Chinese Journal of Chemical Engineering 23 (2015) 162–172

Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/CJCHE

Process Systems Engineering and Process Safety

A new process monitoring method based on noisy time structure independent component analysis☆

Lianfang Cai, Xuemin Tian *

College of Information and Control Engineering, China University of Petroleum, Qingdao 266580, China

ARTICLE INFO

Article history:
Received 7 April 2013
Received in revised form 5 June 2013
Accepted 16 June 2013
Available online 1 November 2014

Keywords:
Process monitoring
Independent component analysis
Measurement noises
Kurtosis
Mixing matrix
Contribution plot
Sensitivity analysis

ABSTRACT

Conventional process monitoring method based on fast independent component analysis (FastICA) cannot take the ubiquitous measurement noises into account and may exhibit degraded monitoring performance under the adverse effects of the measurement noises. In this paper, a new process monitoring approach based on noisy time structure ICA (NoisyTSICA) is proposed to solve such problem. A NoisyTSICA algorithm which can consider the measurement noises explicitly is firstly developed to estimate the mixing matrix and extract the independent components (ICs). Subsequently, a monitoring statistic is built to detect process faults on the basis of the recursive kurtosis estimations of the dominant ICs. Lastly, a contribution plot for the monitoring statistic is constructed to identify the fault variables based on the sensitivity analysis. Simulation studies on the continuous stirred tank reactor system demonstrate that the proposed NoisyTSICA-based monitoring method outperforms the conventional FastICA-based monitoring method.

1. Introduction

As modern industrial processes become more and more complex, process monitoring plays a key role in ensuring the process safety, product quality and economic profit. With a large number of process variables measured in industrial processes, multivariate statistical process monitoring (MSPM) techniques [1–4] which are a popular kind of data-driven methods are developing rapidly for the process fault detection and identification. The MSPM methods transform high-dimensional measured data into low-dimensional space to extract meaningful information for detecting and identifying abnormal situations of industrial processes. Among the numerous MSPM methods, principal component analysis (PCA) is a classical approach. It extracts uncorrelated latent variables called principle components (PCs) which capture the most variances of the original variables and has many extended versions for fault detection and identification [5–8]. However, PCA can only consider up to the second-order variance–covariance statistic and cannot make use of higher-order statistical information contained in the process data [9], which may lead to inadequate feature extraction and degraded monitoring performance. Furthermore, PCA makes a strict assumption that the extracted PCs follow multivariate Gaussian distributions to determine the control limits of the monitoring statistics. In most cases, the essential latent variables of industrial processes obey non-Gaussian distributions [10], and thus, there is a great possibility that this assumption cannot be in accordance with realistic industrial situations.

Recently, a newly emerging MSPM approach called independent component analysis (ICA) is attracting more and more attention from both the academic researchers and process engineers. Different from PCA, ICA can further utilize the higher-order negentropy statistic [11] or the second-order time-delayed covariance statistic [12] to recover mutually independent non-Gaussian latent variables called independent components (ICs) from the original measured variables and can be applied to deal with non-Gaussian processes which are more practical in the real-world manufacturing environment [13]. Kano *et al.* [14] proposed an ICA-based univariate statistical process monitoring (USPM) method and demonstrated its superiority over the PCA-based MSPM. But the number of ICs' monitoring charts is comparatively large, which would raise the burden on the process monitoring. To solve such problem, Lee *et al.* [15] constructed three Mahalanobis-type monitoring statistics based on the extracted ICs and thus developed an ICA-based MSPM method. On the basis of this work, various improved versions of ICA were proposed by taking different process characteristics into account. Stefatos and Hamza [16] proposed a dynamic independent component analysis (DICA) method for capturing process dynamic pattern. Odiowei and Cao [17] combined canonical variate analysis (CVA) with ICA and developed a state-space ICA method for dynamic

☆ Supported by the National Natural Science Foundation of China (61273160), the Natural Science Foundation of Shandong Province (ZR2011FM014), the Fundamental Research Funds for the Central Universities (12CX06071A), and the Postgraduate Innovation Funds of China University of Petroleum (CX2013060).

