Fault Detection of Multimode Processes
Using Concurrent Projection to Latent Structures

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Abstract: Process monitoring based on Concurrent Projection to Latent Structures (CPLS) has been proposed recently as an efficient process monitoring tool to detect the input-relevant and output-relevant faults. In this paper, a novel multimode process monitoring approach is proposed to introduce external analysis into the CPLS monitoring framework. The process variables are divided into external variables, main variables and the output variables. The mode change is detected by monitoring the variation of the external variables through a mode-detection CPLS. The prediction of the main and quality variables by external variables is done by a PLS. After the influence of the external variables is removed from the main and quality variables, another process-monitoring CPLS is built to detect the main-variable-relevant and quality-variable-relevant faults. The proposed approach is illustrated with a simulation process.

Keywords: multiple mode operation, concurrent partial least squares, external analysis.

1. INTRODUCTION

Process monitoring is important to ensure the safety of operation and quality of products. For many industrial cases, multivariate projection methods such as principal component analysis (PCA) and projection to latent structures (PLS) are powerful technology used to detect and identify changes and faults. Wise and Gallagher (1996), and Qin (2003) gave a review of the PCA and PLS-based process monitoring methods which use the statistics of process and quality data collected from normal operations. Both PCA and PLS can reduce the dimensionality of monitoring space and handle large numbers of correlated data. While if the quality related faults is required to be detected, PLS is chosen as an efficient tool instead of PCA since it is based on the covariance between the input process data and the output quality data (Chiang et al., 2001).

However, a standard PLS contains the variations orthogonal to the output which is useless for its prediction, and large variations in the input-residual is not proper to monitor with the Q-statistic. To completely monitor the output-relevant and input-relevant variations, Qin and Zheng (2013) proposed a concurrent PLS (CPLS) algorithm which concisely decompose the data space into the following subspaces: the covariation subspace (CVS) relevant to the predictable variations of the output; the output principal subspace (OPS) and output-residual subspace (ORS) which related to the unpredicted output variations, and an input-principal subspace (IPS) and input-residual subspace (IRS) to which the input variations irrelevant to the output are further projected.

CPLS can effectively detect the output-relevant and input-relevant faults. However, as other traditional statistical process monitoring (SPM) methods, it can only be applied to one nominal operation mode only, which limits its application to industrial process. In general manufacturing industries, due to the alteration of the feedstock and production strategies, the manufacturing process will be operated in different modes. To apply CPLS in multimode process will improve not only its feasibility, but also the monitoring performance of the multimode processes.

To handle the multimode problems, many methods have been proposed in recent years. Some literature considered global or mixture models for process monitoring, such as Gaussian mixture models (Yu and Qin, 2008, Feitäl et al. 2013, Chen and Zhang, 2010), a mixture Bayesian regularization method of PPCA (Ge and Song, 2010), hidden Markov models (Yu, 2010), mode clustering and unfolding integration modeling method (Tong et al., 2013), and the subspace separation (Zhang et al., 2013), etc. Besides the global model based method, adaptive model based approach using different tools, such as recursive algorithms (Qin, 1998; Li et al., 2000) and a signed digraph (Lee et al., 2006), to focus on the local mode information, such as the nonlinearity of processes (Haghani et al., 2014), cross-mode and within-mode correlations (Ma and Shi, 2014), and the transition between two models (Ma and Shi, 2014), Singhal and Seborg, 2006). Since there are effective approaches for single mode process monitoring, the multimode process monitoring is easily implemented if the different modes are identified. A PCA similarity factor (Singhal and Seborg, 2006), the loading matrices of the PCA model (Tan et al., 2012), the similarity metric for PLS models (Zhao et al., 2006) are proposed for process mode identification.

Since mode change is caused only by part of the process variables, it can be eliminated if the influence of the mode-
related variables is removed. Kano et al. proposed a method based on external analysis. They divided process variables into two parts: main variables and external variables which represent operation mode changes. When the effect of external variables on the main variables is removed, the rest of the information from the main variables can be monitored. Ge et al. (2008) developed an online external analysis based monitoring approach and Ge et al. (2014) also constructed an additional regression model for soft sensing, which considered the quality variables and was robust to the change of operation modes.

