EVOLUTION OF MULTIVARIATE STATISTICAL PROCESS CONTROL: APPLICATION OF INDEPENDENT COMPONENT ANALYSIS AND EXTERNAL ANALYSIS

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Abstract

Univariate and multivariate statistical process control (USPC and MSPC) methods have been widely used in process industries for fault detection. However, their practicability and achievable performance are limited due to the assumptions that a process is operated in a steady state and that variables are normally distributed. In the present work, external analysis is proposed to distinguish from faults from normal changes in operating conditions. To further improve the monitoring performance, a new MSPC method based on independent component analysis (ICA) is proposed. The simulation results of a CSTR process have clearly shown the superiority of the proposed ICA-based SPC over USPC and PCA-based SPC, and also the usefulness of external analysis.

Keywords

Statistical process control, Fault detection, Independent component analysis, External analysis

Introduction

In the last decade or so, various multivariate statistical process control (MSPC) methods have been proposed (Kano et al., 2002a). The most well-known MSPC is based on principal component analysis (PCA). In PCA-based SPC (PCA-SPC), Hotelling T^2 statistic of principal components and the sum of squared residuals Q are monitored (Jackson and Mudholkar, 1979). PCA-SPC has been widely accepted in process industries. However, their practicability and achievable performance are limited due to the assumptions that a process is operated in a steady state and that variables are normally distributed. Operating conditions cannot be constant in many processes due to load changes, product grade transitions, or other causes. In the present work, external analysis is proposed to distinguish between faults in a process and normal changes in operating conditions. In addition, to further improve the monitoring performance, a new MSPC method using independent component analysis (ICA) is proposed based on the idea that extracting essential variables from measured variables and monitoring them will improve the monitoring performance. The effectiveness of ICA-based SPC (ICA-SPC) integrated with external analysis is evaluated with its application to monitoring problems of a continuous-stirred-tank-reactor (CSTR) process.

External Analysis

In the present work, measured variables are classified into two groups. Variables in the first group cause changes in operating conditions, which should be distinguished from faults. Those variables are referred to as external variables, because they are given from the outside of a process as a feed flow rate, set-points of controllers, and so on. The other variables, classified into the second group, are affected by external variables and other disturbances. Those variables are called main variables.

The external analysis was originally developed as a part of constrained PCA for enhancing the performance of PCA by using external information (Takane and Shibayama, 1991). In this section, it is shown that the external analysis can be used for removing the influence of external variables from operation data.

Static External Analysis

Consider a data matrix $\boldsymbol{X}$ consisting of k samples of m variables. For simplicity, each variable is assumed to be normalized. The data matrix $\boldsymbol{X}$ is described as $\boldsymbol{X}=[\ \boldsymbol{H}, \boldsymbol{G}\ ]$, where $\boldsymbol{G}$ consists of external variables and $\boldsymbol{H}$ consists of main variables. The main data matrix $\boldsymbol{H}$ should be decomposed into two parts: a part explained by the external data matrix $\boldsymbol{G}$ and the other part not explained. For this purpose, regression analysis such as ordinary least squares and partial least squares (PLS) can be used by regarding external variables and main variables as inputs and outputs, respectively. A regression coefficient matrix $\boldsymbol{C}$ is determined so that the sum of squared errors or the squared Frobenius norm of an error matrix $\boldsymbol{E}$ is minimized. The error matrix is defined as $\boldsymbol{E}=\boldsymbol{H}-\boldsymbol{GC}$. As a result, the main data matrix $\boldsymbol{H}$ can be decomposed into $\boldsymbol{GC}$ and $\boldsymbol{E}$. Any SPC method can be used for monitoring the error part $\boldsymbol{E}$, which is not affected by the external variables.

