FAULT DETECTION AND IDENTIFICATION BASED ON DISSIMILARITY OF PROCESS DATA

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Abstract

Multivariate statistical process control (MSPC) has been widely used for process monitoring. When a fault is detected, it is important to identify an actual cause of the fault. Fault identification methods are classified into two groups by availability of historical data sets obtained from faulty situations. When such historical data sets are not available, contributions from process variables to a monitored index can be used for identifying the variables that contribute significantly to an out-of-control value of the index. On the other hand, when historical data sets are available, a fault can be identified by comparing a data set representing the current faulty situation and historical data sets representing past faulty situations. In recent years, a new MSPC method termed “DISSIM,” which is based on the dissimilarity of process data, has been developed. In the present work, DISSIM is extended for fault identification with or without historical data sets. The fault detection and identification performance of DISSIM is compared with that of the conventional MSPC using principal component analysis by applying those methods to monitoring problems of a continuous-stirred-tank-reactor (CSTR) process. The simulated results show that DISSIM as well as cMSPC functions well for fault detection and that DISSIM works better than cMSPC for fault identification.

1 Introduction

In chemical processes, statistical process control (SPC), which is a data-based approach for process monitoring, has been used widely and successfully. As chemical processes become more heavily instrumented and process data are more frequently recorded, this situation causes a data overload, and multivariate SPC (MSPC) has been developed in order to extract useful information from process data and utilize it for process monitoring [1,7].

Many successful applications have shown the practicability of MSPC. To improve the performance of process monitoring, two kinds of statistical process monitoring methods, focusing on the correlation among process variables, were proposed and their performance is investigated [3-6]. One of the two methods, which was termed DISSIM, is based on the idea that a change of operating condition can be detected by monitoring a distribution of time-series data, which reflects the corresponding operating condition.

After a fault is detected, it is important to identify an actual cause of the fault. The fault identification methods are classified into two groups by availability of historical data sets obtained from faulty situations. When such historical data sets are not available, contributions from process variables to a monitored index can be used for identifying the variables that contribute significantly to an out-of-control value of the index [8]. On the other hand, when historical data sets are available, a fault can be identified by comparing a data set representing the current faulty situation and historical data sets representing past faulty situations [9].

In the present work, DISSIM is extended for fault identification with or without historical data sets. First, a contribution of each process variable to the dissimilarity index is introduced for identifying the variables that contribute significantly to an out-of-control value of the dissimilarity index. Then, another fault identification method, which is based on the similarity of data sets representing the current operating situation and past faulty situations, is proposed. The fault detection and identification performance of DISSIM is compared with that of the conventional MSPC (cMSPC) by applying those methods to monitoring problems of a continuous-stirred-tank-reactor (CSTR) process.

2 Fault Detection and Identification with PCA

In the conventional MSPC approach based on PCA, two statistics, $T^2$ and $Q$, are used for monitoring.

$$T^2 = \sum_{r=1}^{R} \frac{t^2_r}{s^2_r}$$

(1)

$$Q = \sum_{p=1}^{P} (x_p - \hat{x}_p)^2$$

(2)

where $t_r$ is the $r$-th score of measurements and $s^2_r$ is the variance of $t_r$. $x_p$ and $\hat{x}_p$ are a measurement of the $p$-th variable and its predicted (reconstructed) value, respectively. $R$ and $P$ denote the number of principal components retained in the PCA model and the number of process variables, respectively.
The $T^2$ statistic is a measure of the variation within the PCA model, and the $Q$ statistic is a measure of the amount of variation not captured by the PCA model.

When an out-of-control signal is detected by $T^2$ or $Q$, it is necessary to identify the process variables that cause the out-of-control signal. This information helps operators to further diagnose an actual cause of the fault. For this purpose, contribution plots can be used. A contribution of the $p$-th variable to the $Q$ statistic is defined as

$$C_p^{(Q)} = (x_p - \bar{x}_p)^2$$

because the $Q$ statistic is a sum of squared prediction errors. On the other hand, a contribution of each variable to the $T^2$ statistic cannot be easily defined. If only one principal component is related to the detected fault, a contribution of the $p$-th variable to the important score can be used. However, this contribution is not sufficient when several scores are related to the fault. Nomikos derived the contribution of the $p$-th variable to the $T^2$ statistic:

$$C_p^{(T^2)} = t^T S_T^{-1} x_p p_p$$

where $t$ and $p_p$ denote a score vector and the transposed $p$-th row vector of the loading matrix $P$, respectively [8]. This contribution can be positive or negative, although the $T^2$ statistic is always positive. In practice, however, only a few variables whose contributions are positive large are important [10].

