Chemometrics and Intelligent Laboratory Systems 159 (2016) 69–79

Contents lists available at ScienceDirect

Chemometrics and Intelligent Laboratory Systems

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

Distributed model projection based transition processes recognition and quality-related fault detection

Yuchen He[a], Le Zhou[b], Zhiqiang Ge[a], Zhihuan Song[a,*]

[a] State Key Laboratory of Industrial Control Technology, College of Control Science and Engineering, Zhejiang University, Hangzhou 310027, Zhejiang, China
[b] School of Automation and Electrical Engineering, Zhejiang University of Science and Technology, Hangzhou 310023, Zhejiang, China

ARTICLE INFO

Keywords:
Transition process
Distributed model projection
Hierarchical clustering
Transition identification
Fault detection

ABSTRACT

In this paper, a novel transition process identification algorithm based on distributed model projection (DMP) is proposed for clustering nonlinear transition data and monitoring the variations in the transition process. Compared to several alternative identification methods, the DMP algorithm considers both the correlations between variables and correlations between samples. Also, a framework is proposed to combine DMP algorithm and hierarchical clustering to derive an optimal clustering results through a large amount of individual trials of the DMP algorithm. Based on the offline classification results, a transition process is divided into several sub-segments and each of them can be characterized by a stable model. Then the online identification and monitoring methods are carried out based on the sub-models established in those segments. Finally, the Tennessee Eastman (TE) benchmark process is utilized to demonstrate the performance of the proposed process identification and monitoring strategy. Compared to previous works, the proposed algorithm is shown to be superior both in identification and monitoring.

1. Introduction

Recently, data-based multivariate calibration methods have been widely used in modern industries for the purpose of process monitoring and diagnosis [1,2]. Among them, the classical multivariate statistical process control (MSPC) algorithms have achieved great successes in the last few decades, such as principal component analysis (PCA), partial least squares (PLS), principle component regression (PCR), kernel partial least squares (KPLS) and their advanced variants [3–7].

However, most of these methods are assumed to run in a single and stable operating condition. In most cases, the real industrial processes are operated in different conditions due to fluctuations in raw materials, set-point changes, aging of equipment and seasoning effects. In order to solve this problem, many methods have been proposed for the purpose of multimode modeling and process monitoring [1,8–13]. Particularly, Zhu et al. [14] proposed a clustering method for multimode recognition in which an ensemble clustering algorithm is employed. However, the performance of ensemble clustering depends on the proper choice of the initial value of the clustering method. Zhang et al. [12] proposed a subspace separation method where a common subspace and a specific space are used to describe the multimode characteristics. Practically, it is difficult to construct such two subspaces explicitly due to the complexity of multimode processes.

It is also noticed that a stable operation status cannot be immediately switched to another one, indicating that there are transitions between two adjacent stable modes. These unstable processes should also be considered for multimode modeling and monitoring. It is always a challenging and sophisticated issue using traditional methods. For the purposes of transition identification and monitoring, Zhao et al. [15,16], Ge et al. [17], Wang et al. [18], Tan et al. [19] and Yao et al. [20] proposed different algorithms for stable and transient process identification as well as multimode monitoring in recent years. In the above methods, transitions should be identified from multimode process in the offline step so that calibration models can be established using proper training transient data. In Zhao's method [15], the duration of a transient process was defined from the center of a stable mode to the center of its neighboring mode so that the transition process is able to be described using adequate observations. The transition process recognition method was set manually instead of being identified based on the process data. It is quite unreasonable that stable modes would disappear and the whole process only consists of several transitions according to such definition. Process information was taken into account in Wang's method where a complete transition process recognition and modeling method was proposed. In Wang's

* Corresponding author.
E-mail address: songzhihuan@zju.edu.cn (Z. Song).

http://dx.doi.org/10.1016/j.chemolab.2016.10.001
Received 4 December 2015; Received in revised form 11 September 2016; Accepted 4 October 2016
Available online 06 October 2016
0169-7439/

methods [18], a transient process was separated into several sub-segments by the k-means method and each of them was characterized using linear models. Unfortunately, the Euclidean distance between different samples cannot fully reveal the variations and trends of complicated chemical process [21,22]. In the past few decades, the MSPC methods have proved itself in chemical process modeling. Hence, Yao et al. [20] used a series of different PCA models to describe the behavior of a chemical process. A single PCA model was created for each sub-segment and the PCA similarity index was adopted to analyze the difference between each sub-segments. It indicates that the unstable nonlinear transition process is divided into several approximately stable linear processes where the classical MSPC methods can be employed. However, the assumption that variable relationships in each sub-model are linear correlated is still invalid in practice.

