Computers and Chemical Engineering 76 (2015) 1–16

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Topological preservation techniques for nonlinear process monitoring

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ARTICLE INFO

Article history:
Received 26 June 2014
Received in revised form 7 January 2015
Accepted 5 February 2015
Available online 12 February 2015

Keywords:
Process monitoring
Fault detection
Fault diagnosis
Self-organizing maps
Gaussian mixture model

ABSTRACT

This work proposes a novel approach for the offline development and online implementation of data-driven process monitoring (PM) using topological preservation techniques, specifically self-organizing maps (SOM). Previous topological preservation PM applications have been restricted due to the lack of monitoring and diagnosis tools. In the proposed approach, the capabilities of SOM are further extended so that all aspects of PM can be performed in a single environment. First for fault detection, using SOM's vector quantization abilities, an SOM-based Gaussian mixture model (GMM) is proposed to define the normal region. For identification, an SOM-based contribution plot is proposed to identify the variables most responsible for the fault. This is done by analyzing the residual of the faulty point and an SOM model of the normal region used in fault detection. The data points are projected on the model by locating the best matching unit (BMU) of the point. Finally, for fault diagnosis a procedure is formulated involving the concept of multiple self-organizing maps (MSOM), creating a map for each fault. This allows the ability to include new faults without directly affecting previously characterized faults. A Tennessee Eastman Process (TEP) application is performed on dynamic faults such as random variations, sticky valves and a slow drift in kinetics. Previous studies of the TEP have considered particular feed-step-change faults. Results indicate an excellent performance when compared to linear and nonlinear distance preservation techniques and standard nonlinear SOM approaches in fault diagnosis and identification.

1. Introduction

Modern process monitoring is marked by the extensive use of advanced computer systems and large numbers of sensors to determine if a plant is operating in a safe state and to detect when a problem occurs. Identifying these states can be difficult due to the large number of variables measured, but data driven methods offer ways to quickly and efficiently extract useful information from large data sets common in process industries. Improved process monitoring can minimize downtime, increase safety, reduce manufacturing costs, and improve performance, which all contribute to safer and more profitable operations.

Process monitoring tasks include fault detection, fault identification, fault diagnosis, and process recovery. Fault detection recognizes a deviation from the normal operating regime from process measurements. Fault identification can help personnel identify the fault by finding the measured variables most related to the fault. Fault diagnosis determines the root causes of the fault and process recovery is the manual correction for the effect of the fault.

The essence of process monitoring is to quantify the process with measures that are sensitive and robust to faults. Measures to aid in process monitoring have been divided into three categories: knowledge-based, analytical, and data-driven methods (Chiang et al., 2001). Analytical methods create a prediction of the process with a model often derived from first principles. Knowledge-based methods are mostly based on causality and expert systems. Most applications of these systems are for small inputs-outputs systems. For large-scale systems, these techniques require a detailed model or a large amount of knowledge. Data-driven methods are derived directly from process data without using any underlying laws.

Among the data driven methods, self-organizing maps (SOMs), also known as Kohonen Networks (Kohonen, 2001), are a type of neural network used to visualize complicated, high-dimensional data. SOM has been previously applied to chemical process data analysis with success. Deventer et al. (1996) used SOM in tandem with textural analysis for monitoring of a mineral flotation process. Jamsa-Jounela et al. (2003) utilizes SOM to detect several faults in a smelter and an online tool to assist in its implementation. Garcıa and Gonzalez (2004) used SOM and k-means clustering for system state estimation and monitoring with an application to a wastewater treatment plant. Ng and Srinivasan (2008a) and Ng and Srinivasan (2008b) created an effective training strategy using

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http://dx.doi.org/10.1016/j.compchemeng.2015.02.002
0098-1354/

SOM for multistate operations in addition to a sequence comparison algorithm with applications to a lab scale distillation unit, a refinery hydrocracker, and the Tennessee Eastman Process. They also resample the training data in order to achieve an equal representation of the different operating regimes. Corona et al. (2010) and Corona et al. (2012) applied SOM to the classification of different operating regimes of an industrial deethanizer and included a method to consider quality specifications. Throughout these applications, the use of SOM's visualization tools was a key advantage in the analysis over other process monitoring techniques.

