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ISA Transactions ∎ (∎∎∎∎) ∎∎∎–∎∎∎

Contents lists available at ScienceDirect

ISA Transactions

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

Research Article

Batch process monitoring based on multiple-phase online sorting principal component analysis

Zhaomin Lv, Xuefeng Yan*, Qingchao Jiang

Key Laboratory of Advanced Control and Optimization for Chemical Processes of Ministry of Education, East China University of Science and Technology, P.O. Box 293, MeiLong Road No. 130, Shanghai 200237, PR China

ARTICLE INFO

Article history:
Received 10 January 2015
Received in revised form
16 February 2016
Accepted 20 April 2016
This paper was recommended for publication by Dr. Steven Ding.

Keywords:
Batch process monitoring
Multiple-phase
Phase number
Principal component analysis

ABSTRACT

Existing phase-based batch or fed-batch process monitoring strategies generally have two problems: (1) phase number, which is difficult to determine, and (2) uneven length feature of data. In this study, a multiple-phase online sorting principal component analysis modeling strategy (MPOSPCA) is proposed to monitor multiple-phase batch processes online. Based on all batches of off-line normal data, a new multiple-phase partition algorithm is proposed, where k-means and a defined average Euclidean radius are employed to determine the multiple-phase data set and phase number. Principal component analysis is then applied to build the model in each phase, and all the components are retained. In online monitoring, the Euclidean distance is used to select the monitoring model. All the components undergo online sorting through a parameter defined by Bayesian inference (BI). The first several components are retained to calculate the T^2 statistics. Finally, the respective probability indices of P_{T^2} is obtained using BI as the moving average strategy. The feasibility and effectiveness of MPOSPCA are demonstrated through a simple numerical example and the fed-batch penicillin fermentation process.

1. Introduction

As important manufacturing types, batch and fed-batch processes are important in producing high-quality, low-volume products, such as special chemicals, food, pharmaceuticals, and semiconductors. The safe operation of a batch process and the quality consistency of products should be ensured. Given the finite duration, batch-to-batch variations, and multiple operating phases that characterize batch process monitoring, this method is a challenging task and has drawn increasing attention.

Multivariate statistical methods such as principal component analysis (PCA) and partial least square (PLS) have been successfully employed to model multivariate processes [1–7]. Multi-way PCA (MPCA) and multi-way PLS (MPLS) are two of the most popular methods used for batch process monitoring [8–10]. Conventional multivariate statistical process monitoring methods based on MPCA or MPLS, which consider an entire batch data as a sample, may deteriorate monitoring performance because the unknown future status until the end of the batch requires estimation, which may not reflect the actual potential relationship in the process. Variable-wise unfolding methods do not require future status prediction [11,12]. However, such methods rely on the assumption that batch process data originate from a single operating phase. Significant batch processes are typically conducted in a series of steps called multiple operating phases. Moreover, diverse variable correlation structures exist at different time regions. The aforementioned traditional methods consequently fail to detect faults in multiple-phase batch processes.

Numerous phase-based approaches have been developed to address the multiple operating phase problem of batch processes [13–25]. Kosano-vich et al. and Dong and McAvoy developed two MPCA models to analyze batch processes [13,14]. This phase partition method was based on expert knowledge. Doan and Srinivasan performed phase partition based on singular points in several known key variables [15]. This phase partition method was based on process analysis. However, both of the aforementioned methods have a shortcoming, i.e., certain required process features must be determined. To overcome this problem, data-based phase partition methods that do not require prior process knowledge have been developed [16–25]. Lu et al. and Zhao et al. developed numerous automatic phase partition methods based on the clustering time-slice PCA model [16,17]. Since the development of these methods, phase-based modeling methods have been widely used in multiple-phase batch processes [18–25]. However, many data-based phase partition methods have two problems. First, the number of phase is difficult to determine, and a biased estimation

* Corresponding author. Tel.: +86 21 64251036.
E-mail address: xfyan@ecust.edu.cn (X. Yan).

http://dx.doi.org/10.1016/j.isatra.2016.04.022
0019-0578/

Please cite this article as: Lv Z, et al. Batch process monitoring based on multiple-phase online sorting principal component analysis. ISA Transactions (2016), http://dx.doi.org/10.1016/j.isatra.2016.04.022

may affect monitoring performance. Second, many phase partition methods may require batch-wise normalization for data, which cannot be performed properly because of the uneven length feature that is a common phenomenon in batch process. Although many data synchronization methods have been introduced into monitoring strategies, these methods may not reflect the actual potential relationship in the process and may reduce modeling accuracy.

Aside from the aforementioned problems, the selection of components is an essential concern when a PCA-based method is used for process monitoring. Numerous methods, such as cumulative percent variance, cross validation, variance of reconstruction error, and fault signal-to-noise ratio, have been used to determine principal components to be extracted [26–30]. These methods exhibit a common problem, i.e., the importance of components are defined by the variance information of each component, and only the first several components with large variances are selected, whereas the last several components with small variances are rejected. Numerous studies have demonstrated that components with small variances can be equally important as those with large variances [31,32]. Lv et al. placed equal importance on all the components and separated all components into two subspaces according to the classification of the denotative matrix of loading matrices [33]. In this method, variation information in fault data may be divided into two subspaces, and monitoring performance may deteriorate. Jiang et al. proposed the just-in-time reorganized PCA method, which concentrates most deviation information into a dominant subspace [34]. The importance of the components is evaluated via online kernel density estimation, and this method exhibits good monitoring performance in a continuous process. However, estimating kernel density may require a huge amount of normal data, and thus, this method may be difficult to perform in some phases of batch processes with few historical data. Consequently, further applications of this method in batch processes may be limited.

