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Research Article

A nonlinear quality-related fault detection approach based on modified kernel partial least squares

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ABSTRACT

In this paper, a new nonlinear quality-related fault detection method is proposed based on kernel partial least squares (KPLS) model. To deal with the nonlinear characteristics among process variables, the proposed method maps these original variables into feature space in which the linear relationship between kernel matrix and output matrix is realized by means of KPLS. Then the kernel matrix is decomposed into two orthogonal parts by singular value decomposition (SVD) and the statistics for each part are determined appropriately for the purpose of quality-related fault detection. Compared with relevant existing nonlinear approaches, the proposed method has the advantages of simple diagnosis logic and stable performance. A widely used literature example and an industrial process are used for the performance evaluation for the proposed method.

1. Introduction

In the field of process monitoring, model-based methods have been deeply studied and a lot of research results have been achieved [1–3]. Unfortunately, the model-based methods present some implementation difficulties in complex industrial systems such as chemical, metallurgy, bio pharmaceutical and etc., where the analytical models of plants cannot be modeled easily [4]. For such applications, multivariate statistical process monitoring (MSPM) approaches [5–9] are the preferred technologies thanks to their data-based nature. Recently, the research and industrial practices indicate that not all of the process faults will inevitably lead to the fluctuation of product quality. On the contrary, if ignore the alarms of the faults that have no effects on product quality, the unnecessary downtime and maintenance of factory can be significantly reduced, which finally brings considerable economic benefits. Motivated by the potential economic benefits, quality-related process monitoring gradually causes attentions in the past five years [10–16].

Since quality variables are usually hard to be measured online or sampled with significant time-delay [17], it is reasonable to model these quality variables and process variables, then utilize the model to guide the implementation of fault detection scheme. For such a purpose, the MSPM methods are typically limited to significantly utilized partial least squares (PLS) based methodologies [18]. Based on PLS model, many successful monitoring approaches have been developed [5,19]. Recently, Li [20] revealed the geometric nature of PLS, indicating that PLS's principal elements contain many variations that orthogonal to output while the PLS's residual elements contain many variations that associated with output. Based on Li's result, Zhou [10] first analyzed the inherent flaw of PLS for quality-related fault detection and proposed a total PLS (T-PLS) model with a more detailed decomposition for process variables matrix. Zhou's work opened up the studies of quality-related fault detection. Subsequently, Qin [14] proposed C-PLS method according to a similar idea. Soon later, Yin [21] proposed a more simple method utilizing SVD to decompose process variables space into two orthogonal subspaces. Different from the above PLS-based approaches, Peng [22] and Wang [16] used principal component regression (PCR) model to realize another two linear methods. However, relevant nonlinear research has not yet attracted enough attention and existing achievements are limited. By extending T-PLS to a nonlinear version, Peng [23] proposed the first nonlinear quality-related fault detection method based on KPLS model, called total KPLS (T-KPLS). Soon later, Zhang [24] extended the linear method of [14] to a nonlinear case. Very recently, Jia [25] utilized KPLS model and SVD to realize another nonlinear method.

In fact, the current research for nonlinear quality-related fault detection has just started and is far from perfect. As a useful supplement, this paper aims to propose a simple nonlinear method based on KPLS model. Similar to the existing approaches, the proposed method deals with the nonlinearities among process variables by a nonlinear projection function, mapping original

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process variables into high-dimensional feature space in which the linear relationship between kernel matrix and output matrix is realized by means of KPLS. The kernel matrix is then decomposed into two orthogonal parts by SVD and the test statistics for each part are appropriately designed for the purpose of quality-related fault detection. It is satisfactory that the proposed new method has more simple diagnosis logic and more stable performance than most of the existing nonlinear approaches.

The remaining sections are arranged as follows: Section 2 introduces preliminaries. Section 3 gives the specific implementation steps of the new method. In Section 4, simulations on a widely used literature example and an industrial benchmark will be carried out to verify the effectiveness of the new method. Finally, conclusions are drawn in Section 5.