Distance-preservation fault-detection techniques, including principal component analysis (PCA), have previously been applied to the Tennessee Eastman Process with great success. The ease with which training data can be generated using the Tennessee Eastman Process has allowed it to become the benchmark for any new process monitoring scheme. Raich and Cinar (1996) demonstrated the use of standard PCA for fault detection and diagnosis on the Tennessee Eastman Process. Zhu et al. (2011) applied an ensemble clustering method based on a dynamic PCA-ICA model to label process transitions to the TEP and achieve transition process monitoring using PCA based dimensionality reduction. A thorough treatment of PCA and other statistical techniques to the Tennessee Eastman Process is presented in Chiang et al. (2001). A comparison of these standard techniques applied to TEP can be found in Yin et al. (2012). Wang and He (2010) created an alternative approach that monitors the statistics generated from the variance and covariance of process variable statistics. Previous applications of linear data-driven techniques to the TEP have included detection, identification, and diagnosis rates. These previous works may be limited by the use of distance preservation techniques and are more applicable to step changes faults. Nonlinear techniques have been explored as well, some based on linear counterparts. Kramer (1991) and Dong and McAvoy (1996) explored a nonlinear extension of PCA using feedforward neural networks for dimensionality reduction. Several other nonlinear process monitoring techniques are explored in Zhang (2009), including a kernel based nonlinear extension of PCA and ICA. Some researchers have applied SOMs nonlinear topological-preservation features to the TEP. Chen and Yan (2012, 2013) improved the performance of their SOM algorithm using two linear dimensionality reduction techniques, CCA and FDA. Gu et al. (2004) presented the visualization of several step faults in the Tennessee Eastman Process. These works include multiple step faults on a single map. They have not included a method of fault identification and were not applied to faults with any time dependency.

This work proposes a novel SOM-based framework for the offline development and online implementation of data-driven process monitoring schemes. One of the main advantages of linear projections tools such as PCA is its simplicity and the range of tools it provides which covers all three PM tasks of fault detection, identification and diagnosis. Our intention is to develop a nonlinear (topological preservation) approach that will mimic PCA by defining similar measures for process monitoring and fault detection and diagnosis. Here, SOMs are extended to aiding all aspects of process monitoring and the fault diagnosis is performed in a more flexible way. Specifically, for fault detection, using SOM's vector quantization abilities a SOM-based Gaussian mixture model (GMM) is proposed to define the normal region. For identification, an SOM-based contribution plot is proposed to identify the variables most responsible for the fault by analysing the residual of the faulty point and the SOM model of the normal region used in fault detection. The data points are projected on the model by locating the best matching unit (BMU) of the point. Previous topological preservation applications in PM use a single SOM (1-SOM) for all process operating regimes. This presents challenges when a new state is encountered because the map must be trained again to monitor for the new condition. In the proposed approach, fault diagnosis is done by creating a map for each fault, known as MSOM. This allows the ability to include new faults without directly affecting previously characterized faults.

The proposed methodology is applied to the Tennessee Eastman Process (TEP). Previous studies of the TEP have considered particular step-change faults where the root causes of the disturbance are generally limited to one variable. Here, in order to fully utilize SOM's nonlinear topology preservation features, a focus on analyzing more challenging faults such as random variations, sticky valves and slow drift in kinetics is included to effectively illustrate the advantage afforded by SOM. Implementing the proposed methodology indicates that MSOM is able to improve upon linear distance preservation techniques such as PCA as well as nonlinear approaches like NLPCA and more standard SOM based approach to process monitoring tasks.

2. Background

In this section the data-driven techniques utilized in this work are introduced. A brief overview of PCA approaches to process monitoring, SOM, and SOM visualization tools and other advantages.

2.1. Principal component analysis in process monitoring

Principal component analysis (PCA) is a linear distance-preservation technique which determines a set of orthogonal vectors which optimally capture the variability of the data in order of the variance explained in the loading vector directions (Chiang et al., 2001). Given a set of n observations and m process variables in the $n \times m$ matrix X with covariance S, the loading vectors are determined from an eigenvalue decomposition of S:

$$S = \frac{1}{n-1} X^T X = V \Lambda V^T \tag{1}$$

where Λ is the diagonal matrix containing the non-negative real eigenvalues of the covariance matrix in order of decreasing magnitude, and V holds their corresponding eigenvectors. In order to reduce the misclassification rate, it is often desirable to remove directions that may contain little useful information or simple statistical noise. In PCA this is achieved by selecting the columns of the loading matrix which correspond to the largest eigenvalues $P \in R^{m \times a}$. The projections of the observations in X into the lower dimensional space, also known as the scores, can be found from:

$$T = XP \tag{2}$$

PCA process monitoring can also be performed using multi-model PCA (MPCA or PCAm) as described in Chiang et al. (2001). Using the lower dimensional representation calculated in Eq. (2), the Hotelling's T2 statistic is calculated for each observation and for each class's PCA model. The algorithm classifies the new observation into the class whose PCA model has the smallest T2 statistic. For a full discussion of PCA and MPCA based process monitoring, the reader is directed to Chiang et al. (2001).

Extending linear PCA, nonlinear PCA (NLPCA) has also been proposed by Kramer (1991) and Dong and McAvoy (1996). A critical result for NLPCA is the proof by Cybenko (1989) that arbitrary decision regions can be well approximated by continuous feedforward neural networks with only one hidden layer and continuous sigmoidal nonlinearity. Like linear PCA, NLPCA seeks to remove noise variables and weight statistically important variables in the detection and diagnosis of faults. While PCA uses multivariate statistics, NLPCA performs the reduction in dimensionality using a feedforward neural network. The neural network consists of a mapping or "bottleneck" layer, which reduces the input data to the intrinsic dimension, and a de-mapping that, can reconstruct the original