독립요소분석을 이용한 통계 공정 모니터링

이종민, 유창규, 이인범
포항공과대학교 화학공학과

Statistical Process Monitoring with Independent Component Analysis

Jong-Min Lee, ChangKyoo Yoo, In-Beum Lee
Department of Chemical Engineering, POSTECH

Introduction

For a safe operation of chemical process, it is important to detect faults, process upsets, or other special events as rapidly as possible and then to find and remove the factors causing those events. Until now, monitoring using multivariate statistical methods such as PCA have been modified and developed to analyze the high dimensional and correlated data [1,2].

It is known that many of the monitored process variables are not independent. They could be combinations of some independent components that may not be directly measurable. Independent component analysis (ICA) can find these underlying factors from multivariate statistical data. ICA is a recently developed method in signal processing where the goal is to find a linear representation of non-Gaussian data so that the components are statistically independent [3]. A number of ICA have been reported in speech processing, biomedical signal processing, feature extraction, financial time series analysis, data mining, and so on. Whereas PCA can only impose independence up to the second order (mean and variance) while constraining the direction vectors to be orthogonal, PCA imposes statistical independence up to more than second order on the individual component and has no orthogonality constraint [4]. Hence, ICA can reveal more useful information than PCA. Furthermore, the conventional SPM (statistical process monitoring) methods using PCA are based on the assumption that the measured values of product quality are normally distributed. However, such assumption is often invalid for the measurements gained from actual chemical processes because of their dynamic and nonlinear nature. In the present work, a new statistical monitoring method based on ICA and kernel density estimation [5] is proposed. For investigating the feasibility of the proposed method, its fault detection performance is evaluated and compared with that of PCA monitoring method by applying those methods to the simulation benchmark of biological wastewater treatment process.

Independent Component Analysis (ICA)

To introduce the ICA algorithm, it is assumed that *d* measured variables $x_1, x_2, \ldots, x_d$ are given as linear combinations of m ($\leq d$) unknown independent components $s_1, s_2, \ldots, s_m$. The independent components and the measured variables are zero mean. The relationship between them is given by

$$\mathbf{X} = \mathbf{AS} + \mathbf{E} \tag{1}$$

where $\mathbf{X} = [\mathbf{x}(1), \mathbf{x}(2), \ldots, \mathbf{x}(n)] \in R^{d\times n}$ is the data matrix, $\mathbf{A} = [\mathbf{a}_1, \ldots, \mathbf{a}_m] \in R^{d\times m}$ is the mixing matrix, $\mathbf{S} = [\mathbf{s}(1), \mathbf{s}(2), \ldots, \mathbf{s}(n)] \in R^{m\times n}$ is the independent component matrix, $\mathbf{E} \in R^{d\times n}$ is the residual matrix, and *n* is the number of sample. Here, we assume $d \geq m$; when d equals m, the residual matrix, $\mathbf{E}$, becomes the zero matrix. The basic problem of ICA is to estimate the original components **S** or to estimate **A** from **X** without any knowledge of them. Therefore, the objective of ICA is to calculate a separating matrix **W** so that components of the reconstructed data matrix **S**, given as

$$\mathbf{S} = \mathbf{WX} \tag{2}$$

becomes as independent of each other as possible. Using ICA algorithm, we can obtain the rows of **S** whose norm is 1.

The initial step in ICA is whitening, which transforms measured variables $\mathbf{x}(k)$ into uncorrelated variables $\mathbf{z}(k)$ with unit variance. The whitening matrix $\mathbf{Q}$ is given by $\mathbf{Q} = \mathbf{\Lambda}^{-\frac{1}{2}}\mathbf{U}^T$, where $\mathbf{\Lambda} = diag[\lambda_1, \ldots, \lambda_d]$ is diagonal matrix whit the eigenvalues of the data covariance matrix $E(\mathbf{x}(k)\mathbf{x}^T(k))$ and $\mathbf{U}$ is a matrix with the corresponding eigenvalues as its columns. By defining the whitening matrix as $\mathbf{Q}$ and **B**=**QA,** the relationship between **z** and **s** is given as.