Another approach to fault identification is the use of process data obtained from several past faulty operating conditions [9]. When such process data are available, a fault can be identified by comparing the similarity between data sets representing past faulty situations. For applying cMSPC-based fault identification, the following procedure is adopted.

1. Apply PCA to data sets representing past faulty situations, and determine reference PCA models.
2. Calculate $T^2$ and $Q$ of the current data using the reference PCA models when a faulty situation is detected.
3. Identify the past faulty situation whose data set gives the smallest $T^2$ and $Q$ of all. Identification with $T^2$ and $Q$ is performed separately.

For fault identification, the data matrix representing the current faulty situation is updated step by step, and it is scaled with the means and the standard deviations obtained from the data set representing the past faulty situations.

3 Monitoring based on Dissimilarity of Process Data

3.1 Fault Detection

Kano et al. proposed a statistical process monitoring method based on the dissimilarity of process data [3,4,6]. The proposed method, termed DISSIM, is based on the idea that a change of operating condition can be detected by monitoring a distribution of process data because the distribution reflects the corresponding operating condition.

On the basis of the fact that the covariance matrix $R$ of the mixture of both data matrices, $X_1$ and $X_2$, can be diagonalized by using an orthogonal matrix $P_0$

$$P_0^T R P_0 = \Lambda,$$

the original data matrices are transformed into

$$Y_i = \sqrt{N_i/(N_1 + N_2)} X_i P_0 \Lambda^{-\frac{1}{2}}$$

where $N_i$ is the number of samples of each data matrix. After this linear transformation, the transformed data matrices, $Y_1$ and $Y_2$, have the same set of principal components and the principal components are reversely ordered. In other words, the most important correlation for one transformed data set $Y_1$ is equivalent to the least important correlation for the other transformed data set $Y_2$, and vice versa. An illustrative example is shown in Fig. 1.

Finally, the following index $D$ was defined for evaluating the dissimilarity of data sets.

$$D = \frac{4}{P} \sum_{j=1}^{P} (\lambda_j - 0.5)^2$$

Here, $P$ is the number of variables and $\lambda_j$ denotes the eigenvalues of the covariance matrix of the transformed data matrix. When data sets are quite similar to each other, the eigenvalues $\lambda_j$ must be near 0.5. On the other hand, when data sets are quite different from each other, the largest and the

![Figure 1: Linear transformation of data sets (from $X_1$ to $Y_1$) for evaluating the dissimilarity. The cases of similar data sets (top) and different data sets (bottom).](image)
smallest eigenvalues should be near one and zero, respectively. Therefore, $D$ must be near zero when two data sets are similar to each other. On the other hand, $D$ should be near one when data sets are quite different from each other.

For applying DISSIM, a reference data set and a control limit must be determined. The following procedure is adopted.

1. Acquire time-series data when a process is operated under a normal condition, and normalize each column (variable) of the data matrix.
2. Determine the size (steps) of time-window, $w$. Generate data sets with $w$ samples from the data by moving the time-window. Then, select a reference data set from the data sets.
3. Calculate the index $D$, and determine the control limit.

For on-line monitoring, the data matrix representing a current operating condition is updated by moving the time-window step by step, and it is scaled with the mean and the variance obtained at step 1. Then, the dissimilarity index $D$ is calculated. If the index is outside the control limit, the process is judged to be out of control.

### 3.2 Fault Identification without historical data

A contribution of each monitored variable to the dissimilarity index is introduced for identifying the variables that contribute significantly to an out-of-control value of the index.

Since the dissimilarity index is a function of eigenvalues of the covariance matrix of the transformed data matrix, the most contributive eigenvalue to $D$ and the corresponding eigenvector can easily be determined. However, the following two problems should be recognized here.

Problem 1: The data matrix is transformed, and therefore each loading is not directly related to each original variable.

Problem 2: The data matrix consists of $w$ samples where $w$ is the size of time-window.