In this study, a new multiple-phase partition algorithm and another type of online component selection method, called online sorting PCA (OSPCA), are integrated into batch process monitoring, i.e., multiple-phase OSPCA (MPOSPCA). In comparison with traditional phase partition methods, most of which have two steps: firstly time-slice PCA models need to be built, and secondly clustering method is used to divide the models to realize the phase partition. The first step has a request that all batch data must have the even length. If the batches are uneven, the time-slice PCA cannot be built well. However, the phase partition method proposed in this work does not need time-slice PCA model. The clustering method is immediately applied on the original data which are two dimensional variable-wise unfolding. Thus, the batch data with uneven length will not influence the proposed phase partition method proposed. Assuming that no prior process knowledge is available, the phase information should be automatically identified by capturing changes of underlying characteristics. Considering the time-varying process characteristics and similarity within a certain time region as well, it is a natural idea to separate the batch process into multiple phases and develop different models to capture their different process characteristics [25]. In off-line modeling, k-means is immediately used to classify all the original batch data with variable-wise unfolding, and thus, the uneven length feature of data cannot affect partition algorithm performance. According to each phase data set, the average Euclidean radius (AER) is defined to ascertain phase number. It can be easily find that the more phase models, the better performance. However, as the phase number increasing, the AER which can reflect the similarity in each phase data firstly decreases quickly and then decreases slowly. It is a better choice to select the turn point. Each variable-wise phase data set is then normalized, PCA is employed to build the model, and all the components are retained. In online monitoring, the Euclidean distance is calculated between each phase data set center and the current sample. The model with the minimum distance is selected as the monitoring model, and all the components of the current data can be obtained. A probability parameter of each component is examined through Bayesian inference (BI). A large probability of the component indicates that this component contains big deviation information of the online data, and represents the importance of the component. This calculation method of each component importance does not require much normal data. All the components are then sorted online using the aforementioned parameter. The first several components are retained to calculate the T^2 statistics. Through online sorting components, most deviation information can be concentrated together, which is beneficial to fault detection. Finally, BI is used to combine T^2 in the time window as a moving average strategy to address self-correlation among different intervals, given that current behavior is affected by past behavior in the dynamic process. Moreover, a moving average strategy can reduce noise in the industry process. By integrating the proposed multiple-phase partition method into the OSPCA method, the batch process monitoring method, i.e., MPOSPCA, can solve the phase number and uneven length problems in multiple phase batch processes and accurately detect different type faults.

The rest of this paper is organized as follows. Section 2 presents PCA. Section 3 explains the proposed multiple-phase partition algorithm, i.e., OSPCA and the MPOSPCA monitoring procedure. Section 4 shows the design of a numerical example and the fed-batch penicillin fermentation process employed to demonstrate the feasibility and effectiveness of MPOSPCA. Finally, Section 5 presents the conclusion of the study.

2. Preliminaries

This section reviews PCA for process monitoring [26]. Two-stage PCA (TPCA) and Hierarchical PCA (HPCA) are compared with the proposed MPOSPCA method through a simple numerical example and the fed-batch penicillin fermentation process.

2.1. PCA

Considering the matrix $\mathbf{X}(m \times n)$ with m samples and n variables, PCA is defined as follows:

$$\boldsymbol{X} = \boldsymbol{T}\hat{\boldsymbol{P}}^T + \boldsymbol{E}, \tag{1}$$

where $\hat{\boldsymbol{P}}(n \times z)$ is the loading matrix, $\boldsymbol{T}(m \times z)$ is the score matrix, $\boldsymbol{E}(m \times n)$ is the residual matrix, and z is the number of principal components.

T^2 and SPE are two online monitoring statistics that correspond to principal component subspace and residual subspace, respectively. The respective calculations of these statistics are as follows:

$$T^2 = \boldsymbol{x}\hat{\boldsymbol{P}}\boldsymbol{\Lambda}_z^{-1}\hat{\boldsymbol{P}}^T\boldsymbol{x}^T, \tag{2}$$

$$SPE = \boldsymbol{e}\boldsymbol{e}^T; \quad \boldsymbol{e} = \boldsymbol{x} - x\hat{\boldsymbol{P}}\hat{\boldsymbol{P}}^T, \tag{3}$$

where $\boldsymbol{\Lambda}_z = diag(\lambda_1, \lambda_2, \cdots, \lambda_z)$ is the eigenvalue matrix, and $\boldsymbol{x}(1 \times n)$ is the monitored sample. Proper control limits are defined as follows to determine whether the process is operated under normal conditions:

$$T^2 \le \frac{z(m^2-1)}{m(m-z)} F_{z,(m-z),\alpha}, \tag{4}$$