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Multimode process monitoring using improved dynamic neighborhood preserving embedding

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ABSTRACT

Complex processes often have multiple operating modes due to different manufacturing strategies. Meanwhile, within-mode process data usually exhibit dynamic behaviors and the data sample obtained at the present time may be correlated with those sampled for the previous and the next moment. In this paper, a novel improved dynamic neighborhood preserving embedding (IDNPE) algorithm is put forward and a new monitoring approach is proposed based on IDNPE. Different from the conventional principal component analysis (PCA) which aims at preserving the global structure of the data set, the proposed IDNPE tries to preserve the local neighborhood structure of the data set. In order to consider the scales of different variables within-mode and those of the same variables mode-to-mode, a novel distance which contains the local standard deviation information is employed in the IDNPE method. Moreover, for the dynamic behaviors of a single mode, the serial correlation is taken into account. Instead of constructing multiple monitoring models for multimode processes, the proposed IDNPE method builds only one global model without priori process knowledge. Finally, to test the modeling and monitoring performance of the proposed method, a numerical example and the Tennessee Eastman (TE) benchmark case studies are provided.

1. Introduction

Process monitoring is important for providing early warnings to operators in order to ensure the safety and enhance the productivity. Because large amounts of process historical data can be easily recorded and collected [1], multivariate statistical process monitoring (MSPM) techniques such as principal component analysis (PCA) and partial least squares (PLS) have received great attention and have been widely applied as one of the most essential tools for chemical process monitoring [2–7]. However, traditional MSPM schemes are based on the assumption that the process has one nominal operating region and process variables are independently sampled. In modern industrial processes, multimodality is one of the most significant features due to the various demands of markets. At the same time, since the regulatory control presents feedbacks to input variables, the impact of disturbances propagates through both the input and output variables. Thus, the within-mode process variables will move around a steady-state condition and exhibit some degree of auto-correlation [8]. In this condition, the monitoring performance of traditional MSPM methods might be unsatisfactory. Therefore, in order to address these problems, it is necessary to develop novel methods.

For traditional MSPM methods, the assumption that processes contain only one nominal operating region becomes invalid in multimode processes. In order to ensure the safety of production, multimode process monitoring has been intensively studied and many statistical monitoring algorithms have been reported. The most intuitive idea is to build several models for monitoring corresponding to multiple modes. However, it is difficult to obtain prior knowledge of how to separate the historical process data into multiple subsets in the offline modeling phase. Besides, in the online monitoring phase, more efforts need to be made to identify the real state of the process from the monitoring results of multiple local models. If only one local model is selected for monitoring, specific rules should be determined to select the most suitable model for every new sample. Alternatively, if all the local monitoring models are used to monitor the new sample, a rule needs to be designed to integrate the detection results of the local models [9]. Tan and Wang [10] presented a novel monitoring method based on the similarity of data characteristics. This method developed different models to capture the major tendencies of process variables. Based on the Bayesian inference and the combination strategy, a two-dimensional Bayesian method for monitoring processes with both nonlinear and multimode characteristics was proposed [11]. Bayesian classification was used to extract multiple operating regions from historical data [12]. What's more, the local Gaussian distribution is appropriate to characterize each subset of observing data from the same operating modes. Therefore, the Gaussian mixture model (GMM) might be suitable for describing the data generated from different operating modes. A method

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integrating GMM with PCA and discriminant analysis (DA) to monitor processes with nonlinearity and multimode properties was performed [13]. By constructing a probability monitoring index, a Bayesian inference based on the GMM method was developed [14]. Xie and Shi [15] proposed an adaptive Gaussian mixture model that can model different operating modes as well as trace process variations. In order to monitor industrial processes with time-varying and multimode characteristics, a numerically efficient moving window local outlier factor (LOF) algorithm was designed [16]. In addition, the hidden Markov model (HMM) has been successfully applied in multimode processes. Rashid and Yu [17] built the hidden Markov model from measurement data to estimate dynamic mode sequence and used HMM based state estimation to classify the monitored samples into the corresponding modes. Besides, in order to obtain satisfactory monitoring performance, the characteristics of within-mode process data should also be taken into account.

Since the slow property changing of feed stocks, the drift of process characteristics and process controllers designed in the manner of run-to-run adjustment always result in some dynamic behaviors, processes rarely remain at steady state [18]. Due to these dynamic characteristics, the data sample obtained at the present time may be correlated with those sampled for the previous and the next moment. Traditional MSPM methods such as PCA and PLS assume that the observations at the present moment are statistically independent from previous observations and they all inadvertently ignore process dynamics. However, for conventional industrial processes, this assumption is valid only for long sampling intervals. Particularly, when the fault only influences the dynamic change of process variables, the monitoring performance will be seriously deteriorated if the dynamic relationships have not incorporated for modeling [1]. Therefore, for process monitoring with dynamic behavior and fast sampling intervals, the serial correlation needs to be taken into consideration. Ku et al. proposed dynamic PCA (DPCA) that used an augmented matrix with time-lagged variables. In DPCA, a matrix with current and past measurements was built [19]. DPCA and canonical variate analysis (CVA) are data dimensionality techniques which consider the serial correlation. They were applied to the Tennessee Eastman process simulator to test their effectiveness in detecting faults [20]. Considering both within-batch and batch-to-batch dynamics simultaneously, Lu and Yao proposed the two-dimensional dynamic principal component analysis (2-D-DPCA) to model and monitor batch processes [21]. Based on the 2-D-DPCA method, several improved algorithms have been proposed and have been successfully used in batch processes [22–26]. In order to deal with nonlinear and dynamics characteristics of the batch processes at the same time, the two-dimensional dynamic kernel PCA (2-D-DKPCA) and the two-dimensional dynamic kernel Hebbian algorithm (2-D-DKHA) were presented [27]. To handle the problem of monitoring statistics present significant auto-correlation, a set of multivariate statistics based on DPCA and the generation of de-correlated residuals were designed [28].

