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Quality-related fault detection approach based on dynamic kernel partial least squares

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ABSTRACT

In this paper, a new dynamic kernel partial least squares (D-KPLS) modeling approach and corresponding process monitoring method are proposed. The contributions are as follows: (1) Different from standard kernel partial least squares, which performs an oblique decomposition on measurement space. D-KPLS performs an orthogonal decomposition on measurement space, which separates measurement space into quality-related part and quality-unrelated part. (2) Compared with the standard KPLS algorithm, the new KPLS algorithm, D-KPLS, builds a dynamic relationship between measurements and quality indices. (3) By introducing the forgetting factor to the model, i.e., the samples gathered at the different history time are assigned to different weights, so the D-KPLS model builds a more robust relationship between input and output variables than standard KPLS model. On the basis of proposed D-KPLS algorithm, corresponding process monitoring and quality prediction methods are proposed. The D-KPLS monitoring method is used to monitor the numerical example and Tennessee Eastman (TE) process, and faults are detected accurately by the proposed D-KPLS model. The case studies show the effeteness of the proposed approach.

1. Introduction

In the industrial production process, the quality-related indices are the most important monitoring indicator. However, the quality-related indices usually can't be measured easily or acquired online. Thus, quality indices always are monitored by prediction, when process measurements are obtained. Data-driven techniques have been receiving considerable attention in the process monitoring field due to their major advantage of easy implementation and less requirement for the prior knowledge and process mechanism. Multivariate statistical process monitoring (MSPM) methods including principal component analysis (PCA) (Dunteman, 1995; Jackson, 1991; Misra et al., 2002; Jackson, 1980), partial least squares (PLS) (Geladi and Kowalshi, 1986; Hoskuldsson, 1988; Dayal and MacGregor, 1997; Wang, 1999), and independent component analysis (ICA) have been developed over the past two decades (Kano et al., 2003; Tsai et al., 2013; Hsu and Su, 2011). MSPM techniques are the most widely used data-driven techniques in the process monitoring field, which have been successfully applied to the typical industrial processes such as continuous processes, batch processes, and dynamic processes. In addition, data measured in the process industry has the following characteristics: high dimensionality, non-Gaussian distribution, nonlinear relationships, time-varying and multimode behaviors and data autocorrelations (Ge et al., 2013). Thus, many extended methods based on PCA, PLS, and ICA have also been proposed to overcome the drawbacks of the methods mentioned above in the field of industrial process monitoring.

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PLS modeling has been a useful tool for building the relationship between measurements and the quality indices in the multivariate industrial process monitoring field. PLS as a prevalent data-driven modeling method has satisfactory performance in the field of quality prediction, and industrial process monitoring. The process monitoring based on the PLS approach is to extract a few latent variables from highly correlated measurements according to the covariance between measurements and quality variables. By projecting the measurements on the latent space, the quality-related part and quality-unrelated part can be parted and monitored, respectively. For the purpose of process monitoring, extend PLS methods have also been proposed. For example, Herman Wold and Svante Wold proposed a multivariate projection method for multi-blocks data (Wold, 1982; Wold et al., 1987). Helland et al. (1992) proposed a recursive PLS (RPLS) algorithm to update the PLS model with the latest process data. Several preprocessing and postprocessing modification methods of PLS, such as orthogonal signal correction PLS (OSC-PLS) (Antti et al., 1998) and total projection to latent structures (T-PLS) (Zhou et al., 2010; Qin et al., 2001; Li et al., 2010, 2011a) have been proposed. With T-PLS models, which decompose the measurement space further, quality-related fault diagnosis can be performed effectively for multivariate process. For the nonlinear input and output data, polynomial PLS (Wold, 1992; Malthouse et al., 1997), neural PLS (Kramer, 1992; Qin and McAvoy, 1992), and kernel PLS (KPLS) (Zhang and Teng, 2010; Zhang and Hu, 2011) have been proposed. Especially, KPLS is the most common and prevalent method. With the KPLS method, the nonlinear input data are mapped into a high-dimensional feature space in which the input data are more nearly linear. Although KPLS has been used to monitor multivariate industrial processes, there are still some problems for process monitoring base on KPLS technique. Since standard KPLS performs oblique projection to input space, it has limitations in distinguishing quality-related and quality-unrelated faults.

Standard KPLS mentioned above consider only static relations between measurements and quality variables. However, the true relationship between measurements and quality-related data is dynamic. Standard KPLS models are not suitable to model this kind of processes and there are a number of approaches to cope with this problem. A widely accepted way is to include a relatively large number of lagged values of the input and output variables in the measurement block. The model built by those measurements is called dynamic KPLS (D-KPLS) that can reflect the true relations between measurements and quality indices.

