Neural Component Analysis for Fault Detection

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Abstract—Principal component analysis (PCA) is largely adopted for chemical process monitoring and numerous PCA-based systems have been developed to solve various fault detection and diagnosis problems. Since PCA-based methods assume that the monitored process is linear, nonlinear PCA models, such as autoencoder models and kernel principal component analysis (KPCA), has been proposed and applied to nonlinear process monitoring. However, KPCA-based methods need to perform eigen-decomposition (ED) on the kernel Gram matrix whose dimensions depend on the number of training data. Moreover, prefixed kernel parameters cannot be most effective for different faults which may need different parameters to maximize their respective detection performances. Autoencoder models lack the consideration of orthogonal constraints which is crucial for PCA-based algorithms. To address these problems, this paper proposes a novel nonlinear method, called neural component analysis (NCA), which intends to train a feedforward neural work with orthogonal constraints such as those used in PCA. NCA can adaptively learn its parameters through backpropagation and the dimensionality of the nonlinear features has no relationship with the number of training samples. Extensive experimental results on the Tennessee Eastman (TE) benchmark process show the superiority of NCA in terms of missed detection rate (MDR) and false alarm rate (FAR). The source code of NCA can be found in [https://github.com/haitaozhao/Neural-Component-Analysis.git].

Note to Practitioner: Online monitoring for chemical process has been considered as a critical and hard task in real industrial applications. In this paper, an innovative method called neural component analysis (NCA) is proposed for fault detection. NCA is a unified model including a nonlinear encoder and a linear decoder. Due to its simple and intuitive format, NCA has superior performance in both computational efficiency and fault detection which makes it suitable for process monitoring in real industrial applications. Moreover, the experimental results presented can be reproduced effortlessly.

Index Terms—Process monitoring, Fault detection, Feedforward neural network, Autoencoder

I. INTRODUCTION

Monitoring process conditions is crucial to its normal operation [1]. Over last decades, data-driven multivariate statistical process monitoring (MSPM) has been widely applied to fault diagnosis for industrial process operations and production results [2], [3]. Due to the data-based nature of MSPM, it is relatively convenient to apply to real processes of large scale comparing to other methods based on theoretical modelling or rigorous derivation of process systems [4], [5].

The task of MSPM is challenging mainly due to the “curse of dimensionality” problem and the “data rich but information poor” problem. Many methods have been proposed to transform original high dimensional process data into a lower dimensional feature space and then performing fault detection or fault diagnosis in that feature space [6]. Principal component analysis (PCA) [7], [8], [9] is one of the most widely used linear techniques for fault detection. Due to orthogonal linear projection, PCA separates data information into two subspaces: a significant subspace which contains most variation in training data and a residual subspace which includes noises or outliers in training data.

PCA-based methods to inherently nonlinear processes may lead to unreliable and inefficient fault detection, since a linear transformation is hard to tackle the nonlinear relationship between different process variables [10], [11]. To deal with this problem, various nonlinear extensions of PCA have been proposed for fault detection. These extensions can be divided into 3 categories.

The first category is kernel approaches. Kernel PCA (KPCA) is one of the mostly used kernel approaches for fault detection [12]. KPCA implicitly maps the data from an input space into some high dimensional nonlinear feature space, where linear PCA can be applied. KPCA need to perform eigen decomposition (ED) on the kernel Gram matrix whose size is the square of the number of data points. When there are too many data points, the calculation of ED becomes hard to perform [13]. Moreover, KPCA need to determine the kernel and the associated parameters in advance.

The second category is based on linear approximation of nonlinear process. In the linear approximation, several local linear models are constructed and then integrated by Bayesian inference [14]. Linear approximation is simple and easy to realize, but it may not be able to handle strong nonlinearities in the process.

The third category is neural-network-based models, such as robust autoencoder (RAE) [13] and autoassociative neural network [15]. These models train a feedforward neural network to perform the identity encoding, where the inputs and the outputs of the network are the same. The network contains an internal “bottleneck” layer (containing fewer nodes than the output and input layers) for feature extraction. In autoassociative neural network [15], the mapping from the input layer to the “bottleneck” layer can be considered as encoding, while de-mapping from the “bottleneck” layer to the output layer can be considered as decoding. Although the encoding can deal with the nonlinearities present in the data, it has no consideration of the orthogonal constraints used in PCA.