Neighborhood preserving embedding (NPE) is a linear dimensionality reduction algorithm. Different from PCA which aims at preserving the global structure of the data set, NPE aims to preserve the local neighborhood structure of the data set. In multimode process monitoring, the PCA method employs the global information which contains multiple modes and blank area between modes. Therefore, the PCA method cannot describe characteristics of any single mode and the feature space cannot be a low-dimensional representation of original data space. However, the NPE method only employs the local information of a single mode data. Given a set of data points in the space, firstly build a weight matrix which describes the relationship between the data points. Specifically, for each data point, it is represented as a linear combination of the neighboring data points and the combination coefficients are specified in the weight matrix. Then find an optimal embedding such that the neighborhood structure can be preserved in the dimensionality reduced space. In multimode process monitoring, the NPE method can preserve local manifold structure of different modes. The NPE method can describe different characteristics of different modes and the feature space can be a low-dimensional representation of original data space. Therefore, NPE may show a better performance when dealing with the multimode process data. Recently, the efficiency of NPE based method has been validated through a fed-batch process [29].

To develop an efficient monitoring method for complex multimode processes with dynamic behaviors of the within-mode process data, a novel improved dynamic neighborhood preserving embedding (IDNPE) method is proposed in this work. First, the original matrix is augmented with time-lagged variables by considering the serial correlation. Due to the multimodality of the original matrix, the augmented matrix is contaminated by several samples which contain two mode original samples in one augmented sample. Consequently, a new filtering strategy based on the local outlier factor (LOF) method is applied to get rid of these contaminated samples. Second, the IDNPE algorithm is applied to conduct the dimensionality reduction and compute the low dimensional embedding in which nearby points in the high dimensional space remain nearby and similarly co-located with respect to one another. Put another way, the embedding is optimized to preserve the local configurations of the nearest neighbors. Although the z-score method can make the overall data set with sample-mean zero and sample-standard deviation one, the scales of the same variables mode-to-mode are different and so are those of different variables within-mode. Considering the scales of the same variables mode-to-mode and those of different variables within-mode, a novel distance which contains the local standard deviation information is proposed. Then, the T^2 monitoring statistic is constructed in the feature space for fault detection. In the IDNPE method, the multimodality of the data distribution is taken into account and the dynamic characteristics of the within-mode process data are also considered. In particular, no priori process knowledge is required during the modeling and monitoring phases. Finally, the feasibility and efficiency of the proposed method are illustrated through a numerical example and the Tennessee Eastman process.

The remainder of this paper is organized as follows: In Section 2, the basic outline of traditional NPE is briefly introduced. The proposed IDNPE algorithm is detailed in Section 3.1. Section 3.2 shows how to construct the monitoring statistic and how to determine the corresponding control limit. The offline modeling and online monitoring procedures of the proposed method are described in Section 3.3. The results and discussions of a numerical example and the Tennessee Eastman benchmark are presented in Section 4. Finally, some conclusions are drawn in Section 5.

2. Neighborhood preserving embedding (NPE)

NPE is a linear dimensionality reduction technique that aims at preserving the local structure of the data set. Local structure means that each data point can be represented as a linear combination of its neighbors. Recently, the NPE algorithm has been reported in detail and successfully applied in the area of face recognition [30,31]. NPE is a linear approximation to the locally linear embedding (LLE) algorithm. The linear property of NPE makes it fast and suitable for practical applications [32]. Compared to PCA, NPE reveals the intrinsic structure of the observed data and can find more meaningful low dimensional information in the high dimensional space.

The NPE algorithm seeks a transformation matrix $\boldsymbol{A}$, which projects a set of high dimensional points $\boldsymbol{X}^T = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n\} \in \boldsymbol{R}^{m \times n}$ into a set of low dimensional points $\boldsymbol{Y}^T = \{\boldsymbol{y}_1, \boldsymbol{y}_2, \cdots, \boldsymbol{y}_n\} \in \boldsymbol{R}^{p \times n}$, $(p < m)$. The algorithmic procedure is stated as follows:

(1) *Constructing an adjacency graph*: The k-nearest neighbors method is adopted to construct the adjacency graph. Put a directed edge from node i to j if x_j is among the k-nearest neighbors of x_i.