For solving the first problem, the data matrix has to be inverse-transformed into the original matrix. Since the linear transformation of $X_i$ into $Y_i$ can be simply expressed by

$$Y_i = X_i A$$

from Equation (6), the score vector related to the most contributive eigenvector is given by

$$t_1^T = Y_i w_1^{(i)} = X_i A w_1^{(i)} = \sum_{p=1}^P x_p^{(i)}(A w_1^{(i)})_p$$

where $x_p^{(i)}$ is the $p$-th column vector in $X_i$ and $(A w_1^{(i)})_p$ denotes the $p$-th element of $A w_1^{(i)}$.

### 3.3 Fault Identification with historical data

When several past faulty operating data sets are available, a fault can be identified by comparing the similarity between data sets representing faulty operating conditions in the past and the data set representing an operating condition when the fault is detected. Therefore, DISSIM can be easily extended, and it can be used for fault identification as well as fault detection.

Since data sets can be compared on the basis of the dissimilarity index $D$, the similarity index $S = 1 - D$ can be defined. For applying DISSIM-based fault identification, the following procedure is adopted.

1. Prepare reference data sets representing past faulty situations. Each data set consists of $w$ samples.
2. Calculate the similarity index $S$ between the current data set and the reference data sets when a faulty situation is detected.
3. Identify the past faulty situation whose data set has the largest $S$ of all.

### 4 Application

In this section, univariate SPC (USPC), the conventional MSPC (cMSPC), and DISSIM are applied to monitoring problems of a CSTR process [2].

#### 4.1 CSTR

The CSTR process used for dynamic simulations is shown in Fig. 2. The process has two manipulated variables and five continuous process measurements. A total of nine variables used for monitoring are listed in Table 1. Process data are

| $x_1$ | reactor temperature |
| $x_2$ | reactor level |
| $x_3$ | reactor outlet flow rate |
| $x_4$ | coolant flow rate |
| $x_5$ | reactor feed flow rate |
| $x_6$ | MV of level controller |
| $x_7$ | MV of outlet flow controller |
| $x_8$ | MV of temperature controller |
| $x_9$ | MV of coolant flow controller |

Table 1: Process variables used for monitoring.
Figure 2: CSTR with feedback control.

<table>
<thead>
<tr>
<th>Case</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>normal operation</td>
</tr>
<tr>
<td>F1</td>
<td>catalyst deactivation - ramp</td>
</tr>
<tr>
<td>F2</td>
<td>heat exchanger fouling - ramp</td>
</tr>
<tr>
<td>F3</td>
<td>dead coolant flow measurement</td>
</tr>
<tr>
<td>F4±</td>
<td>bias in reactor temperature measurement</td>
</tr>
<tr>
<td>F5</td>
<td>coolant valve stiction</td>
</tr>
<tr>
<td>F6±</td>
<td>feed flow rate - step</td>
</tr>
<tr>
<td>F7±</td>
<td>feed concentration - ramp</td>
</tr>
<tr>
<td>F8±</td>
<td>feed temperature - ramp</td>
</tr>
<tr>
<td>F9±</td>
<td>coolant feed temperature - ramp</td>
</tr>
<tr>
<td>F10±</td>
<td>upstream pressure in coolant - step</td>
</tr>
<tr>
<td>F11±</td>
<td>downstream pressure in outlet line - step</td>
</tr>
<tr>
<td>S1±</td>
<td>reactor temperature set-point change - step</td>
</tr>
</tbody>
</table>

Table 2: Process disturbances for the CSTR process. The symbol ± indicates that there are two types of changes, i.e. increase (+) and decrease (−).

generated from a normal operating condition and 20 abnormal operating conditions listed in Table 2. All variables are measured every five seconds.

4.2 Settings for Monitoring

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 a normal condition. On the basis of these control limits, the fault detection performance is evaluated by the following steps.

1. Each monitoring method is applied to the data in all cases, and each index is calculated.

2. For the data obtained after the occurrence of a fault, the percentage of the samples outside the control limit is calculated in each simulation. This percentage is termed “reliability” in the present work.

3. The average reliability of 100 simulations is calculated in each case.

Figure 3: Monitoring results in case F7+. $T^2$, $Q$, and $D$ are shown from the top (solid line) with their control limits (dotted line). A disturbance occurs at step 101.