Dynamic External Analysis

When process dynamics cannot be ignored, the influence of changes in external variables cannot be removed from operation data by using static external analysis. In such a case, a dynamic model must be built. The simplest approach is the use of past measurements of external variables as inputs. Therefore, the main data matrix $\boldsymbol{H}$ and the external data matrix $\boldsymbol{G}$ are modified as follows:

$$\boldsymbol{H} = \boldsymbol{H}_0 = \left[\boldsymbol{h}^T(s) \quad \cdots \quad \boldsymbol{h}^T(k-1) \quad \boldsymbol{h}^T(k)\right]^T \tag{1}$$

$$\boldsymbol{G} = \left[\boldsymbol{G}_0 \quad \boldsymbol{G}_1 \quad \cdots \quad \boldsymbol{G}_{s-1}\right] \tag{2}$$

$$\boldsymbol{G}_i = \left[\boldsymbol{g}^T(s-i) \quad \cdots \quad \boldsymbol{g}^T(k-i-1) \quad \boldsymbol{g}^T(k-i)\right]^T \tag{3}$$

where s is the number of steps. That is, external data at total s sampling points, $\boldsymbol{g}(t)$, $\boldsymbol{g}(t-1)$, ..., $\boldsymbol{g}(t-s+1)$, are used for estimating main data $\boldsymbol{h}(t)$. This external analysis, proposed in this work, is referred to as dynamic external analysis. It is regarded as identification of an impulse response model.

Independent Component Analysis

ICA (Jutten and Herault, 1991) is a signal processing technique for transforming observed multivariate data into statistically independent components. In this section, an ICA algorithm and ICA-SPC (Kano et al., 2002b) are briefly described.

Algorithm and Example of ICA

It is assumed that each of m measured variables is given as a linear combination of n ($\leq m$) unknown independent components. The independent components and the measured variables are zero mean. The relationship between a measured-variable data matrix $\boldsymbol{X}$ and an independent-component data matrix $\boldsymbol{S}$ is given by $\boldsymbol{X}=\boldsymbol{SA}$, where $\boldsymbol{A}$ is an unknown full-rank matrix, called the mixing matrix. The basic problem of ICA is to estimate the independent-component matrix $\boldsymbol{S}$ or to estimate the mixing matrix $\boldsymbol{A}$ from the measured data matrix $\boldsymbol{X}$ without any knowledge of $\boldsymbol{S}$ or $\boldsymbol{A}$. The practical problem of ICA is to calculate a separating matrix $\boldsymbol{W}$ so that components of the reconstructed data matrix $\boldsymbol{Y}$, given as $\boldsymbol{Y}=\boldsymbol{XW}$, become as independent of each other as possible.

Finding the local extrema of the fourth-order cumulant is equivalent to estimating the non-Gaussian independent components (Delfosse and Loubaton, 1995). In the present work, a fixed-point algorithm (Hyvarinen and Oja, 1997) is used to minimize or maximize the fourth-order cumulant. To perform ICA, measured variables are first transformed into uncorrelated variables with unit variance, because statistical independence is more restrictive than uncorrelation. This pretreatment can be accomplished by PCA, and it is called sphering or prewhitening.

An example of ICA is shown in Fig. 1. Original variables are a sinusoidal variable and a random variable. These two variables s_1 and s_2 are transformed into measured variables x_1 and x_2. First, x_1 and x_2 are sphered by using PCA, and uncorrelated variables z_1 and z_2 are obtained. Then, to obtain independent variables y_1 and y_2, ICA is applied to z_1 and z_2. Figure 1 clearly shows that the original variables can be reconstructed by ICA without any knowledge of the original variables or the mixing matrix.

Monitoring of Independent Components

The procedure of ICA-SPC is similar to USPC. That is, each independent component is monitored. If one or more of the independent component is outside the control limit, the process is judged to be out of control.

In order to realize an advantage in using independent components for process monitoring, the fitness of control limits for monitored variables is illustrated in Fig. 2. The control limits for measured variables x_1 and x_2 are far from the region representing a normal operating condition because these variables are highly correlated. In Fig. 2 (center), two types of control limits for the sphered variables z_1 and z_2 are drawn. The control limits become rectangular when sphered variables are monitored independently. On the other hand, the control limits are integrated into an ellipse when sphered variables are monitored together. The fitness, however, is not perfect. This characteristic limits the achievable performance of PCA-SPC. On the other hand, the control limits perfectly fit the independent components y_1 and y_2. Therefore, ICA-SPC functions better than the others.

