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Semi-supervised mixture discriminant monitoring for chemical batch processes

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ABSTRACT

In order to ensure operation safety and consistent product quality, multivariate statistical methods have been widely adopted in chemical batch process monitoring. In this paper, a semi-supervised mixture discriminant monitoring (SMDM) scheme is proposed, which integrates the strengths of both supervised and unsupervised techniques. The semi-supervised characteristic enables SMDM to fully make use of both labeled and unlabeled data, leading to more reliable process models. In addition, SMDM is suited to handling non-Gaussian distributed data that are commonly observed in batch processes. Inheriting from supervised learning, SMDM has better online fault diagnosis capability of known faults compared to the unsupervised multivariate statistical process monitoring methods. Meanwhile, the utilization of control charts makes SMDM capable to detect unknown faults. After an unknown fault is detected, the process variables most contributing to the fault can be identified through missing variable analysis. Such information is valuable for process engineers to find out the root cause of the fault. The collected data of the new faults are then used to update the monitoring model. By doing so, the fault diagnosis performance of the monitoring model can be improved online. The proposed method is demonstrated through its application to an injection molding process.

1. Introduction

In chemical industrial applications, batch processing is of great importance due to its flexibility in manufacturing low-volume, high-value added products. In order to ensure operation safety as well as consistent and high product quality, historical data based batch process monitoring has attracted much research interest [1,2]. According to Chiang et al. [3], the entire procedure of process monitoring consists of fault detection, fault identification, fault diagnosis, and process recovery. In Chiang et al.'s definition that will be followed in this paper, fault detection is for the recognition of process abnormality, while the purpose of fault identification is to find out the variables contributing mostly to the detected process faults. Different from fault identification, fault diagnosis aims to determine the root causes of the abnormal behaviors. With such information, it is possible to conduct process recovery. Unsupervised techniques, such as principal component analysis (PCA), independent component analysis (ICA), and Gaussian mixture model (GMM), are frequently used in fault detection and identification [4]; while supervised techniques, such as Fisher discriminant analysis (FDA), artificial neural network (ANN), and support vector machine (SVM), are commonly adopted for fault diagnosis via classification, after a fault is detected [3].

Various multivariate statistical process monitoring (MSPM) approaches have been applied to batch processes, some of the most typical of which are the following. The well-known multiway principal component analysis (MPCA) method was proposed by Nomikos and MacGregor [5,6] in 1994, tracking the progress of batch runs by projecting variable trajectory information to lower dimensional latent variable spaces. Multiway partial least squares (MPLS) [7] conducts batch process monitoring in a similar way as MPCA does, which considers product quality during process modeling. To track the time-varying characteristic of variable trajectories in batch operations, Rännar et al. developed the adaptive hierarchical PCA (AHPCA) method [8]. Chen and Liu [9], Lu et al. [10] as well as Yao and Gao [11] integrated PCA with time-series model structures to better present batch process dynamics. For improving the analysis of processes, multiblock PCA/PLS [12,13] were also utilized in batch process modeling and monitoring. In recent years, pioneered by Lu and Gao [14], many researchers showed interest in the phase-based modeling and fault detection of batch processes [15]. Besides these linear PCA/PLS-based methods, nonlinear techniques have also been applied to batch processes, e.g. the multiway kernel PCA [16]. To cope with the non-Gaussian data distribution caused by various process conditions or operation phases, ICA has also been utilized in batch process monitoring [17,18]. GMM handles the non-Gaussianity contained in batch process data in another way [19–21], which approximates the distribution of normal operating data with a mixture of Gaussians.

