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ORIGINAL ARTICLE

New fault detection method based on reduced kernel principal component analysis (RKPCA)

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Abstract This paper proposes a new method for fault detection using a reduced kernel principal component analysis (RKPCA). The proposed RKPCA method consists on approximating the retained principal components given by the KPCA method by a set of observation vectors which point to the directions of the largest variances with the retained principal components. The proposed method has been tested on a chemical reactor and the results were satisfactory.

Keywords KPCA · RKPCA · PCs · SPE · Fault detection

Nomenclature

T^2	Hotelling statistic
SPE	Squared prediction error
m	Number of variables
$x(k) \in R^m$	Observation vector
$x_i(k)$	ith variable of the measurement vector $x(k)$
$X \in R^{N \times m}$	Data matrix
$\sum \in R^{m \times m}$	Correlation matrix
ℓ	Number of principal components
P	Eigenvector matrix
T	Score matrix
$\hat{X}$	Projection of X to R^{ℓ}
E	Error matrix
$\hat{x}(k)$	Projection of $x(k)$ to R^{ℓ}
$e(k)$	Error vector
δ_α^2	Threshold of SPE
$\chi^2_{\ell,\alpha}$	Threshold of T^2
p_i	ith eigenvector of P
λ_i	ith eigenvalue of K
ϕ	Transformation function
K	Kernel matrix

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1 Introduction

The demands for product quality and operation safety in the process industry have spurred the recent development of many fault diagnosis methods. Recently, with the development of measurement and data storage equipment, it is strongly required to use multivariate statistical method for extracting useful information from a large amount of process data. Multivariate statistical projection methods such as principal component analysis (PCA) have been widely applied for monitoring linear system [1, 2]. However, for some complicated cases in industrial chemical and biological processes with particular nonlinear characteristics, PCA performs poorly due to its assumption that the process data are linear. To overcome the nonlinear shortcoming of the traditional MSPC method, several nonlinear extensions of PCA were reported. Kernel PCA (KPCA) is a novel nonlinear PCA technique which is developed in recent years [3, 4]. It can efficiently compute principal components (PCs) in high-dimensional feature spaces by means of integral operators and nonlinear kernel functions. Despite recently reported KPCA-based monitoring applications, the following problems arise: first, the identification of a KPCA monitoring model requires the storage of the symmetric kernel matrix (computation time may increase with the number of samples); second, the fault isolation is a much more

difficult problem in nonlinear PCA than in linear PCA [5] and the monitoring model is fixed which may produce false alarms if the process is naturally time-varying.

This paper deals with the problem of need storage and computation time. In this paper, we propose a new reduced kernel principal component analysis (RKPCA) in which we consider only the set of observations that approximate the retained principal components. The RKPCA method has been tested on a chemical reactor and the results were successful.

The paper is organized as follows. In section 2, the KPCA technique is reminded. The proposed reduced KPCA method for process monitoring is detailed in section 3. Section 4 presents the KPCA method for fault detection. Section 5 validates the proposed algorithm on the CSTR benchmark. Finally, section 6 concludes the paper.

2 Kernel principal components analysis

KPCA is a nonlinear version of PCA method, when the initial data are projected in a new space, with a nonlinear mapping ϕ. PCA is then computed in this feature space F, as done with linear model.

Let $X = [x_1 \quad x_2 \quad \dots \quad x_N]^T$; the training set scaled to zero mean and unit variance. Let $x_i \in R^m, i=1,\dots,N$ to be the data vector at time $i>1$. By nonlinear mapping ϕ, a measured input is projected into an hyper-dimensional feature space F as

$$\phi : x_i \in R^m \mapsto \phi(x_i) = \phi_i \in F \tag{1}$$

Note that the feature space F have an arbitrarily large, possibly infinite dimensionality equal to h. The covariance matrix in the feature space F can be constructed by

$$C_\phi = \frac{1}{N}\sum_{i=1}^{N} \phi(x_i)\phi(x_i)^T = \frac{1}{N}\chi^T\chi \in R^{h\times h} \tag{2}$$

with $\chi = [\phi_1 \quad \phi_2 \quad \dots \quad \phi_N]^T x_i$ is the training data arranged in the feature space. To find the principal components, one has to solve the eigenvalue problem in the feature space such that:

$$\lambda_j \mu_j = C_\phi \mu_j \quad \forall j = 1, \dots, h \tag{3}$$

where $\lambda_j \geq 0$ is an eigenvalue and μ_j is a vector of eigen loadings. Schölkopf in [3] has suggested the following way to find this eigenvalue decomposition and he denote that: all solutions μ_j with $\lambda_j \neq 0$ lie in the span of $\{\phi(x_1),\phi(x_2),\dots,\phi(x_N)\}$. Therefore, there must exist coefficient $\gamma_i^j, i=1,\dots,N$ such every eigenvector μ_j of C_ϕ can be linearly expanded by

$$\mu_j = \sum_{i=1}^{N} \gamma_i^j \phi_i \tag{4}$$

Equation (3) is equivalent to

$$\lambda_j \left\langle \phi(x_i), \mu_j \right\rangle = \left\langle \phi(x_i), C_\phi \mu_j \right\rangle \quad \text{for } j = 1, \dots, h \tag{5}$$

Combining Eqs. (2) and (4) in (5), we obtain for $j=1,\dots,h$

$$\lambda_j \sum_{q=1}^{N} \gamma_q^j \langle \phi(x_i), \phi(x_q) \rangle = \left\langle \phi(x_i), \frac{1}{N}\sum_{k=1}^{N} \phi(x_k)\phi(x_k)^T \sum_{q=1}^{N} \gamma_q^j \phi(x_q) \right\rangle \tag{6}$$

$$\lambda_j \sum_{q=1}^{N} \gamma_q^j \langle \phi(x_i), \phi(x_q) \rangle = \left\langle \phi(x_i), \frac{1}{N}\sum_{k=1}^{N} \sum_{q=1}^{N} \gamma_q^j \phi(x_k) \langle \phi(x_k)\phi(x_q) \rangle \right\rangle \tag{7}$$

$$\lambda_j \sum_{q=1}^{N} \gamma_q^j \langle \phi(x_i), \phi(x_q) \rangle = \frac{1}{N}\sum_{k=1}^{N} \sum_{q=1}^{N} \gamma_q^j \langle \phi(x_i)\phi(x_k) \langle \phi(x_k)\phi(x_q) \rangle \rangle \tag{8}$$

An important property of the feature space is that the dot product of the form $\langle \phi(x_i), \phi(x_j) \rangle$ can be calculated by virtue of kernel tricks as a function of the corresponding vectors x_i and x_j, this is,

$$\langle \phi(x_i), \phi(x_j) \rangle = k(x_i, x_j) = K_{ij} \tag{9}$$

Then, the inner product of $\langle \phi(x_i), \phi(x_j) \rangle$ of Eq. (8) is changed by the kernel function $k(x_i,x_j)$. Then, Eq. (8) can be expressed as

$$\lambda_j \sum_{q=1}^{N} \gamma_q^j K_{qk} = \frac{1}{N}\sum_{k=1}^{N} \sum_{q=1}^{N} \gamma_q^j K_{ik} K_{kq} \quad \forall k = 1, \dots, N \tag{10}$$

Now, let us define a vector $\gamma^j = [\gamma_1^j, \gamma_2^j, \dots, \gamma_N^j]^T \in R^N$, so we have

$$\lambda_j K \gamma^j = \frac{1}{N} K^2 \gamma^j \tag{11}$$

To find solutions of Eq. (11), we solve the eigenvalue problem

$$N\lambda_j \gamma^j = K\gamma^j \quad \forall j = 1, \dots, N \tag{12}$$

In the following, for simplicity, we will denote λ_j as the eigenvalues of K, i.e., the solutions $N\lambda_j$ in Eq. (12). We rewrite Eq. (12) in the following matrix form:

$$\Lambda V = KV \tag{13}$$

with $\Lambda = diag(\lambda_1 \quad , \dots, \quad \lambda_N)$ is the diagonal matrix of the corresponding eigenvalues and $V = [\gamma^1 \quad , \dots, \quad \gamma^N]$ is the matrix containing the eigenvectors of the kernel matrix K. In order to insure the normality of $\mu_1,\mu_2,\dots,\mu_N$. In Eq. (3), the corresponding vectors $\gamma^1,\gamma^2,\dots,\gamma^N$ should be scaled such that