* Corresponding author.
E-mail address: tianxm@upc.edu.cn (X. Tian).

http://dx.doi.org/10.1016/j.cjche.2014.10.006
1004-9541/

process monitoring. Tian *et al.* [18] proposed a multiway kernel independent component analysis (KICA) method for monitoring nonlinear batch process. Considering the extraction of non-Gaussian feature and the preservation of the local neighborhood structure simultaneously, Cai *et al.* [19] integrated KICA with locality preserving projections (LPP) for nonlinear process monitoring. To account for the process multimodal characteristic, Zhang *et al.* [20] developed a modified KICA based process monitoring method by the introduction of the Kronecker product. Rashid and Yu [21] proposed a hidden Markov model based adaptive ICA approach for monitoring processes with multimodality. In these studies, the well-known fast ICA algorithm (FastICA) [22] was adopted as a promising feature extraction technique. However, these FastICA-based process monitoring methods commonly used noise-free ICA model and thus could not take the influence of measurement noises into consideration. In fact, measurement noises always exist in industrial processes and thus inevitably contaminate measured data [23,24]. Under the adverse effects of measurement noises, the monitoring performances of these FastICA-based monitoring methods may decline drastically. Consequently, developing an improved ICA-based monitoring method which can eliminate or attenuate the effects of measurement noises is extremely important for enhancing the process monitoring performance. To the best of our knowledge, currently, there is one monitoring method based on probabilistic ICA (PICA) [24] that can consider the measurement noises explicitly and can obtain the ICs without noises from the normal offline data. Nevertheless, the ICs calculated online are still corrupted by noises and thus cannot effectively reflect the real process information.

Motivated by the above analysis, a new process monitoring method based on noisy time structure ICA (NoisyTSICA) is proposed in this paper. The process data are described with a noisy ICA model and conducted robust prewhitening with the covariance matrix of the measurement noises to obtain the whitened data. The NoisyTSICA objective function is then constructed based on the time structure of the whitened data and optimized by the gradient descent algorithm to estimate the mixing matrix and extract the ICs. Furthermore, a monitoring statistic is built to conduct fault detection by using the recursive kurtosis estimations of the dominant ICs. Lastly, a contribution plot for the constructed monitoring statistic is established to identify the fault variables by applying sensitivity analysis. A simple example of estimating the mixing matrix and a process monitoring example of the continuous stirred tank reactor are used to demonstrate the effectiveness of the proposed monitoring method.

2. FastICA-based Monitoring Method

The conventional monitoring methods based on ICA usually adopt the noise-free ICA model as follows

$$\boldsymbol{x} = \boldsymbol{A}\boldsymbol{s} \tag{1}$$

where $\boldsymbol{x} = [x_1, x_2, \cdots, x_m]^{\mathrm{T}} \in R^{m\times 1}$ denotes the vector of the zero-mean measured variables, $\boldsymbol{s} = [s_1, s_2, \cdots, s_m]^{\mathrm{T}} \in R^{m\times 1}$ is the vector of the zero-mean ICs and $\boldsymbol{A} \in R^{m\times m}$ is the unknown mixing matrix.

ICA tries to estimate both $\boldsymbol{A}$ and $\boldsymbol{s}$ only from $\boldsymbol{x}$. Equivalently, the objective of ICA can be defined as follows: to find a de-mixing matrix $\boldsymbol{W} \in R^{m\times m}$ which can make the elements of the estimated vector $\hat{\boldsymbol{s}} \in R^{m\times 1}$ given by

$$\hat{\boldsymbol{s}} = [\hat{s}_1, \hat{s}_2, \cdots, \hat{s}_m]^{\mathrm{T}} = \boldsymbol{W}\boldsymbol{x} \tag{2}$$

be as independent of each other as possible.