All the previously mentioned methods require a fault-free training data set of normal operation for model building, and belong to the class of unsupervised monitoring techniques. Therefore, they mainly aim at fault detection, and can also provide fault identification information

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with the help of contribution plots [22] or fault reconstruction algorithms [23]. However, the root causes of the faults are not discovered by these methods. In real industry, the process data always contain a certain number of faulty samples due to various types of sensor faults and process abnormalities. Hence, it is natural to think about extending the utilization of supervised techniques to online process monitoring for both fault detection and diagnosis. In continuous process applications, FDA, an efficient tool for fault classification, has been considered as an alternative for online monitoring [24]. A limitation of the conventional FDA algorithm is that it relies on the assumption of within-class Gaussianity. To handle the multimodality within each normal or faulty class, Yu [25] adopted the localized Fisher discriminant analysis (LFDA) approach. In the field of batch process monitoring, Zhang et al. [26] utilized kernel Fisher discriminant analysis (KFDA) to detect and diagnose the faults occurring in a nonlinear process, while Yu [27] extended the kernelized LFDA to batch process applications and named his method multiway kernel LFDA (MLKFDA).

Despite their advantages, the conventional supervised monitoring techniques have two major shortcomings. First, most of these methods rely on data classification. As a result, they are not capable of dealing with unknown faults not contained in the training data set, although such faults are often observed in industrial processes. In addition, as discussed in [28], even for known faults, monitoring solely based on classification results may lead to detection delay. It is effective to integrate control charts with supervised monitoring techniques. Second, the performance of supervised learning tends to be degraded when a part of historical samples are unlabeled. In process monitoring, such situation is common, which occurs if the status of parts of the historical measurements is unclear. In such cases, the supervised techniques often lead to models over-fitted to the labeled samples. As a result, the monitoring performance may seriously deteriorate. Most recently, an MDA-based monitoring approach [28] has been proposed to overcome the first shortcoming. However, the second problem still exists.

To solve the above problems, this paper proposes a semi-supervised mixture discriminant monitoring (SMDM) approach for batch process applications. First, the mixture discriminant analysis (MDA) [29,30] model is extended from supervised learning to semi-supervised learning. Inherited from MDA, the developed semi-supervised mixture discriminant analysis (SMDA) approach is able to deal with non-Gaussian distributed data. In the meantime, benefiting from semi-supervised learning, SMDA outperforms MDA when parts of the data are unlabeled. Then, a batch process monitoring scheme, i.e. SMDM, is proposed by combining the statistical process control (SPC) charting technique and the SMDA model. Such a combination enables the proposed SMDM method to efficiently detect both known and unknown faults. For known faults, root-cause diagnosis results can be achieved automatically through fault classification, while for unknown faults in which the exact type information is unavailable, the identification of the most contributing variables is carried on using missing data analysis. In addition, the newly collected data are then utilized to update the monitoring model, which makes it possible to continuously improve the fault diagnosis ability.

The rest of the paper is organized as follows. In Section 2, the conventional MDA approach for data classification is reviewed, followed by the development of the SMDA model in Section 3. Then, the entire procedure of SMDM is described in Section 4, including the SMDA based process modeling, the development of control chart, the steps of online fault detection, the root-cause diagnosis of known faults, the identification of unknown faults, as well as the model update. In Section 5, the application to an injection molding process verifies the capability of the proposed approach. Finally, the conclusions are drawn in Section 6.

2. Mixture discriminant analysis

MDA was firstly proposed by Hastie and Tibshirani [29] for handling within-class non-Gaussianity in discriminant analysis, in which the class densities are modeled as mixtures of Gaussians. In the original work, different classes are assumed to have a common covariance matrix. Later, Fraley and Raftery [30] relaxed such assumption and allowed the utilization of different class covariance matrices in MDA. The details of the MDA approach are as follows.

Without losing generality, assume that the training data set $\mathbf{X} = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \cdots \quad \mathbf{x}_n]^T$ has the dimensions of $n \times m$, where m is the number of variables and n is the number of samples. All the training sample vectors x_i ($i = 1, 2, \ldots, n$) are known to belong to a class j, where $j = 1, 2, \ldots, J$. Divide each class j into R_j artificial subclasses, denoted by c_{jr}, $r = 1, \ldots, R_j$, and define $R = \sum_{j=1}^{J} R_j$. Each subclass has a multivariate Gaussian distribution with a mean vector $\boldsymbol{\mu}_{jr}$ and a covariance matrix $\boldsymbol{\Sigma}_{jr}$. The prior probability for class j is denoted by Π_j, while the mixing probability for the rth subclass within class j is presented by the parameter π_{jr}. $\sum_{r=1}^{R_j} \pi_{jr} = 1$. Usually, the Π_j are known or easily estimated from the training data, and the π_{jr} are unknown.