Motivated by the external analysis method, a novel multimode process monitoring approach which combines CPLS and external analysis is proposed in this paper. The process variables are divided into external variables, main variables and the quality variables. For the process monitoring, the mode-detection CPLS is trained with the external variables as the input and the main quality variables as the output to monitor the variations of the external variables. When the mode transition is detected, an additional PLS with enough data from multiple modes is used for the prediction of the main quality variables by the external variables. The influence of the external variables is removed from the main variables and external variables. Choosing the updated main variables as the input and the updated quality variables as the output, the process-monitoring CPLS is built to detect the main-variable-relevant faults and quality-variable-relevant faults. The approach inherently utilizes steady state information of different modes and does not require the knowledge of the process dynamics.

The rest of this paper is organized as follows. Section 2 introduces the concurrent PLS. Section 3 proposes the external analysis based CPLS for multimode process monitoring. The effectiveness of our approach is demonstrated in Section 4 by a simulation example. The last section gives conclusions.

2. CONCURRENT PLS

For normalized process input \( X \in R^{nxp} \) which consists of \( n \) samples with \( p \) variables and output data matrices \( Y \in R^{nyq} \) which consists of \( n \) samples with \( q \) variables, the CPLS algorithm is given by Qin and Zheng (2013) as following four steps:

**Step 1:** Perform PLS on \( X \) and \( Y \) by (1).

\[
X = \sum_{i=1}^{a} t_i p_i^T + E = TP^T + E
\]

\[
Y = \sum_{i=1}^{a} u_i q_i^T + \tilde{Y} = TQ^T + \tilde{Y}
\]

where \( T = [t_1, \ldots, t_a] \) is the scores, \( P = [p_1, \ldots, p_a] \) and \( Q = [q_1, \ldots, q_a] \) are the loading vectors for \( X \) and \( Y \), \( E \) and \( \tilde{Y} \) are PLS residuals corresponding to \( X \) and \( Y \), and \( a \) is the number of PLS factors which is usually determined by cross-validation.

**Step 2:** Perform singular value decomposition (SVD) of the predictable output \( \tilde{Y} \) as follows,

\[
\tilde{Y} = TQ^T = T_c D V_c^T = T_c Q_c^T
\]

where \( Q_c = V_c D_c \) and

\[
R_c = RQ_c^T V_c D_c^{-1}
\]

\[
R = W \left( W^T W \right)^{-1}
\]

**Step 3:** Form the unpredictable output \( \tilde{Y}_a \) in (1), and perform PCA on \( \tilde{Y}_a \) with \( l_p \) principal components:

\[
\tilde{Y}_a = Y - T_p Q_p^T = T_p P_p^T + \hat{Y}
\]

**Step 4:** Form the output-relevant input by \( \hat{X}_a \), and perform PCA on \( \hat{X}_a \) with \( l_x \) principal components:

\[
\hat{X}_a = X - T_x R_x^+ = T_x P_x^T + \tilde{X}
\]

where \( R_x^+ = \left( R_x^T R_x \right)^{-1} R_x^T \).

Overall, the CPLS model decomposes the input \( X \) and output \( Y \) as follows:

\[
X = T_y R_y^+ + T_p P_p^T + \hat{X}
\]

\[
Y = T_x Q_x^+ + T_p P_p^T + \tilde{Y}
\]

Thus, for each row of the monitoring input data \( x \) and the output data \( y \), the co-variation subspace is monitored by the \( T^2 \) statistics:

\[
T^2 = (n-1)x^T R_y^+ x \leq \frac{a(n^2 - 1)}{n(n-1)} F_{a,a,a} \tag{7}
\]

where \( F_{a,a,a} \) is \( F \)-distribution with \( a \) and \( a \times a \) degrees of freedom and confidence level \((1-\alpha)\times100\%\). The OPS and ORS of the unpredicted output variation are monitored by the \( T^2 \) statistics and \( Q \) statistics, respectively:

\[
T^2 = \frac{1}{n-1} \tilde{Y}_a^T P_y (T_y^T T_y)^{-1} P_y \tilde{Y}_a \leq \frac{I_y (n^2 - 1)}{n(n-1)} F_{I_y,a-I_y,a} \tag{8}
\]

\[
Q = \| \tilde{Y} \|^2 \leq g_{x_h,a} \tag{9}
\]

where \( \tilde{Y} \) and \( \tilde{Y} \) is a specific row of \( \tilde{Y}_a \) and \( \tilde{Y} \) respectively, and \( x_h \) is the \( x^2 \)-distribution with \( h \) degrees of freedom. Moreover, the IPS and IRS of the input variations are monitored by the following \( T^2 \) statistics and \( Q \) statistics, respectively:

\[
T^2 = \frac{1}{n-1} \tilde{X}_a^T P_x (T_x^T T_x)^{-1} P_x \tilde{X}_a \leq \frac{I_x (n^2 - 1)}{n(n-1)} F_{I_x,a-I_x,a} \tag{8}
\]

where \( \tilde{X}_a \) is a specific row of \( \tilde{X}_a \) and \( \tilde{X} \), respectively.

3. CPLS WITH EXTERNAL ANALYSIS FOR MULTIMODE PROCESS MONITORING

Mode changes of the process are mostly related to different process operation conditions. Some of the process variables are related to the operation conditions directly, such as throughput rate, process setpoints, and the operation temperature. Kano et al. (2004) referred to these variables as external variables. Besides, the other process variables are
variables that are irrelevant to mode changes. Ge et al. (2014) considered the quality-related variables and extended this definition. All variables are divided into three categories: the external variables, the main variables and the quality variables. So all the process variables \( V \in \mathbb{R}^{m} \) will be decomposed as:

\[
V = [E \quad M \quad Z]\tag{10}
\]

where \( E \in \mathbb{R}^{m} \) consists of external variables, \( M \in \mathbb{R}^{m} \) consists of main variables, and \( m = m_e + m_m + m_q \). The proposed CPLS method with external variables is to first build a CPLS model using E as input and \([M \ Z]\) as outputs. This model, referred to as mode-detection CPLS model, is used to discriminate between mode changes and input sensor faults. In the next step, the mode-detection CPLS model is used to remove the impact of E on both M and Z before building another CPLS model between Z and M for process monitoring that is insensitive to mode changes.

### 3.1 The mode-detection CPLS

For process monitoring, a mode-detection CPLS is trained by choosing external variables E as the input, while main variables M and quality variables Z are the output. Assume \( X_1 \) and \( Y_1 \) denote the normalized input and output of the mode-detection CPLS respectively, we will have

\[
X_1 = [E]
\]

\[
Y_1 = [M \quad Z]^T
\]

And the mode-detection CPLS is represented as

\[
X_1 = T_{1e} R_{1e} + T_{1m} P_{1m} + \hat{X}_1
\]

\[
Y_1 = T_{1q} Q_{1q} + T_{1p} P_{1p} + \hat{Y}_1
\]

where \( T_{1e}, R_{1e}, Q_{1q}, T_{1m}, P_{1m}, \hat{X}_1, T_{1p}, P_{1p}, \hat{Y}_1 \) are defined as \( T, R, Q, T, P, \hat{X}, T, P, \hat{Y} \) in section 2. And the monitor indices \( T_{1}^2, T_{1}^2, Q_{1}, T_{1}^2 \) and \( Q_{1} \) are the corresponding \( T^2 \) statistics and Q statistics which is introduced in section 2.

Since the indices \( T_{1}^2 \) and \( Q_{1} \) will monitor the input-relevant variations, they can be adopted to detect the mode changes especially when they cannot be observed directly through the external variables. However, to exclude the sensor faults which will also cause variations of the external variables, \( T_{1}^2 \), \( T_{1}^2 \) and \( Q_{1} \) must also be used. Consequently, if the \( T_{1}^2 \) and/or \( Q_{1} \) are above the control limit but \( T_{1}^2 \) and \( Q_{1} \) are not, the mode transition is not the possible cause. There must be any external-variable-relevant fault such as the sensor failure occurred in the process.