In this paper, we propose a D-KPLS algorithm for building a more robust relationship between measurement and quality indices. And the new model, called dynamic kernel partial least squares, is built in reproducing kernel Hilbert space. In addition, for the purpose of process monitoring, D-KPLS decomposes the feature space into two orthogonal subspaces. And the fault detection approaches based on the new model are proposed.

The remainder of this paper is organized as follows. In Section 2, the standard KPLS algorithm is reviewed. In Section 3, the new D-KPLS algorithm is proposed. The corresponding fault detection methods are proposed in Section 4. Numerical example and Tennessee Eastman process cases studies are given out in Section 5 to show the effectiveness of new models for industrial process monitoring. The conclusions are summarized in the last section.

2. KPLS model

Given input matrix $\mathbf{X}$ consisting of N samples with m process variables, and output matrix $\mathbf{Y}$ containing N observations with J quality variables, i.e.,

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_N \end{bmatrix} \in \mathbf{R}^{N\times m}, \quad \mathbf{Y} = \begin{bmatrix} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_N \end{bmatrix} \in \mathbf{R}^{N\times J},$$

where $\mathbf{x}_i \in \mathbf{R}^m$ and $\mathbf{y}_i \in \mathbf{R}^J$ $(i=1, \ldots, N)$ are row vectors, respectively.

The main idea of the KPLS algorithm is to map the input data $\mathbf{x}_i \in \mathbf{R}^m$ on a high-dimensional feature space through a non-linear mapping, which is a reproducing kernel Hilbert space. And the dimension of feature space may be arbitrarily large even infinite. The non-linear structure in input space is more likely to be linear in feature space, which a linear KPLS regression can be applied.

Chosen a Mercer kernel $k(\cdot, \cdot)$, then the non-linear mapping $\varphi(\cdot)$ can be obtained by the following inner products.

$$k(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)\varphi(\mathbf{x}_j)^T \tag{1}$$

with $\varphi(\mathbf{x}_i) \in R^{1\times S}$, $i=1, \ldots, N$. S is the dimension of feature space.

The kernel function $k(\cdot, \cdot)$ selected must satisfy the Mercer's theorem conditions. And a specific kernel function implicitly determines the associated mapping $\varphi(\cdot)$ and the feature space.

By substituting the $k(\mathbf{x}_i, \mathbf{x}_j)$ for $\varphi(\mathbf{x}_i)\varphi(\mathbf{x}_j)^T$, knowing the explicit non-linear mapping and calculating the inner product can be avoided.

According to Eq. (1), the Gram matrix $\mathbf{K} \in \mathbf{R}^{N\times N}$ can be obtained as follows:

$$\mathbf{K} = \Phi(\mathbf{X})\Phi(\mathbf{X})^T \tag{2}$$

with $\Phi(\mathbf{X}) = [\varphi(\mathbf{x}_1)^T, \ldots, \varphi(\mathbf{x}_N)^T]^T \in \mathbf{R}^{N\times S}$.

Before building the KPLS model, the mapped sample $\varphi(x_i)$ need to be centered as follows:

$$\varphi(\mathbf{x}_i)^T = \varphi(\mathbf{x}_i)^T - \Phi^T\mathbf{e} \tag{3}$$

where $\mathbf{e}$ is a column vector with all the entries equal to $1/N$. And the centered Gram matrix $\mathbf{K}$ is calculated by Eq. (4).

$$\mathbf{K} = \Phi(\mathbf{X})\Phi(\mathbf{X})^T = (\mathbf{I}-\mathbf{E})\mathbf{K}(\mathbf{I}-\mathbf{E}) \tag{4}$$

where $\mathbf{E}$ is a $(N \times N)$ matrix with all its entries equal to $1/N$ and the element (i,j) of $\mathbf{K}$ is $k(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)\varphi(\mathbf{x}_j)^T$.

According to KPLS algorithm, the regression function between $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_N]^T$ and $\Phi(\mathbf{X})$ can be expressed by the following matrix forms (Zhang and Teng, 2010):

$$\hat{\mathbf{Y}} = \Phi(\mathbf{X})\mathbf{C} = \mathbf{T}\mathbf{T}^T\mathbf{Y} \tag{5}$$

$$\begin{cases} \mathbf{T} = \Phi(\mathbf{X})\mathbf{R} \\ \mathbf{R} = \Phi(\mathbf{X})^T\mathbf{U}(\mathbf{T}^T\mathbf{K}\mathbf{U})^{-1} \end{cases} \tag{6}$$

with $\mathbf{C} = \Phi(\mathbf{X})^T\mathbf{U}(\mathbf{T}^T\mathbf{K}\mathbf{U})^{-1}\mathbf{T}^T\mathbf{Y}$ is regression coefficient, and $\hat{\mathbf{Y}}$ is the prediction of $\mathbf{Y}$.