Usually, the measured variables need to be whitened firstly. The whitened variables $\boldsymbol{z} \in R^{m\times 1}$ are obtained by

$$\boldsymbol{z} = \boldsymbol{Q}\boldsymbol{x} \tag{3}$$

where $\boldsymbol{Q} = \mathrm{diag}(\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \cdots, \boldsymbol{\lambda}_m)^{-1/2}[\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \cdots, \boldsymbol{\beta}_m]^{\mathrm{T}} \in R^{m\times m}$ denotes the whitening matrix, $\boldsymbol{\lambda}_i, i = 1, 2, \cdots, m$ are the eigenvalues of the measured variables' covariance matrix $\mathbf{C}_x = \mathrm{E}(\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}) \in R^{m\times m}$ and satisfy the condition $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$, $\mathrm{diag}(\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \cdots, \boldsymbol{\lambda}_m)$ denotes the $m \times m$ diagonal matrix with $\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \cdots, \boldsymbol{\lambda}_m$ as its diagonal elements, $\boldsymbol{\beta}_i$, $i = 1, 2, \cdots, m$ are the eigenvectors of $\mathbf{C}_x$ and $\mathrm{E}(\cdot)$ denotes the expectation operator.

Then, the whitened variables satisfy the condition

$$\mathrm{E}\left(\boldsymbol{z}\boldsymbol{z}^{\mathrm{T}}\right) = \boldsymbol{I}_m \tag{4}$$

where $\boldsymbol{I}_m \in R^{m\times m}$ is the identity matrix.

For the mathematical convenience, all the ICs can be assumed to have the unit variance without loss of generality. Then Eq. (2) is reformulated as

$$\hat{\boldsymbol{s}} = \boldsymbol{W}\boldsymbol{x} = \boldsymbol{U}\boldsymbol{Q}\boldsymbol{x} = \boldsymbol{U}\boldsymbol{z} \tag{5}$$

where $\boldsymbol{W} = \boldsymbol{U}\boldsymbol{Q}$, $\boldsymbol{U} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_m]^{\mathrm{T}} \in R^{m\times m}$ is an orthogonal matrix due to the reason that $\mathrm{E}(\hat{\boldsymbol{s}}\hat{\boldsymbol{s}}^{\mathrm{T}}) = \mathrm{E}(\boldsymbol{U}\boldsymbol{z}\boldsymbol{z}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}}) = \boldsymbol{U}\mathrm{E}(\boldsymbol{z}\boldsymbol{z}^{\mathrm{T}})\boldsymbol{U}^{\mathrm{T}} = \boldsymbol{U}\boldsymbol{U}^{\mathrm{T}} = \boldsymbol{I}_m$.

Thus, the problem of estimating the ordinary matrix $\boldsymbol{W}$ is converted to a simpler problem of estimating the orthogonal matrix $\boldsymbol{U}$. To calculate $\boldsymbol{U}$, the FastICA algorithm based on the maximum negentropy criterion [22] is widely used in the conventional ICA-based monitoring methods [13–18]. The optimization objective of FastICA is defined as follows

$$\begin{aligned} &\max_{\boldsymbol{u}^{\mathrm{T}}\in\boldsymbol{U}} J_1\left(\boldsymbol{u}^{\mathrm{T}}\right) = \max_{\boldsymbol{u}^{\mathrm{T}}\in\boldsymbol{U}} \left(\mathrm{E}\left(\mathrm{G}\left(\boldsymbol{u}^{\mathrm{T}}\boldsymbol{z}\right)\right) - \mathrm{E}(\mathrm{G}(\upsilon))\right)^2 \\ &\text{s.t. } \mathrm{E}\left(\left(\boldsymbol{u}^{\mathrm{T}}\boldsymbol{z}\right)^2\right) = 1,\ \boldsymbol{u}^{\mathrm{T}}\boldsymbol{u} = 1 \end{aligned} \tag{6}$$