$$\langle \mu_k, \mu_k \rangle = 1 \text{ for all } k = 1, \ldots, N \tag{14}$$

Using Eq. (4), this lead to

$$1 = \left\langle \sum_{i=1}^{N} \gamma_i^k \phi(x_i), \sum_{j=1}^{N} \gamma_j^k \phi(x_j) \right\rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} \gamma_i^k \gamma_j^k \langle \phi(x_i), \phi(x_j) \rangle \tag{15}$$

$$\begin{aligned} 1 = \sum_{i=1}^{N} \sum_{j=1}^{N} \gamma_i^k \gamma_j^k K_{ij} &= \langle \gamma^k, K\gamma^k \rangle \\ &= \lambda_k \langle \gamma^k, \gamma^k \rangle \end{aligned} \tag{16}$$

Thus, the associated orthogonal eigenvectors $\gamma^1, \gamma^2, \ldots, \gamma^N$ can be expressed as

$$\langle \gamma^k, \gamma^k \rangle = \frac{1}{\lambda_k} \text{ for all } k = 1, \ldots, N \tag{17}$$

which shows that $\mu_1, \mu_2, \ldots, \mu_N$ are given by

$$\mu_i = \sum_{j=1}^{N} \frac{\gamma_j^i}{\sqrt{\lambda_i}} \phi_j = \lambda_i^{-1/2} \chi^T \gamma^i \tag{18}$$

The matrix with the ℓ first leading eigenvectors are the KPCA principal loadings in the feature space, denoted as $\hat{P}_f = [\mu_1 \quad \mu_2 \quad \ldots \quad \mu_\ell]$. From Eq. 18, $\hat{P}_f$ is related to the loadings in the measurement space as

$$\begin{aligned} \hat{P}_f &= \left[\frac{1}{\sqrt{\lambda_1}} \chi^T \gamma^1 \quad \ldots \quad \frac{1}{\sqrt{\lambda_\ell}} \chi^T \gamma^\ell \right] \\ &= \chi^T \hat{P} \hat{\Lambda}^{-\frac{1}{2}} \end{aligned} \tag{19}$$

Where $\hat{P} = [\gamma^1 \quad \ldots \quad \gamma^\ell]$ and $\hat{\Lambda} = diag\ (\lambda_1 \quad \ldots \quad \lambda_\ell)$ are the ℓ principal eigenvectors and eigenvalues of K, respectively, corresponding to the largest eigenvalues in descending order.

For a given measurement x and its mapped vector $\phi = \phi(x)$, the model scores are calculated as

$$\begin{aligned} \hat{t} = \hat{P}_f^T \phi &= \hat{\Lambda}^{-\frac{1}{2}} \hat{P}^T \chi \phi \\ &= \hat{\Lambda}^{-\frac{1}{2}} \hat{P}^T k(x) \end{aligned} \tag{20}$$

where

$$\begin{aligned} k(x) = \chi \phi &= [\phi_1 \quad \phi_2 \quad \ldots \quad \phi_N]^T \phi \\ &= [\phi_1^T \phi \quad \phi_2^T \phi \quad \ldots \quad \phi_N^T \phi]^T \\ &= [k(x_1, x) \quad k(x_2, x) \quad \ldots \quad k(x_N, x)]^T \end{aligned} \tag{21}$$

Before applying KPCA, mean centering and variance scaling in high-dimensional space should be performed. Mean centering can be done by substituting the kernel matrix K with

$$\tilde{K} = K - I_N K - K I_N + I_N K I_N \tag{22}$$

where $I_N = \frac{1}{N} \begin{bmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} \in R^{N \times N}$. Also, the variance scaling of kernel matrix can be done by the following equation.

$$K_{scl} = \frac{\tilde{K}}{trace\left(\tilde{K}\right)/N} \tag{23}$$

If we apply eigenvalue decomposition to K_{scl}.

$$\Lambda V = K_{scl} V \tag{24}$$

We can obtain the orthogonal eigenvectors $\gamma^1, \gamma^2, \ldots, \gamma^\ell$ corresponding to ℓ largest eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_\ell$