### 3.2 Prediction of main/quality variables

PLS is based on the covariance between the input data and the output data. In this paper, a PLS is used with external variables as the input and the main/quality variables as the output to predict the influence of external variables E on main variables M and quality variables Z, i.e.,

\[
E = T_p P_p^T + F
\]

\[
[M \ Z]^T = T_p Q_p^T + \hat{M} \quad \hat{Z}^T
\]

where \( T_p \) is the scores, \( P_p \) and \( Q_p \) are the loading vectors, \( F \) and \( \hat{M} \quad \hat{Z}^T \) are PLS residuals corresponding to \( E \) and \( [M \ Z]^T \). So the prediction of \([M \ Z]^T\) is

\[
\hat{M} \quad \hat{Z}^T = T_p Q_p^T
\]

It must be noted that if more data, especially data from different modes, are incorporated in the PLS model, the prediction performance will be improved. Therefore, although the mode-detection CPLS can predict the output which is represented by \( \hat{Y}_1 = T_{1q} Q_{1q} \), an additional PLS predictor with more available training data will have better prediction performance.

### 3.3 The process-monitoring CPLS

After the mode-detection CPLS gives the result that the process is possibly operated in multiple modes, the process-monitoring CPLS needs to be built. Since the prediction of M and Z by E, i.e., \( \hat{M} \) and \( \hat{Z} \), has been achieved by PLS, the influence of the mode transition will be diminished if \( \hat{M} \) and \( \hat{Z} \) are removed from the original M and Z. Thus, taking \( M - \hat{M} \) as the input \( X_{2} \), \( Z - \hat{Z} \) as the output \( Y_{2} \), i.e.,

\[
X_{2} = M - \hat{M}
\]

\[
Y_{2} = Z - \hat{Z}
\]

the process-monitoring CPLS is trained as

\[
X_{2} = T_{2e} R_{2e} + T_{2m} P_{2m} + \hat{X}_{2}
\]

\[
Y_{2} = T_{2q} Q_{2q} + T_{2p} P_{2p} + \hat{Y}_{2}
\]

where \( T_{2e}, R_{2e}, Q_{2q}, T_{2m}, P_{2m}, \hat{X}_{2}, T_{2p}, P_{2p}, \hat{Y}_{2} \) are defined as \( T, R, Q, T, P, \hat{X}, T, P, \hat{Y} \) in Section 2. The process-monitoring CPLS divides the input and output space into CVS, OPS, ORS and IRS, and monitor them by \( T_{2}^2, T_{2}^2 \) and \( Q_{2}, T_{2}^2 \) and \( Q_{2} \), respectively.

### 3.4 The proposed algorithm

The detailed process monitoring procedure is shown below. 

**Step 1:** Collect the normal process variables, normalize them and classify them into three categories: external variables E, main variables M and quality variables Z.

**Step 2:** Choose E as the input \( X_1 \) and \( M \quad Z \) as the output \( Y_1 \), and construct the mode-detection CPLS model as (12). The indices \( T_{1}^2, Q_{1}, T_{1}^2, T_{1}^2 \) and \( Q_{1} \) are computed.

**Step 3:** If the indices \( T_{1}^2 \) and/or \( Q_{1} \) of the mode-detection CPLS are above the control limit, and any of \( T_{1}^2, T_{1}^2 \) and
are above the control limit, a PLS (13) is trained and the prediction $\hat{M}, \hat{Z}$ are achieved by (14).

**Step 4:** Compute $X_2 = M - \hat{M}$ and $Y_2 = Z - \hat{Z}$. Choose $X_2$ and $Y_2$ as the input and the output respectively, and construct the process-monitoring CPLS model as (16). If some of the indices $T_{x_2}^2, T_{y_2}^2, Q_{x_2}$ and $Q_{y_2}$ are above the control limit, there are output-relevant faults in the process. If any of the index $2\hat{c}_T, 2\hat{y}_T, 2\hat{x}_T$ are below the control limit, which is done by a PLS with 550 samples. We end up with $\hat{M}$, so $\hat{x}_1, \hat{y}_1, \hat{z}_1$ are main variables, and $\hat{x}_2, \hat{y}_2, \hat{z}_2$ are quality variables.