$$\mathbf{z}(k) = \mathbf{Qx}(k) = \mathbf{QAs}(k) = \mathbf{Bs}(k) \tag{3}$$

Since **s** are mutually independent and **z** are mutually uncorrelated,

$$E\{\mathbf{z}(k)\mathbf{z}^T(k)\} = \mathbf{B}E\{\mathbf{s}(k)\mathbf{s}^T(k)\}\mathbf{B}^T = \mathbf{B}\mathbf{B}^T = \mathbf{I}\ . \quad (4)$$

We have therefore reduced the problem of finding an arbitrary full-rank matrix **A** to the simpler problem of finding an orthogonal matrix **B**, which then gives

$$\mathbf{s}(k) = \mathbf{B}^T\mathbf{z}(k) = \mathbf{B}^T\mathbf{Q}\mathbf{x}(k)\ . \quad (5)$$

From Eqs. (2) and (5), the relation between **W** and **B** can be expressed as

$$\mathbf{W} = \mathbf{B}^T\mathbf{Q}\ . \quad (6)$$

To calculate **B**, it should be updated so that $\mathbf{s}$ may have great non-Gaussianity. There are two common measures of non-Gaussianity: kurtosis and negentropy [3]. Kurtosis is sensitive to outliers. On the other hand, negentropy is based on the information-theoretic quantity of (differential) entropy. Tthe negentropy J can be approximated as follows [3]:

$$J(y) \approx [E\{G(y)\} - E\{G(v)\}]^2 \quad (7)$$

where y is assumed to be of zero mean and unit variance, v is a Gaussian variable of zero mean and unit variance, and G is any non-quadratic function. Hyvärinen and Oja (2000) suggests a number of functions for G:

$$G_1(u) = \frac{1}{a_1}\log\cosh(a_1 u)\ ,\quad G_2(u) = \exp(-a_2 u^2/2)\ ,\quad G_3(u) = u^4 \quad (8)$$

where $1 \le a_1 \le 2$. Among these three functions, G_1 is a good general-purpose contrast function and was therefore selected for use in the present study.

Based on their approximate form for the negentropy, Hyvärinen and Oja (2000) introduced a very simple and highly efficient fixed-point algorithm for ICA, calculated over sphered zero-mean vectors $\mathbf{z}$. This algorithm calculates one column of the separating matrix **B** and allows the identification of one independent component; the corresponding IC can then be found using Eqs. (5). The algorithm is repeated to calculate each independent component. The algorithm is as follows,

1. Take a random initial vector $\mathbf{b}_0$ of unit norm. Let $i = 1$.
2. Let $\mathbf{b}_i{*} = E\{\mathbf{z}g(\mathbf{b}^T{}_{i-1}\mathbf{z})\} - E\{g'(\mathbf{b}^T{}_{i-1}\mathbf{z})\}\mathbf{b}_{i-1}$, where g is one of the derivatives of G_s presented in Eqs. (15), (16) and (17).
3. Divide $\mathbf{b}_i = \dfrac{\mathbf{b}_i{*}}{\|\mathbf{b}_i{*}\|}$
4. If $|\mathbf{b}_i{}^T\mathbf{b}_{i-1}|$ differs from 1 by more than a predetermined tolerance, let $i = i + 1$ and go back to Step 2. Otherwise, output the vector $\mathbf{b}_i$.

In order to estimate more than one solution, up to a maximum of m solutions, the algorithm can be run as many times as required. After one has estimated p vectors, $\mathbf{b}_1, \mathrm{K}\ , \mathbf{b}_p$, the decorrelation procedure entails two simple additional steps for $\mathbf{w}_{p+1}$. First, let

$$\mathbf{b}_{p+1} = \mathbf{b}_{p+1} - \sum_{j=1}^{p}\mathbf{b}_{p+1}{}^T\mathbf{b}_j\mathbf{b}_j \quad (9)$$

and then

$$\mathbf{b}_{p+1} = \frac{\mathbf{b}_{p+1}}{\|\mathbf{b}_{p+1}\|} \quad (10)$$

Note that the final vector $\mathbf{b}_i$ given by the algorithm equals one of the columns of the (orthogonal) mixing matrix **B** shown in Eq. (5). After calculating **B**, we can obtain demixing matrix **W** from Eq. (6). For more details on the FastICA algrothm, see Hyvärinen and Oja (2000).