3 Reduced kernel principal components analysis

We select a reduced number of observations $x_b^{(j)} \in \{x^i\}_{i=1,\ldots,N}$ among the N measurement variables of the information matrix. The retained observations can be used as a new data matrix. The proposed reduced KPCA method (RKPCA) approaches each vector $\{\mu_j\}_{j=1,\ldots,\ell}$ by a transformed input data $\phi(x_b^j) \in \{\phi(x^{(i)})\}_{i=1,\ldots,N}$ having a high projection value in the direction of μ_j [6]. For each principal component $\{\mu_j\}_{j=1,\ldots,\ell}$ the proposed RKPCA method selects among the set of $\{\phi(x^{(i)})\}_{i=1,\ldots,N}$ the closest vectors, $\phi(x_b^{(j)})$ to μ_j To achieve that we project all the $\{\phi(x^{(i)})\}_{i=1,\ldots,N}$ on the principal component μ_j and we retain the observations $\phi(x_b^j) \in \{\phi(x^{(i)})\}_{i=1,\ldots,N}$ that satisfied

$$\begin{cases} \phi\left(x_b^{(j)}\right)_j = \underset{i=1,\ldots,N}{Max} \tilde{\phi}\left(x^{(i)}\right)_j \\ \phi \quad \left(x_b^{(j)}\right)_{i \neq j} < \quad \zeta \end{cases} \tag{25}$$

where $\tilde{\phi}\left(x^{(i)}\right)_j$ is the j^{th} component projection of $\phi(x^{(i)})$ on μ_j and ζ is a given threshold.

The RKPCA algorithm is summarized by the seven following steps:

1. Given an initial standardized block of training data, construct the kernel matrix K and scale it.
2. Determine the nonzero eigenvalues $\{\lambda_j\}_{j=1,\ldots,N}$ and the eigenvectors $\{\gamma_j\}_{j=1,\ldots,N}$ of Gram matrix K.
3. Determine the number ℓ of principal component PCs and organize the $\{\gamma_j\}_{j=1,\ldots,\ell}$ on the decreasing order with respect to the corresponding eigenvalues.
4. For the ℓ retained principal components, choose the $\{(x_b^j)\}_{j=1,\ldots,\ell}$ that satisfy (25).

5. Construct the reduced kernel matrix.
6. Estimate the reduced KPCA model (the eigenvalues and vectors of the reduced kernel matrix).
7. Determine the control limits of the SPE chart.

4 RKPCA for fault detection

The KPCA-based monitoring method is similar to that using PCA in that the *Spe* statistic in the feature space can be interpreted in the same way. The *Spe* index is defined as the norm of the residual vector in the feature space [7, 8]. Let $\tilde{t}$ be the residual components and $\tilde{P}_f$ the corresponding loading matrix

$$\tilde{t} = \tilde{P}_{f\,f}\phi = [\,\mu_{\ell+1} \quad \mu_{\ell+2} \quad \ldots\,]^T\phi \tag{26}$$

The *Spe* index is calculated as the squared norm of the residual components

$$Spe = \tilde{t}^T\tilde{t} = \phi^T\tilde{P}_f\tilde{P}_f^T\phi \tag{27}$$

Since we do not know the dimension of the feature space, it is not possible to know the number of residual components there. Thus, we cannot calculate explicitly the loading matrix $\tilde{P}_f$. However, we can calculate the product $\tilde{P}_f\tilde{P}_f^T$ as the projection orthogonal to the principal component space, which is

$$\hat{C}_f = \tilde{P}_f\tilde{P}_f^T = I_N - \hat{P}_f\hat{P}_f^T \tag{28}$$

and leads to

$$Spe = \phi^T\left(I_N - \hat{P}_f\hat{P}_f^T\right)\phi = \phi^T\phi - \phi^T\hat{P}_f\hat{P}_f^T\phi \tag{29}$$

From Eqs. 9 and 19, the *Spe* is calculated as a function of input vectors as

$$\begin{aligned} Spe &= k(x,x) - \phi^T\chi^T\hat{P}\hat{\Lambda}^{-1}\hat{P}^T\chi\phi \\ &= k(x,x) - k(x)^T\hat{P}\hat{\Lambda}^{-1}\hat{P}^T k(x) \\ &= k(x,x) - k(x)^T\hat{C}\,k(x) \end{aligned} \tag{30}$$

where $\hat{C} = \hat{P}\hat{\Lambda}^{-1}\hat{P}^T$, assuming that the prediction errors are normally distributed, the confidence limits for the *Spe* are calculated from the χ^2 distribution and are given by [9]:

$$Spe_{\lim,\,a} \sim g\chi^2_{h,a}; g = \frac{v}{2m}; h = \frac{2m^2}{v} \tag{31}$$

with m and v are the estimated mean and variance, respectively, of the *Spe* from the training data.