Recent years, a new trend in neural-network-based techniques known as deep learning has become popular in artificial intelligence and machine learning [16]. Deep-learning-based models are widely used in unsupervised training to learn the representation of original data. Although these models are often derived and viewed as extensions of PCA, all of them...
lack the consideration of the orthogonal constraints used in PCA. The orthogonal constraints are quite important, since they can largely reduce the correlations between extracted features. Figure 1 shows simple plots of features of Vector $X$ obtained by orthogonal projections and non-orthogonal projections respectively. From Figure 1b it is easy to find PC$_1$ and PC$_2$ are largely correlated. It means that the extracted features contain redundant information and may distort the reconstruction of the original vector $X$.

Motivated by the above analysis, this paper proposes a novel unified model, called neural component analysis (NCA), for fault detection. NCA firstly utilizes a nonlinear neural network as an encoder to extract features. Then linear orthogonal transformation is adopted to decode the features to the original data space. Finally, this unified model is trained by minimizing the reconstruction error between original data and the decoded data. After training, NCA can be used as an unsupervised learning method to extract the key features of process data. In this paper, Hotelling $T^2$ statistic and the squared prediction error (SPE) statistic are used for fault detection. The merits of the proposed NCA method are demonstrated by both theoretical analysis and case studies on the Tennessee Eastman (TE) benchmark process.

II. AUTOENCODER AND PCA

An autoencoder model is an artificial neural network adopted for unsupervised feature extraction [13]. An autoencoder model tries to learn a representation (encoding) for original data, specifically for the purpose of dimensionality reduction. Recently, due to the research works in deep learning, the autoencoder concept has been widely accepted for generative models of data [19].

We assume that there are $N$ input samples $x_i = [x_{i1}, x_{i2}, \ldots, x_{in}] \in \mathbb{R}^{1 \times n}$ ($i = 1, 2, \ldots, N$). The simplest structure of an autoencoder model is a feedforward neural network which consists of one input layer with $n$ inputs, one hidden layer with $p$ ($p < n$) units and one output layer with the same number of nodes as the input layer (see Figure 2). The purpose of this structure is to reconstruct its own inputs. Therefore, an autoencoder model belongs to unsupervised learning.

An autoencoder model includes both the encoder part and the decoder part, which can be defined as transitions $\alpha$ and $\beta$, such that:

$$\alpha : \mathbb{R}^{1 \times n} \rightarrow \mathcal{F}$$
$$\beta : \mathcal{F} \rightarrow \mathbb{R}^{1 \times n}$$

$$\alpha, \beta = \arg \min_{\alpha, \beta} \sum_{i=1}^{N} \|x_i - \beta(\alpha(x_i))\|^2. \tag{1}$$

In this paper, we only consider the case $\mathcal{F} = \mathbb{R}^{1 \times p}$. The encoder part takes the input $x$ and maps it to $z \in \mathbb{R}^{1 \times p}$:

$$z = \alpha(x) \triangleq \sigma(Wx + b).$$

This feature $z$ is usually referred to as latent code, latent feature or latent representation. Here, $\sigma(\cdot)$ is an element-wise activation function such as a sigmoid function or a hyperbolic tangent function. Matrix $W$ is a parameter matrix and $b$ is a bias vector.

The decoder part maps the feature vector $z$ to the reconstruction $\tilde{x}$ of the same dimensionality as $x$:

$$\tilde{x} = \beta(z) \triangleq \tilde{\sigma}(\tilde{W}z + \tilde{b})$$

where $\tilde{\sigma}$, $\tilde{W}$ and $\tilde{b}$ for the decoder part may be different from the corresponding $\sigma$, $W$ and $b$ for the encoder part, depending on the applications of the autoencoder model.

In order to learn the parameters in the activation functions, an autoencoder model is often trained to minimize reconstruction error:

$$W, b, \tilde{W}, \tilde{b} = \arg \min_{W, b, \tilde{W}, \tilde{b}} \sum_{i=1}^{N} \|x_i - \tilde{\sigma}(\tilde{W}\sigma(Wx + b) + \tilde{b})\|^2. \tag{2}$$

If linear activation functions are used, the optimal solution to an autoencoder is strongly related to PCA [20]. In this case, Equation (1) can be written as:

$$A, B = \arg \min_{A, B} \sum_{i=1}^{N} \|x_i - x_iAB^T\|^2$$

or

$$A, B = \arg \min_{A, B} \|X - XAB^T\|_F^2. \tag{2}$$

Figure 1: Projections of Vector $X$ on non-orthogonal and orthogonal directions respectively.