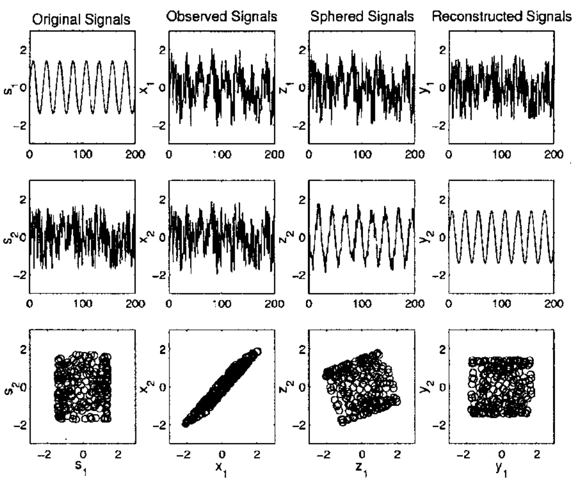

Figure 1. A simple example of ICA.

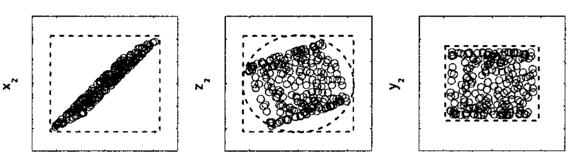

Figure 2. The fitness of control limits for USPC (left), PCA-SPC (center), and ICA- SPC (right).

Application: CSTR Process

In this section, several SPC methods integrated with dynamic external analysis are applied to monitoring problems of a CSTR process (Johannesmeyer and Seborg, 1999) to show the usefulness of dynamic external analysis.

The CSTR process is shown in Fig. 3. The reactor is equipped with a cooling jacket. Operation data sets are generated from 13 operating conditions listed in Table 1. One hundred simulations are carried out in each case. The control limit of each index or variable is determined so that the number of samples outside the control limit is 1% of the entire samples while the process is operated under normal conditions.

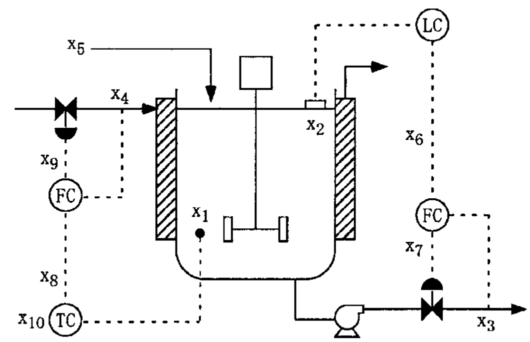

Figure 3. CSTR with feedback control.

Table 1. Faults and condition changes.

Case	Operation Mode
N	normal operation
N1	feed flow rate – step
N2	set-point of reactor temperature – step
F1	catalyst deactivation – ramp
F2	heat exchanger fouling – ramp
F3	dead coolant flow measurement
F4	bias in reactor temp. measurement – step
F5	coolant valve sticking
F6	feed concentration – ramp
F7	feed temperature – ramp
F8	coolant feed temperature – ramp
F9	upstream pressure in coolant line – step
F10	downstream pressure in outlet line – step

Dynamic External Analysis

In this case study, N1 and N2 are regarded as normal changes in operating condition, which should be distinguished from faults. Therefore, the reactor feed flow rate x_5 and the setpoint of temperature controller x_{10} are classified as external variables. The other eight variables are main variables. The results of dynamic external analysis are shown in Fig. 4. After the set-point (SV) of temperature x_{10} is increased stepwise at 40 min., the output (MV) of coolant flow controller x_9 is manipulated, and the coolant flow rate x_4 is decreased. As a result, the reactor temperature x_1 follows its set-point x_{10}. Since this set-point change considerably affects process variables, it is judged to be abnormal if control limits are designed especially for the operating condition at the lower temperature. On the other hand, the fault detection speed deteriorates significantly if control limits are extended for judging both operating conditions to be normal.