The Hotelling's T^2 index is calculated in the feature space as $T^2 = \hat{t}^T\hat{\Lambda}^{-1}\hat{t}$. The T^2 is calculated using kernel functions as [10]

$$T^2 = k(x)^T\hat{P}\Lambda^{-2}\hat{P}^T k(x) = k(x)^T D k(x) \tag{32}$$

where $D = \hat{P}\Lambda^{-2}\hat{P}^T$. The $100(1-\alpha)\%$ control limit for the T^2 is calculated using the F distribution such as

$$T^2_{\lim,\alpha} = \frac{p\left(N^2-1\right)}{N(N-p)}F_{p,N-p,\alpha} \tag{33}$$

where N is the number of observation in the model, p the number of principal components, and α the significance level.

5 Simulation results

To evaluate the performances of the proposed RKPCA fault detection method, a simulation on a chemical reactor CSTR is presented.

5.1 The chemical reactor description

The process is a continuous stirred tank reactor (CSTR) which is a nonlinear system used to conduct chemical reactions [11, 12] so that two reactants 1 and 2, with concentration Cb_1 and Cb_2 and feed w_1 and w_2, respectively, are mixed to provide a final product with feed w_0 and concentration Cb. A diagram of this reactor is given in Fig. 1.

The physical equations describing the process are

$$\begin{aligned} \frac{dh(t)}{dt} &= w_1(t) + w_2(t) - 0.2\sqrt{h(t)} \\ \frac{dC_b(t)}{dt} &= (C_{b1}(t) - C_b(t))\frac{w_1(t)}{h(t)} + (C_{b2}(t) - C_b(t))\frac{w_2(t)}{h(t)} - \frac{k_1 \cdot C_b(t)}{(1 + k_2 \cdot C_b(t))^2} \end{aligned} \tag{34}$$

where $h(t)$ is the level of the mixture in the reactor and k_1 and k_2 are consuming reactant rates. The temperature in the reactor is assumed constant and equal to the ambient temperature.

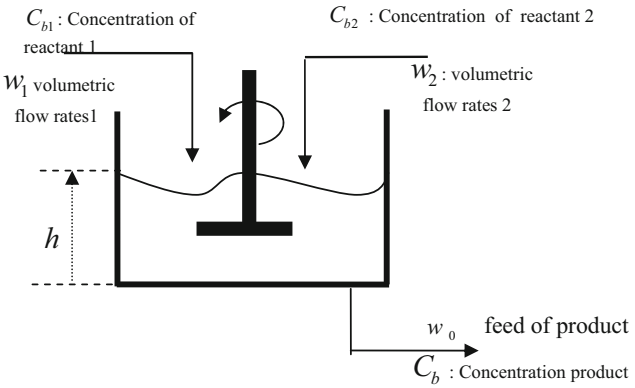

Fig. 1 Chemical reactor diagram

5.2 Results

To build the RKPCA model, we use the radial basis function (RBF) kernel defined as

$$k(x,x') = \exp\left(-\frac{\|x-x'\|^2}{2\sigma^2}\right) \quad (35)$$

with σ=8. Therefore, we have used 50 observations to build the reduced KPCA model and 750 new observations in the validation phase. The number of significant PCs is selected using CPV method, such that the variance explained is approximately 95 % of the total variance. The number of retained principal component is equal to ≈3.

A fault affecting the variable w_1 is simulated between samples 600 and 700 with the magnitude of 60 % of the range of variation of w_1. Control limits are calculated at the confidence level of 95 and 99 %, respectively.