Process Monitoring Statistics based on ICA

We can obtain $\mathbf{B}$, $\mathbf{W}$, and $\mathbf{S}_{normal}$ from applying ICA to the normal operating data. Then, they are separated into the deterministic part ($\mathbf{B}_d$, $\mathbf{W}_d$, $\mathbf{S}_d$) and excluded part ($\mathbf{B}_e$, $\mathbf{W}_e$, $\mathbf{S}_e$). The monitoring statistics $I^2(k) = \mathbf{s}_d(k)^T \mathbf{s}_d(k)$, $I_e^{\,2}(k) = \mathbf{s}_e(k)^T \mathbf{s}_e(k)$, $SPE(k) = \sum_{j=1}^{d}(x_j(k) - \hat{x}_j(k))^2$ of normal operating condition are calculated and their confidence limits are obtained by kernel density estimation. For on-line monitoring, new independent data matrices, $\mathbf{S}_{newd}$ and $\mathbf{S}_{newe}$ can be obtained if new data $\mathbf{X}$ ($\mathbf{X}_{new}(J \times k)$) is transformed through the separating matrices $\mathbf{W}_d$ and $\mathbf{W}_e$, i.e., $\mathbf{S}_{newd} = \mathbf{W}_d \mathbf{X}_{new}$ and $\mathbf{S}_{newe} = \mathbf{W}_e \mathbf{X}_{new}$, respectively. After calculating the monitoring statistics for new data, they are compared against the normal operating data.

Illustrative Example

The proposed ICA monitoring algorithm is applied to the detection of various disturbances in the simulated data on the basis of benchmark simulation. The IAWQ model No. 1 and a ten-layer settler model are used to simulate the biological reactions and the settling process, respectively. Fig. 1 shows the flow diagram of the modeled WWTP system. Influent data and operation parameters developed by a working group on benchmarking of wastewater treatment plants, COST 624, are used in the simulation [6]. We used seven variables among many variables used in the benchmark to build monitoring system since they are typically monitored and important variables in real WWT systems. The variables are listed in Table 1. We used 14 days as a normal data set developed by the benchmark, where the training model was based on a normal operation period for one week of dry weather and validation data was used on data set for last 7 days. The internal disturbance was imposed by decreasing nitrification rate in the biological reactor, the specific growth rate for the autotrophs is decreased in benchmark. The autotrophic growth rate at sample 288 is decreased rapidly from 0.5 to 0.4 day^{-1} and linearly decreased from 0.4 to 0.2 day^{-1} until sample 480. In this case, as shown in Fig. 2, PCA indicates many false alarms even under normal operating data and cannot detect the internal disturbance when disturbance occurs since the periodic features of wastewater plant are dominant and indicate. The same condition is applied to ICA. In this case, the fault detection is allowable. The ICA monitoring charts are shown in Fig. 3. I^2 value increases rapidly around sample 288 and reveals a diurnal variation, which indicates successive fault detection. And there is no false alarm under normal operating data. In Fig. 4, contribution plots for ICA monitoring charts are displayed. From contribution plot for I^2 at sample 600, we can conclude that variable 1 ($S\text{-}NH_{in}$), variable 4 ($S\text{-}O_3$) and variable 5($S\text{-}NO_2$) are primarily contributed to the I^2 statistic.

Conclusions

This paper proposes a new monitoring approach using ICA method for multivariate statistical process control. Monitoring using ICA gives more sophisticated results rather than conventional method using PCA since ICA imposes statistical independence up to more than second order on the individual component and has no orthogonality constraint. Especially, when the measured variables have non-Gaussian distribution, monitoring using ICA with kernel density estimation can give better result. The proposed monitoring method is applied to the simulation benchmark of biological wastewater treatment process and shows the power and advantages of the ICA monitoring over PCA monitoring.

Acknowledgement

This work was supported by the Brain Korea 21 project.