In this example, three different modes with different $s_1$ are simulated. 500 normal samples for each mode are simulated. The first 300 samples are used to train the mode-detection CPLS which choose $r_1$ as the input $x_1$ and other 6 variables as the output $y_1$. We end up with $a = 1, l_x = 1, l_y = 6$, so that $Q_{x_1}$ and $Q_{y_1}$ are null. As shown in Fig.1, all the indices $T_{x_1}^2, T_{y_1}^2$ of 501$^{st}$-1500$^{th}$ samples are above the 95% control limit, which shows there are multiple modes in the process.

![Fig.1 The indices $T_{x_1}^2, T_{y_1}^2$ and $T_{z_1}^2$ of the mode-detection CPLS](image)

<table>
<thead>
<tr>
<th>$r(i)$</th>
<th>$s_1$</th>
<th>$s_2$</th>
<th>$s_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.894</td>
<td>0.058</td>
<td>0.353</td>
</tr>
<tr>
<td>0</td>
<td>0.445</td>
<td>0.932</td>
<td>0.466</td>
</tr>
<tr>
<td>0</td>
<td>0.846</td>
<td>0.525</td>
<td>0.203</td>
</tr>
</tbody>
</table>

where $s_i \sim U(0,1)$ is uncorrelated random signals which follow the uniform distribution, and $v(k) \sim N(0,0.2^2)$ and $w(k) \sim N(0,0.1^2)$ are noise vectors which follow the normal distribution. A signal with random value between 0 and 10 is added on $s_1$ every 500 data points to generate different modes of the process. According to (17), $r_1$ is affected only by the change of $s_1$, so $r_1$ should be regarded as external variables. And other variables $r_2 \sim r_6$ are main variables, and $z_1$ and $z_2$ are quality variables.

After removing the prediction $\hat{M}, \hat{Z}$ from the original $M$ and $Z$ we obtain the prediction error which is stationary, which indicates the mode change is removed from the original data. Using 400 normal samples, the process-monitoring CPLS is trained with $M - \hat{M}$ as the input $x_2$ and $Z - \hat{Z}$ as the output $y_2$. We end up with $a = 3, l_x = 2, l_y = 2$, so that $Q_{x_2}$ and $Q_{y_2}$ are null. And other matrices are

$$R_y = \begin{bmatrix} -0.0167 & -0.0365 \\ 0.0450 & 0.0191 \\ 0.0205 & -0.0007 \\ -0.0051 & -0.0258 \end{bmatrix}, \quad P_y = \begin{bmatrix} -0.1090 & -0.6243 \\ -0.4547 & -0.1555 \\ 0.8594 & 0.0226 \\ -0.2068 & 0.7652 \end{bmatrix}$$

$$P_x = \begin{bmatrix} -0.1610 & 0.9869 \\ 0.9869 & 0.1610 \end{bmatrix}$$

The monitoring result is shown in Fig.3. In Fig.3, all the indices $T_{x_2}^2, T_{y_2}^2$, and $T_{z_2}^2$ are below the control limit, which

4. **CASE STUDY**

The simulated numerical example which has five process variables and two quality variables is as follows (Ge et al., 2014):

$$\begin{bmatrix} r(i) \\ z(i) \end{bmatrix} = \begin{bmatrix} 1 & 0.894 & 0.058 & 0.353 & 0.813 \\ 0.445 & 0.932 & 0.466 & 0.419 & 0.846 & 0.525 & 0.203 & 0.672 & 1.110 & 0.307 & 1.159 & 0.703 & 0.374 & 1.909 & 0.879 & -1.094 & -0.139 & 0.296 \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \\ s_3 \end{bmatrix} + \begin{bmatrix} v(i) \\ w(i) \end{bmatrix}$$

where $s_i \sim U(0,1)$ is uncorrelated random signals which follow the uniform distribution, and $v(k) \sim N(0,0.2^2)$ and $w(k) \sim N(0,0.1^2)$ are noise vectors which follow the normal distribution. A signal with random value between 0 and 10 is added on $s_1$ every 500 data points to generate different modes of the process. According to (17), $r_1$ is affected only by the change of $s_1$, so $r_1$ should be regarded as external variables. And other variables $r_2 \sim r_6$ are main variables, and $z_1$ and $z_2$ are quality variables.