Figure 2: The autoencoder model.
where \( X = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_N \end{batrix} \) and \( \| \cdot \|_F \) is the Frobenius norm.

\( A \in \mathbb{R}^{n \times p} \) and \( B \in \mathbb{R}^{n \times p} \) are two linear transformation matrices. Baldi and Hornik \([21]\) showed that, if the covariance matrix \( \Sigma_x \) associated with the data \( X \) is invertible, a unique local and global minimum to Equation (2) corresponds to an orthogonal projection onto the subspace spanned by the first principal eigenvectors of the covariance matrix \( \Sigma_x \). More precisely, the optimal solutions to (2) can be obtained by \( A = B = U_{n \times p} \), where \( U_{n \times p} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_p] \) are the \( p \) eigenvectors corresponding to the \( p \) largest eigenvalues of the covariance matrix \( \Sigma_x \). In PCA, \( \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_p \) are defined as loading vectors or principal components and \( T = XU \) is the score matrix corresponding to the loading matrix \( U \).

Although there is no orthogonal constraints of the transformation matrices \( A \) or \( B \), the solutions to Equation (3) are composed by orthogonormal bases. Due to the orthogonal decomposition, PCA can transform an original data space into two orthogonal subspaces, a principal subspace which contains most variation in original data and a residual subspace which includes noises or outliers. \( T^2 \) statistic and SPE statistic are often adopted as indicators for fault detection corresponding to the principal subspace and the residual subspace respectively. The orthogonal decomposition minimizes the correlations between these two subspaces and makes the linear reconstruction of original data with the least distortion \([22], [23]\). Because of this orthogonal property, PCA is widely used in process monitoring and many other fault detection methods can be considered as the extensions of PCA \([1]\).

### III. NEURAL COMPONENT ANALYSIS

A nonlinear autoencoder model can be trained to extract latent features. However, due to the lacking of the orthogonal property, the significant information of original data and the information of noises or outliers are largely combined in this model. An autoencoder model turns to overfit original data and learns to capture as much information as possible rather than reducing correlations in original data and extracting the significant information. Because of this problem, nonlinear autoencoder models are not used as widely as PCA.

In the section, we propose a novel unified model, called neural component analysis (NCA), for fault detection. NCA firstly utilizes a nonlinear neural network as an encoder to extract features. Then linear orthogonal transformation is adopted to decode the features to the original data space. In this way, NCA can be considered as a combination of nonlinear and linear models.

In NCA, we use linear transformation \( B \) instead of nonlinear transition \( \beta \) used in Equation (1). The optimization problem of NCA is

\[
W, b, B = \arg \min_{W, b, B} \sum_{i=1}^{N} \| x_i - g(\mathbf{x}_i; W, b) B^T \|_F^2 \quad (3)
\]

subject to \( B^T B = I_{p \times p} \)

where \( g(\mathbf{x}_i; W, b) \) is a neural network with \( p \) outputs. Assume \( B = [b_1, b_2, \ldots, b_p] \) where \( b_i \in \mathbb{R}^{n \times 1} \), then the orthogonal normal constraint, \( B^T B = I \), means

\[
b_i^T b_j = \begin{cases} 1 & i = j \\ 0 & \text{otherwise} \end{cases} \quad (i, j = 1, 2, \ldots, p).
\]

Figure 3 illustrates the structure of NCA. Here \( B \) contains three orthogonal bases (plotted in red, blue, and green), i.e. \( B = [b_1, b_2, b_3] \).

Equation (3) shows the difference between NCA and autoencoder. Firstly, NCA is a unified model of nonlinear encoding and linear decoding. For the linear decoding, it will be shown later that the computation of the transformation matrix \( B \) is quite simple and no gradient-descent-based optimization is needed. Secondly, the orthogonormal constraints \( B^T B = I_{p \times p} \) are added to NCA. It means that the decoding from latent features is an orthogonal reconstruction, which can largely reduce the correlation of different variables.

Let

\[
G = \begin{bmatrix} g(\mathbf{x}_1; W, b) \\ g(\mathbf{x}_2; W, b) \\ \vdots \\ g(\mathbf{x}_N; W, b) \end{bmatrix} \in \mathbb{R}^{N \times p}, \quad (4)
\]

the optimization problem of NCA in Equation (3) can also be written as

\[
W, b, B = \arg \min_{W, b, B} \| X - GB^T \|_F^2 \quad (5)
\]

subject to \( B^T B = I_{p \times p} \).