The mixture density for class j is:

$$m_j(\mathbf{x}) = p(\mathbf{x}|j) = \sum_{r=1}^{R_j} \pi_{jr}(2\pi)^{-m/2}\left|\boldsymbol{\Sigma}_{jr}\right|^{-1/2} \exp\left(-\frac{\left(\mathbf{x}-\boldsymbol{\mu}_{jr}\right)^T \boldsymbol{\Sigma} jr^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_{jr}\right)}{2}\right). \quad (1)$$

The parameters, μ_{jr}, Σ_{jr} and π_{jr}, can be estimated by maximizing the log-likelihood function:

$$l^{mix}(\theta) = \sum_{i=1}^{n} \log p(\mathbf{x}_i|\theta), \quad (2)$$

where the parameter $\theta = \{\pi_{jr}, \boldsymbol{\mu}_{jr}, \boldsymbol{\Sigma}_{jr}; r = 1, 2, \cdots, R_j, j = 1, 2, \cdots, J\}$.

The iterative expectation–maximization (EM) algorithm provides a convenient method for maximizing $l^{mix}(\theta)$. Provided that $\mathbf{x}$ is a training sample in class j, the estimated probability of $\mathbf{x}$ belonging to the rth subclass of class j is expressed as:

$$p\left(c_{jr}|\mathbf{x}, j\right) = \frac{\pi_{jr}(2\pi)^{-m/2}\left|\boldsymbol{\Sigma}_{jr}\right|^{-1/2} \exp\left(-\frac{\left(\mathbf{x}-\boldsymbol{\mu}_{jr}\right)^T \boldsymbol{\Sigma}_{jr}{}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_{jr}\right)}{2}\right)}{\sum_{k=1}^{R_j} \pi_{jk}(2\pi)^{-m/2}\left|\boldsymbol{\Sigma}_{jk}\right|^{-1/2} \exp\left(-\frac{\left(\mathbf{x}-\boldsymbol{\mu}_{jk}\right)^T \boldsymbol{\Sigma}_{jk}{}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_{jk}\right)}{2}\right)}. \quad (3)$$

The above equation is known as the expectation step (E-step), followed by the maximization step (M-step) as:

$$\pi_{jr} = \frac{\sum_{\mathbf{x}_i \in \text{class } j} p\left(c_{jr}|\mathbf{x}_i, j\right)}{\sum_{k=1}^{R_j} \sum_{\mathbf{x}_i \in \text{class } j} p\left(c_{jk}|\mathbf{x}_i, j\right)} \quad (4)$$

$$\boldsymbol{\mu}_{jr} = \sum_{\mathbf{x}_i \in \text{class } j} \mathbf{x}_i p\left(c_{jr}|\mathbf{x}_i, j\right) / \sum_{\mathbf{x}_i \in \text{class } j} p\left(c_{jr}|\mathbf{x}_i, j\right), \quad (5)$$

$$\boldsymbol{\Sigma}_{jr} = \frac{\sum_{\mathbf{x}_i \in \text{class } j} p\left(c_{jr}|\mathbf{x}_i, j\right)\left(\mathbf{x}_i-\boldsymbol{\mu}_{jr}\right)\left(\mathbf{x}_i-\boldsymbol{\mu}_{jr}\right)^T}{\sum_{\mathbf{x}_i \in \text{class } j} p\left(c_{jr}|\mathbf{x}_i, j\right)}. \quad (6)$$

The above two steps are repeated iteratively until convergence.