Since the control limits are determined so that they represent 99% confidence limits, a monitoring method is regarded as successful in detecting the abnormal condition if the reliability is considerably higher than 1%. The reliability is affected by the number of samples used for calculating it. In the present work, 200 samples (about 17 min) are used for calculating the reliability.

In addition, the fault identification performance is evaluated by using a success rate of fault identification, $SR_{FID}$.

$$SR_{FID} = \frac{N_{FID}}{N_{FD}} \times 100 \%$$

where $N_{FID}$ is the number of samples at which a fault is detected and correctly identified. $N_{FD}$ is the number of samples at which a fault is detected. The success rate is calculated from 10 simulated data sets in each case.

4.3 Results and Discussion

The fault detection results are summarized in Table 3. To obtain those results, several different design parameters such as the number of principal components and the size of time-window were tried, and then the best parameters were selected.

In many cases, the reliability of cMSPC and DISSIM is considerably better than that of USPC. Those results indicate the importance of taking account of the correlation between variables for fault detection. On the other hand, the reliability of cMSPC and DISSIM is quite similar. In general, DISSIM is better than cMSPC for detecting small changes of operating conditions. In this case study, however, faults, disturbances, and set-point changes are so large that cMSPC and DISSIM give similar performance.

The fault detection results in case F7+ are shown in Fig. 3. It should be noted that the reliability in Table 3 is not equivalent to the reliability estimated from Fig. 3, because the results from one of the 100 realizations are shown in this figure.
Table 3: Fault detection performance (Reliability [%]) of SPC methods.

![Figure 4: Time-series contributions of process variables to the $Q$ statistic in case F3. A disturbance occurs at step 101.](image)

![Figure 5: Time-series contributions of process variables to the dissimilarity index $D$ in case F3. A disturbance occurs at step 101.](image)

To validate the usefulness of the proposed contribution of each process variable to the dissimilarity index, the contribution plots in the case F3 are shown in Figs. 4 and 5. In these figures, a contribution of each variable is zero when an out-of-control signal is not detected.

In the case F3, coolant flow measurement is dead at step 101. This fault can be easily detected by using both cMSPC and DISSIM. The contribution plots to the $Q$ statistic seem to indicate that a fault or disturbance is related to the coolant flow control loop, because PV (process variable) and MV (manipulated variable) of coolant flow rate are contributing significantly to the index. Although contribution plots to $T^2$ are not shown due to the limited space, the variables contributing significantly are $x_1, x_8,$ and $x_9$. This result implies that a fault or disturbance is related to the reactor temperature control loop. On the other hand, the variables contributing significantly to the dissimilarity index $D$ are five variables just after the fault occurs, and then MV of coolant flow rate becomes the most suspected variable. This result can be interpreted as that coolant flow rate should be checked first, because MV is calculated with the control algorithm and it is affected only by PV. Therefore, the information obtained from the contribution plots is useful for investigating the cause of the fault.

In general, fault identification based only on contribution plots is quite difficult. It should be emphasized that not only the information from contribution plots but also knowledge of the process has to be used for fault identification.

The fault identification results with historical data sets are summarized in Table 4. It should be noted that 10 reference data sets are generated for representing each faulty situation by moving a time-window of 150 steps every 36 steps (3 min). The operating condition is time-variant after a fault occurs; therefore, several reference data sets representing the same faulty situation but different time periods should be simultaneously compared with the current data set. Table 4 shows the superiority of DISSIM over cMSPC. In cases F2, F4, F5, F9, F10, and S1, the success rates of fault identification with DISSIM are higher than those of cMSPC. DISSIM-based fault identification functions better than a cMSPC-based method, because a time-window is used for calculating the similarity index and thus more information can be used in the DISSIM-based method.
5 Conclusions

New fault identification methods, based on the similarity of process data sets, were proposed. One of MSPC methods, DISSIM, was extended for fault identification with or without historical data sets. The fault detection and identification performance of the proposed methods was compared with that of the conventional MSPC method by applying those methods to monitoring problems of a CSTR process. The simulated results show that DISSIM as well as cMSPC functions well for fault detection in comparison with USPC and that DISSIM works better than cMSPC for fault identification.

Acknowledgment

The authors gratefully acknowledge the financial support from the Japan Society for the Promotion of Science (JSPS-RFTF96R14301).

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