The evaluated performances are as follows[13]:

- The false alarm rate (FAR) which expresses the ratio of the violated samples (those which exceed the detection thresholds) to the faultless data.

$$FAR = \frac{violated\ samples}{faultless\ data}\% \quad (36)$$

- The missed detection rate (MDR) which is given by the ratio of the faulty data that does not exceed the detection thresholds to all the faulty data.

$$MDR = \frac{missed\ detection}{faulty\ data}\% \quad (37)$$

- The good detection rate (GDR) which expresses the ratio violated samples to the faulty data and not violated samples to faultless data.

$$GDR = \left(\frac{violated\ samples}{faulty\ data} + \frac{not\ violated\ samples}{faultless\ data}\right)\% \quad (38)$$

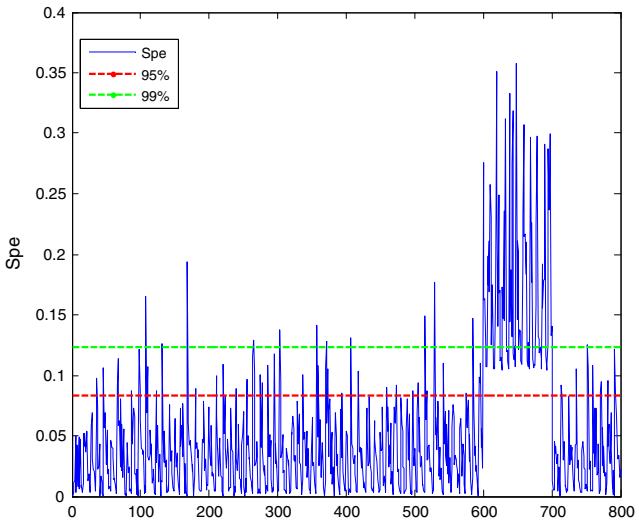

Fig. 2 *Spe* with a fault on the variable w_1

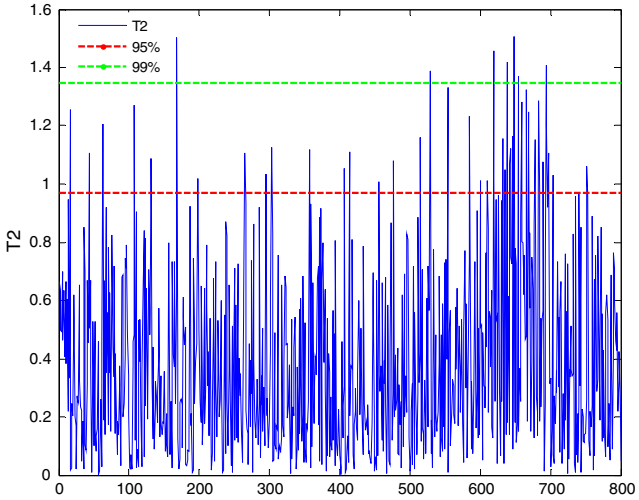

Fig. 3 T^2 with a fault on the variable w_1

The detection results of the reduced kernel principal component (RKPCA) method using the fault detection indices *Spe* and T^2 are shown, respectively, in Figs. 2 and 3.

According to the Fig. 2, the index *Spe* has detected the fault in both thresholds (95 and 99 %) witch confirm the good efficiency of the proposed RKPCA method. But using the T^2, the fault is not detected in both thresholds (Fig. 3).

The performances of the proposed RKPCA method are summarized in the Table 1. According to Table 1, we remark that the proposed RKPCA method for fault detection using SPE index has good results in terms of FAR, MDR, and GDR and especially in the case of the threshold 99 %.

6 Conclusions

In this paper, a new kernel method for nonlinear system fault detection is proposed. The proposed technique is entitled reduced kernel principal component analysis (RKPCA). The principle of the proposed method consists on approximating

Table 1 Performances of reduced KPCA for fault detection

	FAR		MDR		GDR	
	95 %	99 %	95 %	99 %	95 %	99 %
Spe	1.69	0.15	43	63	86	90
T^2	12	11	5	7	28	34

the retained principal components determined by the KPCA method by a set of observation vectors which point to the directions of the largest variances with the selected principal components. In order to evaluate the performances of the RKPCA method, it is applied to detect a fault on a CSTR benchmark and the results were satisfactory. The proposed RKPCA technique for fault detection may be very helpful to design a real time monitoring strategy of nonlinear systems.

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