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Table 1. Variables used in the monitoring of the benchmark model

No.	Symbol	Meaning
1	$S\text{-}NH_{in}$	Influent ammoniac conc.
2	Q_{in}	Influent flow rate
3	TSS_4	Total suspended solid (reactor 4)
4	$S\text{-}O_3$	Dissolved oxygen conc. (reactor 3)
5	$S\text{-}O_4$	Dissolved oxygen conc. (reactor 4)
6	KLa_5	Oxygen transfer coefficient (reactor 5)
7	$S\text{-}NO_2$	Nitrate conc. (reactor 2)

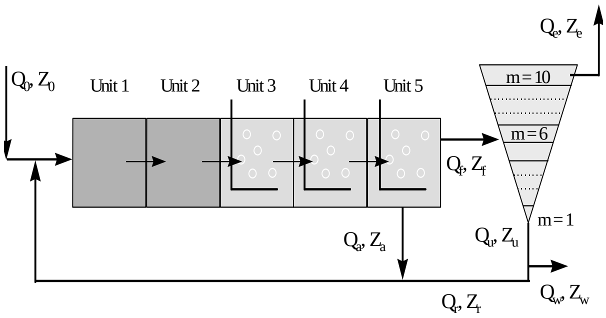

Fig.1. Process layout for the simulation benchmark.

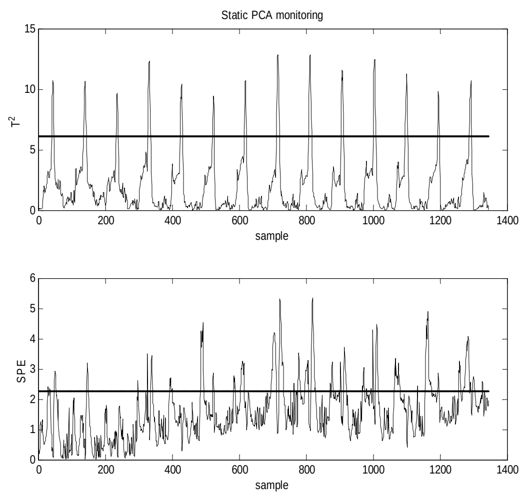

Fig. 2. PCA monitoring charts: T^2 and *SPE* plots when deteriorating nitrification occurs in benchmark simulation.

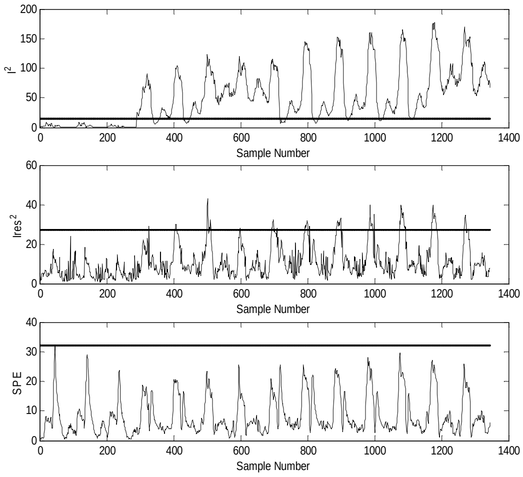

Fig. 3. ICA monitoring charts: I^2, I_e^2 and *SPE* plots when deteriorating nitrification occurs in benchmark simulation.

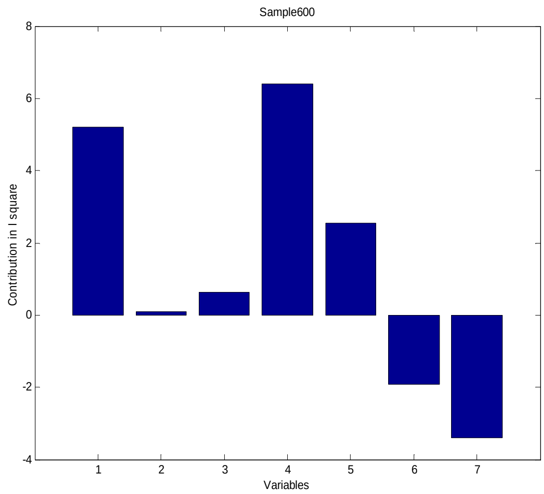

Fig. 4. Variables contributing to the deviation in SPE at sample 60