
</table>

Fig. 2. Monitoring chart for fault 16: (a) PCA; (b) DPCA; (c) TS-PCA;
To better demonstrate the features of TS-PCA, the monitoring charts of PCA, DPCA, and TS-PCA for Fault 5 and Fault 16 are shown in Fig. 1 and Fig. 2.

In the case of Fault 5, the condenser cooling water inlet temperature is step changed. Then the control loops will act to compensate for the change and the temperature in the separator will return to its set-point about 10 hours (200 samples) later. For this fault, PCA (Fig. 1 (a)) and DPCA (Fig. 1 (b)) cannot detect the fault from approximately sample 350 since most variables returned to their set-points that time. However, in fact, even after sample 350 the condenser cooling water inlet temperature is still higher than the normal operating condition and the condenser cooling water flow rate is continuously manipulated, which means a fault remains in the process. As shown in Fig. 1 (c), TS-PCA can still detect the fault even after sample 350. The reason for this phenomenon is that TS-PCA monitors the time-uncorrelated component of the process data and its normalization process is more precise than DPCA, hence it is more sensitive to the abnormal conditions. Fig. 2 indicates that though DPCA has higher detection rate than PCA, its false alarm rate is also much higher than the other two methods. Among all of the three methods, TS-PCA has the best monitoring result, so the discrete–time Two-step structure is a promising dynamic structure for PCA.

V. CONCLUSION

In this paper, discrete–time Two-step model was combined with PCA to handle the dynamic characteristics of industrial processes. Through estimating dynamic relationship among the process data, TS-PCA can successfully extract the time-uncorrelated component from the dynamic data and use it for process monitoring. In addition, the TS-PCA can update the expectation and standard variance of the process data at each step and hence its normalization process is more precise than those of PCA and DPCA. The test results on the simulated dynamic process and TE process show that TS-PCA is more sensitive to the abnormal conditions and it has lower false alarm rate than PCA and DPCA. Hence, TS-PCA is a promising method for dynamic process monitoring.

In this paper, only the first-order dynamic structure was adopted in TS-PCA and hence TS-PCA may work worsen than DPCA in high-order dynamic process. To address this problem, the “time lag shift” structure in DPCA can be integrated into SS–PCA, which will be studied in the near future.

REFERENCES