Matrix \( G \), corresponding to the score matrix of PCA, is the key features which we want to obtain for further analysis, such as fault detection and diagnosis. However, it is difficult to compute the optimal \( W, b \) and \( B \) simultaneously since the
optimization problem in Equation 5 is nonconvex. In this paper, we compute \( W, b \) and \( B \) iteratively as follows. We firstly fix \( W, b \) and obtain \( G \), then \( B \) can be computed by optimizing

\[
B = \arg \min_B \| X - GB^T \|_F^2 \\
\text{subject to } B^T B = I_{p \times p}.
\]

(6)

Once \( B \) is obtained, \( W \) and \( b \) can be updated by solving the following optimization problem:

\[
W, b = \arg \min_{W,b} \| X - GB^T \|_F^2.
\]

(7)

The solution to the optimization problem in Equation 7 can be obtained by the backpropagation algorithm 24 which is widely adopted in training feedforward neural networks. The solution to Equation 6 is to determine an orthogonal matrix, that rotates \( G \) to fit original data matrix \( X \). In linear algebra and statistics 25, Procrustes analysis is a standard technique for geometric transformations between two matrices. The orthogonal Procrustes problem can be viewed as a matrix approximation problem which tries to find the optimal rotation or reflection for the transformation of a matrix with respect to the other. Theorem 1 shows how to solve the reduced rank Procrustes rotation problem.

**Theorem 1.** 26 Reduced Rank Procrustes Rotation. Let \( M_{N \times n} \) and \( N_{n \times p} \) be two matrices. Consider the constrained minimization problem

\[
\hat{H} = \arg \min_H \| M - NH^T \|_F^2 \\
\text{subject to } H^T H = I_{p \times p}.
\]

Suppose the singular value decomposition (SVD) of \( M^T N \) is \( UDV^T \), then \( \hat{H} = UV^T \).

According to Theorem 1, we can design iterative procedures of NCA to obtain \( W, b \) and \( B \) as follows:

1) Perform PCA on original data \( X \) to obtain the loading matrix \( U \in \mathbb{R}^{n \times p} \) and let \( B = U \).
2) Fix \( B \), solve the optimization problem in Equation 7 by the backpropagation algorithm.
3) Form \( G \) by Equation 4 and perform SVD on \( X^TG \), i.e. \( X^TG = UDV^T \).
4) Compute \( \hat{B} = UV^T \).
5) If \( \| B - \hat{B} \| < \epsilon \), break;
else, let \( B = \hat{B} \) and go to Step 2.
6) Output \( W, b \) and \( B \).

After training, \( g(x; W, b) \) can be used for further feature extraction.

IV. FAULT DETECTION BASED ON NCA

A novel fault detection method based on NCA is developed in this section. The implementation procedures are given as follows. Firstly in the modeling stage, the process data are collected under normal process conditions and scaled by each variable; Then NCA is performed to obtain the neural network \( g(x; W, b) \) for nonlinear feature extraction. Finally Hotelling \( T^2 \) and the squared prediction error (SPE) statistics are used for fault detection.

Let \( g_i = g(x_i; W, b) \) be the nonlinear latent features of \( x_i \) \((i = 1, 2, \cdots, N)\) and \( \Sigma_g \) is the covariance matrix associated with the features \( G = [g_1^T, g_2^T, \cdots, g_N^T]^T \). \( T^2 \) statistic of \( g_i \) is computed as follows:

\[
T^2_i = \frac{g_i^T \Sigma_g^{-1} g_i}{\text{E}(g_i^T \Sigma_g^{-1} g_i)}.
\]

(8)

SPE statistic of feature \( g_i \) can be calculated as follows:

\[
\text{SPE}_i = \| x_i - g_i B^T \|_F^2.
\]

(9)

Because of no prior information available about the distribution of \( g_i \), we compute the confidence limit for \( T^2 \) and SPE statistics approximately by kernel density estimation (KDE) 27. Let \( T^2_1, T^2_2, \cdots, T^2_N \) with an unknown density \( \rho(\cdot) \) are the \( T^2 \) statistics of \( g_1, g_2, \cdots, g_N \). The kernel density estimator of \( T^2 \) statistic is

\[
\hat{\rho}_h(T^2) = \frac{1}{N} \sum_{i=1}^N K_h(T^2 - T^2_i) = \frac{1}{hN} \sum_{i=1}^N K \left( \frac{T^2 - T^2_i}{h} \right)
\]

where \( K(\cdot) \) is a non-negative function that integrates to one and has zero mean and \( h > 0 \) is a bandwidth parameter. In this paper, we take the RBF kernel for density estimation, which is given by

\[
\hat{\rho}_h(T^2) = \frac{1}{\sqrt{2\pi}hN} \sum_{i=1}^N \exp \left( -\frac{(T^2 - T^2_i)^2}{2h^2} \right).
\]