Figure 4 (center) shows that the influence of the set-point change can be removed from each measured variable by conducting the dynamic external analysis, and control limits fit variables nicely. In addition, control limits can be adjusted automatically for changes in operating conditions as shown in Fig. 4 (right). The time-variant control limits enable us to monitor measured variables directly. Small fluctuations in time-variant control limits are caused by changes in feed flow rate, which is another external variable.

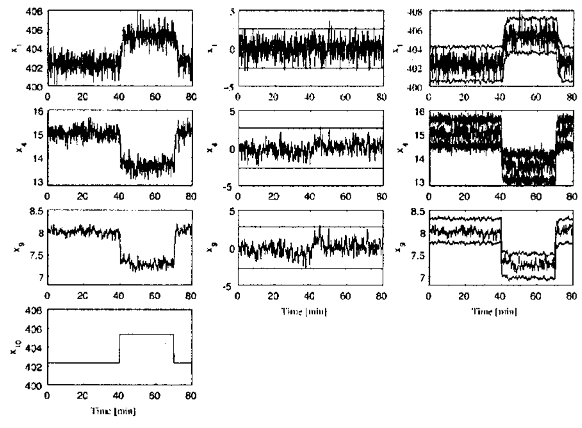

Figure 4. The results of external analysis.

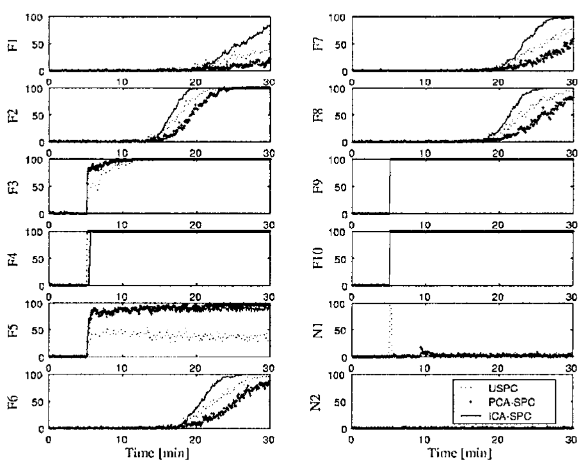

Figure 5. Time-series plots of fault detection rate.

Monitoring Results

Figure 5 shows the fault detection rate in all cases except for case N. The fault detection rate is defined as the percentage (%) of the realizations in which each monitoring method detects the fault at each time step. Therefore, the best monitoring method is the one with the highest fault detection rate. In Fig. 5, each fault or operating condition change occurs at 5 min.

In abnormal cases F1, F2, F6, F7, and F8, the fault detection rate with ICA-SPC is considerably higher than the others. In cases F4, F9, and F10, the fault detection rate reaches 100% within one or two steps. In cases F3 and F5, the fault detection rate of USPC is much lower than the others. These results indicate that the judgment made by ICA-SPC is more reliable than by USPC or PCA-SPC. Higher reliability is an important characteristic of any monitoring method. In cases N1 and N2, changes in the feed flow rate and the set-point of reactor temperature should be judged to be normal, and the fault detection rates should be about 1% throughout the monitoring period because control limits are set as 99% confidence limits. In fact, the fault detection rates are sufficiently low, and it is confirmed that the influence of the external variables could be removed from all main variables.

Conclusions

In the present work, static/dynamic external analysis was proposed to distinguish normal changes in operating conditions from faults, and ICA-SPC was developed to further improve the fault detection performance. The advantages of PCA and ICA can be integrated into combined MSPC (Kano et al., 2002c). The proposed approach based on both external analysis and ICA will be a breakthrough in statistical process monitoring.

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