where $\boldsymbol{u}^{\mathrm{T}} \in R^{1\times m}$ is a row vector of the orthogonal matrix $\boldsymbol{U}$, υ is a Gaussian variable with zero mean and unit variance, and $\mathrm{G}(\cdot)$ is a non-quadratic function and can be chosen as $\mathrm{G}(\boldsymbol{u}^{\mathrm{T}}\boldsymbol{z}) = -\exp(-(\boldsymbol{u}^{\mathrm{T}}\boldsymbol{z})^2/2)$. The specific details of FastICA can be found in reference [22].

Once the orthogonal matrix $\boldsymbol{U}$ is obtained, the ICs are estimated by Eq. (5) and arranged in the descending order according to their non-Gaussian degrees measured by the negentropy statistic [18]. The row vectors of $\boldsymbol{U}$ are also ordered correspondingly. The mixing matrix is then estimated by $\hat{\boldsymbol{A}} = (\boldsymbol{U}\boldsymbol{Q})^{-1}$. To conduct fault detection, the two monitoring statistics are defined as follows [9,11,15–18,24]

$$I^2(t) = (\boldsymbol{U}_d\boldsymbol{Q}\boldsymbol{x}(t))^{\mathrm{T}}(\boldsymbol{U}_d\boldsymbol{Q}\boldsymbol{x}(t)) = \hat{\boldsymbol{s}}_d(t)^{\mathrm{T}}\hat{\boldsymbol{s}}_d(t) \tag{7}$$

$$SPE(t) = \left(\boldsymbol{x}(t) - \boldsymbol{Q}^{-1}\boldsymbol{U}_d{}^{\mathrm{T}}\boldsymbol{U}_d\boldsymbol{Q}\boldsymbol{x}(t)\right)^{\mathrm{T}}\left(\boldsymbol{x}(t) - \boldsymbol{Q}^{-1}\boldsymbol{U}_d{}^{\mathrm{T}}\boldsymbol{U}_d\boldsymbol{Q}\boldsymbol{x}(t)\right) \tag{8}$$

where $\boldsymbol{x}(t)$ denotes the sample value of $\boldsymbol{x}$ at the sample time t, $\boldsymbol{U}_d$ is composed of the first d row vectors of $\boldsymbol{U}$, $\hat{\boldsymbol{s}}_d \in R^{d\times 1}$ is the vector of the d dominant ICs, d is the number of the dominant ICs, $I^2(t)$ is used to monitor the systematic part of the process variation and $SPE(t)$ is used to monitor the residual part of the process variation.

Once a fault is detected by Eqs. (7)–(8), the variable contributions of $\boldsymbol{x}(t)$ to $I^2(t)$ and $SPE(t)$ are calculated to identify the fault variables by using the following equations, respectively [15]

$$CI^2(t) = \frac{\boldsymbol{Q}^{-1}\boldsymbol{U}_d{}^{\mathrm{T}}\boldsymbol{U}_d\boldsymbol{Q}\boldsymbol{x}(t)}{\left\|\boldsymbol{Q}^{-1}\boldsymbol{U}_d{}^{\mathrm{T}}\boldsymbol{U}_d\boldsymbol{Q}\boldsymbol{x}(t)\right\|_2} \cdot \|\boldsymbol{U}_d\boldsymbol{Q}\boldsymbol{x}(t)\|_2 \tag{9}$$

$$CSPE(t) = \boldsymbol{x}(t) - \boldsymbol{Q}^{-1}\boldsymbol{U}_d{}^{\mathrm{T}}\boldsymbol{U}_d\boldsymbol{Q}\boldsymbol{x}(t). \tag{10}$$

3. NoisyTSICA-based Monitoring Method

It is a well accepted fact that the measured data are usually contaminated by the measurement noises with different intensities. Under the