After estimating \( \hat{\rho}_h(T^2) \), for the testing statistic \( T^2_{\text{new}} \), the following condition is checked: If \( \hat{\rho}_h(T^2_{\text{new}}) < \tau \) then \( x_{\text{new}} \) is normal else \( x_{\text{new}} \) is abnormal. The threshold \( \tau \) is assigned globally and could be adjusted in order to lower the percentage of false alarm. Practically, \( \tau \) is often equal to 0.01.

Similarly, we also can obtain

\[
\hat{\rho}_h(\text{SPE}_i) = \frac{1}{\sqrt{2\pi}hN} \sum_{i=1}^N \exp \left( -\frac{(\text{SPE}_i - \text{SPE}_{\text{new}})^2}{2h^2} \right)
\]

where \( \text{SPE}_1, \text{SPE}_2, \cdots, \text{SPE}_N \) with an unknown density \( \rho(\cdot) \) are the \( \text{SPE} \) statistics of \( X_1, X_2, \cdots, X_N \). For the testing statistic \( \text{SPE}_{\text{new}} \), the following condition is checked: If \( \hat{\rho}_h(\text{SPE}_{\text{new}}) < \tau \) then \( x_{\text{new}} \) is normal else \( x_{\text{new}} \) is abnormal.

The offline modeling and online monitoring flow charts are shown in Figure 4. The procedures of offline modeling and online monitoring are as follows:

- **Offline modeling:**
  1) Collect normal process data as the training data.
  2) Normalize the training data by each variable with zero mean and unit variance.
  3) Initialize \( B \) as the loading matrix which contains the first \( p \) eigenvectors of the covariance matrix of the training data.
Figure 4: The steps of the proposed NCA method for fault detection.

4) Fix \( B \) to compute \( W \) and \( b \) by training a neural network optimizing Equation (7).
5) Fix \( W \) and \( b \) to compute \( B \) by Reduced Rank Procrustes Rotation solving Equation (6).
6) Compute \( T^2 \) and SPE statistics of \( x_i \) by Equation (8) and (9) respectively.
7) Determine the control limit of \( T^2 \) and SPE by KDE respectively.

- Online monitoring:
  1) Sample a new testing data point \( x_{new} \). Normalize it according to the parameters of the training data.
  2) Extract the feature \( g_i = g(x_{new}; W, b) \).
  3) Compute \( T^2 \) and SPE statistics of the feature \( g_i \).
  4) Alarm if \( T^2 \) (or SPE) of the extracted feature exceed the control limit; Otherwise, view \( x_{new} \) as a normal data.

V. SIMULATION AND DISCUSSION

The Tennessee Eastman process (TEP) has been widely used by process monitoring community as a source of publicly available data for comparing different algorithms. The simulated TEP is mainly based on an practical industrial process in which the kinetics, operation and units have been altered for specific reasons. The data generated by TEP are nonlinear, strong coupling and dynamic [28], [29]. There are five major units in TEP: a chemical reactor, condenser, recycle compressor, vapor/liquid separator, and stripper. A flow sheet of TEP with its implemented control structure is shown in Figure [5].

The MATLAB codes can be downloaded from [http://depts.washington.edu/control/LARRY/TE/download.html](http://depts.washington.edu/control/LARRY/TE/download.html). Besides normal data, the simulator of TEP can also generate 21 different types of faults in order to test process monitoring algorithms.

A total of 52 variables including 22 continuous process measurements, 19 compositions and 11 manipulated variables1 were selected as the monitoring variables in our experiments. The training data set contained 500 normal data. Twenty-one different faults were generated and 960 data for each fault were chosen for testing, in which the fault happened from 161th data to the end of the data. The 21 fault modes are listed in Table [I].