Notation: Let $\mathbb{R}$ be the set of scalars, $\mathbb{R}^m$ be the set of m-dimensional vectors, $\mathbb{R}^{n\times m}$ be the set of $n \times m$ matrices, and all vectors and matrices are shown in bold. $\mathbf{I}_m$ is an identity matrix with $m \times m$-dimensional. $\langle \mathbf{x}, \mathbf{y}\rangle$ is the inner product of vectors $\mathbf{x}$ and $\mathbf{y}$. $rank(\mathbf{A})$ is the rank of matrix $\mathbf{A}$. '$\star$' represents the elements block of matrix. $\mathcal{N}(\mu, \delta^2)$ is normal distribution with mean μ and variance δ. $\mathcal{F}_\alpha(a, b)$ is $\mathcal{F}$ distribution with confidence limit α and a and b degrees of freedom. $\chi^2_\alpha(h)$ is χ^2 distribution with confidence limit value α, coefficient g and h degrees of freedom.

2. Kernel Partial Least Squares (KPLS)

Assume that, the considered nonlinear process totally contains m process variables $(x_{i,1}, x_{i,2}, \ldots, x_{i,m})$ and l quality variables $(y_{i,1}, y_{i,2}, \ldots, y_{i,l})$. The off-line measurements of these variables are recorded into samples $\mathbf{x}_i$ and $\mathbf{y}_i$, respectively, i.e.:

$$\mathbf{x}_i = [x_{i,1}, x_{i,2}, \ldots, x_{i,m}]^T \in \mathbb{R}^m, \tag{1}$$

$$\mathbf{y}_i = \left[y_{i,1}, y_{i,2}, \ldots, y_{i,l}\right]^T \in \mathbb{R}^l, \tag{2}$$

where $i = 1, 2, \ldots, N$. N is the number of training samples. All the samples satisfy normal distributions and $N \gg m > l \geq 1$. Samples $\mathbf{x}_i$ and $\mathbf{y}_i$ are composed of matrices $\mathbf{X}$ and $\mathbf{Y}$, that:

$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N]^T \in \mathbb{R}^{N\times m}, \tag{3}$$

$$\mathbf{Y} = [\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N]^T \in \mathbb{R}^{N\times l}. \tag{4}$$

Usually, $\mathbf{X}$ is called process variables matrix or input matrix, $\mathbf{Y}$ is called quality variables matrix or output matrix.

To deal with the nonlinear characteristics among process variables, it is a common way [26,23–25] to map the original input data into a high-dimensional feature space, such that the mapped data and the output can be modeled by linear means. To this aim, given a nonlinear projection function ϕ, project the original samples $\mathbf{x}_i (i = 1, 2, \ldots, N)$ into a feature space F, that:

$$\mathbf{x}_i \in \mathbb{R}^m \;\rightarrow\; \phi(\mathbf{x}_i) \in \mathbb{R}^\Omega, \tag{5}$$

where the dimension Ω can be arbitrarily large or even infinite. The input matrix $\mathbf{X}$ turns to feature matrix $\mathbf{\Phi}$:

$$\mathbf{\Phi} = [\phi(\mathbf{x}_1),\ \phi(\mathbf{x}_2),\ \cdots,\ \phi(\mathbf{x}_N)]^T \in \mathbb{R}^{N\times\Omega}. \tag{6}$$

As a necessary step [26], $\phi(\mathbf{x}_i)$ should be zero mean, that:

$$\bar{\phi}(\mathbf{x}_i) = \phi(\mathbf{x}_i) - \bar{\phi}, \tag{7}$$

$$\bar{\phi} = \frac{1}{N}\sum_{i=1}^{N}\phi(\mathbf{x}_i) = \frac{1}{N}\mathbf{\Phi}^T\mathbf{1}_N, \tag{8}$$

where $\mathbf{1}_N = [1,\ 1,\ \cdots,\ 1]^T \in \mathbb{R}^N$. Thus, the zero mean of $\mathbf{\Phi}$ is

$$\begin{aligned}\bar{\mathbf{\Phi}} &= \left[\bar{\phi}(\mathbf{x}_1),\ \bar{\phi}(\mathbf{x}_2),\ \ldots,\ \bar{\phi}(\mathbf{x}_N)\right]^T \\ &= \mathbf{\Phi} - \left[\bar{\phi}, \bar{\phi}, \ldots, \bar{\phi}\right]^T \\ &= \mathbf{\Phi} - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\mathbf{\Phi}.\end{aligned} \tag{9}$$