In order to solve the above problems, we propose a novel algorithm called distributed model projection (DMP) in this paper. In the DMP algorithm, the transition process is recognized by an iterative method. Since the beginning part of a transition is very different from the ending part, it is still assumed that a transition can be divided into several sub-models, in which it can be treated as a stable process. The amount of clusters can be properly determined by the subtractive clustering algorithm (SCM). Each of these clusters is supposed to be a stable mode or a transition. Also, nonlinear relationship between process data and quality data is an important issue in chemical processes. For this purpose, the DMP algorithm is proposed by using the KPLS model to describe the behavior of a process. The algorithm starts with several initial models which are established by the randomly initialized data in each cluster. In order to capture the characteristics of a process accurately and avoid the noises caused by the single observation, the classical moving window strategy is adopted to create several overlapping windows across the whole process. According to the theory of principle-components-similarity [23], two data blocks with similar principle components subspaces may have similar statistical characteristics to each other. In other words, two data blocks with small prediction errors are considered to be similar to each other when these two blocks are projected to the same model. Hence, each moving window in a multimode process is projected to the initial models to calculate corresponding prediction errors. A window having the smallest error with respect to a model is assigned to the corresponding cluster. In such way, a transition process is initially recognized and divided into several segments (sub-models).

On the basis of the current models, the windows in each cluster are statistically similar to each other. However, it is noticed that the initial models are established based on the randomly initialized data. Hence, these models should then be updated using all available samples within each cluster. After the new models are derived, all the windows are projected to these models to determine the new assignment of each window. And the iteration will continue until no further variation is found in the clustering results. In each single cluster, statistically similar windows are grouped together and dissimilar windows are assigned to different clusters. The clustering results of the DMP algorithm indicate the similarity between different moving windows.

Besides, the DMP algorithm is considered as a nonhierarchical clustering method which may converge to a local optimal solution [21,22]. It means that the clustering result in one trial by using DMP algorithm may be different from the result in another one. Compared to nonhierarchical clustering methods, global optimal solutions can be derived using hierarchical clustering methods. In order to obtain global optimal clustering results, a hierarchical clustering method is adopted by combining the clustering results of a large amount of DMP trials. The similarity information derived by the DMP algorithm can be the input of any common hierarchical method.

After the transition process is recognized, the corresponding fault detection methods can be derived. For most multimode process monitoring methods, it only involves the process data where the abnormal situations of process can be monitored while the variations of the final product quality cannot be detected. When the quality data can be measured, the relationships between the process variables and the quality variables should also be included to enhance the ability of process and quality monitoring. In chemometric region, some supervised methods have been proposed for single and multimode process modeling [11,24]. However, little attention has been paid on the quality-related transition process monitoring. Hence, a quality-related transition fault detection method is also studied in this paper.

The rest of the paper is organized as follows: a brief description of transition process is given in Section 2. In Section 3, offline transition recognition by using the DMP algorithm and hierarchical clustering explanation are introduced explicitly. Then an online identification and quality-related process monitoring method is introduced in Section 4. A TE benchmark process is demonstrated in Section 5 to evaluate the performance of the proposed method. Finally, some conclusions are made.

2. Transition process description and analysis

Differing from stable modes, a transition process is a trend from one stable mode to another. Hence, the statistical characteristics of a transition cannot be well depicted using the traditional MSPC method because of intricate relationships between variables. At the beginning of each transition, the statistical characteristic is similar to the previous stable mode. At the end, it is accordingly similar to the following stable mode. Therefore, it is difficult to handle transition modeling and monitoring issues using classical stable mode methods. Furthermore, considering the existence of control loops in an industrial process, 'irregularity' sometimes occurs in a transition [15,16,25]. It means that the present sample may contain similar characteristics with previous samples several sampling intervals before.

Considering the statistical characteristics of transitions, several recognition and modeling steps are used in this paper. Firstly, the observations are divided into several clusters utilizing the DMP algorithm, where a stable process can be demonstrated using a single cluster while the transition process contains several smaller sub-models, so that the traditional MSPC methods can be employed in each cluster. After that, the corresponding process monitoring scheme can be established in each stable and transient mode. A new sample needs to be classified into a certain cluster once it is measured. Then the sample can be monitored using the corresponding fault detection algorithm. In the next two sections, the offline recognition and online identification algorithm will be introduced in detail.

3. Offline multimode identification and transition recognition

A multimode process usually consists of several stable processes and transitions. Commonly, different stable processes and transitions should be identified before online monitoring. The conventional clustering methods were mainly carried out based on the Euclidean distance. Hence, the relationships between different samples were emphasized and two samples with small Euclidean distance between them were considered to belong to one cluster [18,22]. It might work under the assumption that the relationships between different variables are simple. Considering the complexity in the process control, such assumption is often invalid in continuous chemical process. Usually, chemical processes contain variations, especially peaks and valleys, and it is therefore difficult to illustrate the behavior of a process merely by traditional Euclidean-distance-based clustering methods. For the purpose of process control and fault detection, a growing number of successes have achieved by the MSPC methods, such as PCA and PLS. It is more appropriate to introduce MSPC methods into process analysis and multimode identification. Inspired by the principle-components-similarity analysis [23], two data blocks are considered to be similar to each other when both residuals are very small with