![Fig.2 The prediction of main variables $M$ and quality variables $Z$](image)

After removing the prediction $\hat{M}, \hat{Z}$ from the original $M$ and $Z$ we obtain the prediction error which is stationary, which indicates the mode change is removed from the original data. Using 400 normal samples, the process-monitoring CPLS is trained with $M - \hat{M}$ as the input $x_2$ and $Z - \hat{Z}$ as the output $y_2$. We end up with $a = 3, l_x = 2, l_y = 2$, so that $Q_{x_2}$ and $Q_{y_2}$ are null. And other matrices are

$$R_y = \begin{bmatrix} -0.0167 & -0.0365 \\ 0.0450 & 0.0191 \\ 0.0205 & -0.0007 \\ -0.0051 & -0.0258 \end{bmatrix}, \quad P_y = \begin{bmatrix} -0.1090 & -0.6243 \\ -0.4547 & -0.1555 \\ 0.8594 & 0.0226 \\ -0.2068 & 0.7652 \end{bmatrix}$$

$$P_x = \begin{bmatrix} -0.1610 & 0.9869 \\ 0.9869 & 0.1610 \end{bmatrix}$$

The monitoring result is shown in Fig.3. In Fig.3, all the indices $T_{x_2}^2, T_{y_2}^2$, and $T_{z_2}^2$ are below the control limit, which
shows the multimode does not generate the false alarm by the process-monitoring CPLS.

Fig. 3 The indices $T_{2,2}^c$, $T_{2,2}^y$ and $T_{2,2}^x$ of process-monitoring CPLS when no fault occurs. A fault is added in the following form in the input space

$$x_{2,k} = x_{2,k} + \Xi_{2,3} f_{2,3}$$

(18)

or in the output space

$$y_{2,k} = y_{2,k} + \Xi_{2,3} f_{2,3}$$

(19)

500 faulty samples in operation mode 3 produced by (18) or (19) are used to verify the fault detection performance of process-monitoring CPLS. These 500 samples are added after the 1500 normal multimode samples for each following fault scenario.

According to Qin and Zheng (2013), $\Xi_{2,3}$ is chosen to be the first column of $R_c$ and normalized to unit norm, thus the fault occurs in CVS only. The fault detection result is shown in Fig.4. As shown in Fig.4, only index $T_{2,2}^c$ detects the fault, which indicates this is an output-relevant fault. Let $\Xi_{2,3}$ be the first column of $P_x$, thus the fault occurs in IPS only. The fault detection result is shown in Fig.5. As shown in Fig.5 only index $T_{2,2}^x$ detects the fault, which indicates this is an input-relevant fault. Let $\Xi_{2,3}$ be the first column of $P_y$, thus the fault occurs in OPS only. The fault detection result is shown in Fig.6. As shown in Fig.6, only index $T_{2,2}^y$ detects the fault, which indicates this is an output-relevant fault. According to Fig.4 - Fig.6, the process monitoring CPLS can detect main-variable-relevant and quality-variable-relevant faults in the multimode process.

5 CONCLUSIONS

In this paper, an external analysis based CPLS is proposed for multimode industrial process monitoring. The process variables are divided into external variables, main variables and quality variables. Using the external variables as inputs, the mode-detection CPLS model is used to detect mode changes by monitoring the variation of the main variables and
quality variables due to changes in the external variables. After the influence of the external variables is removed from the main and quality variables, another process-monitoring CPLS model is built to detect the main-variable-relevant faults and quality-variable-relevant faults. The proposed method extends the application of CPLS to multimode processes, and is shown to be able to detect mode changes and detect the main-variable-relevant faults and quality-variable-relevant faults.

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