According to Cover's theory [26], nonlinear data set $(\mathbf{X}, \mathbf{Y})$ now turns to approximately linear data set $(\bar{\mathbf{\Phi}}, \mathbf{Y})$, where $\bar{\mathbf{\Phi}}$ contains all the fault information of process variables. According to [26], the KPLS model of $(\bar{\mathbf{\Phi}}, \mathbf{Y})$ is modeled as follows:

$$\begin{cases}\bar{\mathbf{\Phi}} = \mathbf{T}\mathbf{P}^T + \bar{\mathbf{\Phi}}_r \\ \mathbf{Y} = \mathbf{T}\mathbf{Q}^T + \mathbf{Y}_r\end{cases}, \tag{10}$$

where $\mathbf{T} \in \mathbb{R}^{N\times\gamma}$ is called score matrix. $\mathbf{P} \in \mathbb{R}^{M\times\gamma}$ and $\mathbf{Q} \in R^{l\times\gamma}$ are loading matrices of $\bar{\mathbf{\Phi}}$ and $\mathbf{Y}$, respectively. $\bar{\mathbf{\Phi}}_r$ and $\mathbf{Y}_r$ are residuals. γ is the number of laten variables determined by cross validation [27].

Due to the dimension Ω of $\mathbf{\Phi}$ is arbitrarily large or even infinite, the following kernel matrix $\mathbf{K}$ is usually defined [26] to avoid the explicit using of $\mathbf{\Phi}$:

$$\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^T \in \mathbb{R}^{N\times N}, \tag{11}$$

where the element $k_{i,j}$ of the i_{th} row and j_{th} column of $\mathbf{K}$ is

$$k_{i,j} = \langle\phi(\mathbf{x}_i), \phi(\mathbf{x}_j)\rangle = f_{ker}(\mathbf{x}_i, \mathbf{x}_j), \tag{12}$$

where f_{ker} is Gaussian kernel function [26] that:

$$f_{ker}(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x} - \mathbf{y}\|^2}{c}\right), \tag{13}$$

where c is a constant fixed by the method introduced in [23]. The zero mean of $\mathbf{K}$ is also required [26], that:

$$\begin{aligned}\bar{\mathbf{K}} &= \bar{\mathbf{\Phi}}\bar{\mathbf{\Phi}}^T \\ &= \left(\mathbf{\Phi} - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\mathbf{\Phi}\right)\left(\mathbf{\Phi} - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\mathbf{\Phi}\right)^T \\ &= \left(\mathbf{I}_N - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\right)\mathbf{\Phi}\mathbf{\Phi}^T\left(\mathbf{I}_N - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\right) \\ &= \left(\mathbf{I}_N - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\right)\mathbf{K}\left(\mathbf{I}_N - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\right).\end{aligned} \tag{14}$$

Algorithm 1. The calculation algorithm of KPLS [26].

1. Set $i=1$, $\mathbf{Y}_1 = \mathbf{Y}$, $\bar{\mathbf{K}}_1 = \bar{\mathbf{K}}$;
2. Select the first column of $\mathbf{Y}_i$ as $\mathbf{u}_i$;
3. $\mathbf{t}_i = \bar{\mathbf{K}}_i\mathbf{u}_i$;
4. $\mathbf{t}_i = \mathbf{t}_i / \|\mathbf{t}_i\|$;
5. $\mathbf{c}_i = \mathbf{Y}_i^T\mathbf{t}_i$, $\mathbf{u}_i = \mathbf{Y}_i\mathbf{c}_i$;
6. $\mathbf{u}_i = \mathbf{u}_i / \|\mathbf{u}_i\|$;
7. Repeat step 3 to step 6 until $\mathbf{t}_i$ converges;
8. $\bar{\mathbf{K}}_{i+1} = (\mathbf{I}_N - \mathbf{t}_i\mathbf{t}_i^T)\bar{\mathbf{K}}_i(\mathbf{I}_N - \mathbf{t}_i\mathbf{t}_i^T)$, $\mathbf{Y}_{i+1} = (\mathbf{I}_N - \mathbf{t}_i\mathbf{t}_i^T)\mathbf{Y}_i$;
9. Save parameters $\mathbf{T} = [\mathbf{T}, \mathbf{t}_i]$, $\mathbf{U} = [\mathbf{U}, \mathbf{u}_i]$;
10. Set $i = i + 1$ and repeat step 2 to step 9 until $i > \gamma$.

Replacing $\bar{\mathbf{\Phi}}\bar{\mathbf{\Phi}}^T$ by $\bar{\mathbf{K}}$, the KPLS model of Eq. (10) is solved by Algorithm 1.