In this paper, we compare our proposed NCA method with PCA, KPCA and autoencoder. For KPCA, we use the most widely used Gaussian kernel \( k(x_i, x_j) = \exp(\frac{-\|x_i - x_j\|^2}{c}) \) and select the kernel parameter \( c \) as \( 10n\bar{\delta} \), where \( \bar{\delta} \) is the mean of standard deviations of different variables [30].

A. Visualization of data of different methods

In order to intuitively visualize the features of different methods, we extract 2 features for each method and plot them in Figure [6]. In Figure [6], the blue “*” indicates normal data, while the red “o” indicates fault data from Fault 1. It can be found that normal data and fault data are largely overlapped in Figure [6a] and [6c]. In this case, PCA, KPCA and

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1. The agitation speed was not included because it was not manipulated.
autoencoder cannot find the significant information for fault detection. However, in Figure 6d, the overlapping of normal samples and fault samples is much less than those in Figure 6a, 6b, and 6c. Through the nonlinear feature extraction based on orthogonal constraints, NCA directly gives out the key features in a two-dimensional space which include significant information for fault detection.

Figure 7 shows the difference between $B$ of NCA and the loading matrix $U$ of PCA. Figure 7a shows the result of $B^T B$. It is easy to find that $B$ contains orthonormal columns, i.e. $b_i^T b_j = 1$ if $i = j$, otherwise, $b_i^T b_j = 0$. Moreover, the correlations between the columns of $B$ and those of $P$ are plotted in Figure 7b. Obviously with the nonlinear feature extract, the optimum solution $B$ of NCA is utterly different from the loading matrix $U$ of PCA.

Figure 8 plots the reconstruction errors $\|X - GB^T\|^2_p$ in the training stage. It can be found that NCA converges very fast. Thanks for GPU-accelerated computing, the total training time of NCA is 2.58 seconds. We perform the experiment on a computer with Intel Core i7 3.4GHz, 16G RAM, and NVIDIA GeForce GTX 1080Ti. For comparison, KPCA is performed on the same computer and the training time is 1.53 seconds.

B. Case studies

In this subsection, we investigate the performance of our proposed NCA. The performance is compared with PCA, KPCA, and autoencoder. The source codes of NCA and other methods can be found in https://github.com/haitaozhao/Neural-Component-Analysis.git

According to the cumulative percentage variance (CPV) rule, the reduced dimensionality, $p$, was determined as 27 for PCA such that 85% of the energy in the eigenspectrum (computed as the sum of eigenvalues) was retained. In order to give a fair comparison, the same value $p = 27$ was used for KPCA, autoencoder and NCA.

Missed detection rate (MDR) refers to the rate of the abnormal events being falsely identified as normal events in the monitoring process, which is only applied to the fault detection situation. For testing all the 21 faults, MDR is recorded together in Table II where smaller values indicate better performances. False alarm rate (FAR) which refers to the normal process monitoring results of PCA, KPCA, autoencoder and NCA are shown in parentheses. The small FARs also indicate better performances. In Table II the best achieved performance for each fault is highlighted in bold. In this study, we only consider the fault cases where $\text{MDR} \leq 50\%$ and $\text{FAR} \leq 5\%$. Because if $\text{MDR} \geq 50\%$, the detection performance would be even worse than random guess whose MDR is 50%. Moreover, we adopt the threshold value for FAR as 5% which is commonly used in fault detection.

NCA outperforms PCA, KPCA and autoencoder in 11 cases with lower MDRs. Autoencoder gives the best performance with 5 cases, KPCA gives the best performance with 7 cases and PCA gives the best performance with 4 cases. Autoencoder, KPCA, and NCA provide better results than PCA.
Table II: Missed Detection Rate (%) and False Alarm Rate (%) (shown in parentheses) of PCA, LPP, LPP_Markov and DGE in TEP

| No. | $T^2$ | SPE | $T^2$ | SPE | $T^2$ | SPE | $T^2$ | SPE |
|-----|-------|-----|-------|-----|-------|-----|-------|-----|
| 1   | 0.50(4.38) | 0.13(20.6) | 0.57(5.00) | 0.63(5.63) | 0.50(3.13) | 0.75(0.00) | 0.50(0.00) | 0.75(0.00) |
| 2   | 1.67(2.50) | 0.75(18.1) | 1.63(5.00) | 1.75(5.00) | 1.50(1.35) | 2.00(0.00) | 1.75(0.00) | 1.50(0.00) |
| 3   | 9.20(0.63) | 71.90(0.00) | 88.51(2.5) | 93.80(6.63) | 96.41(1.88) | 99.90(0.00) | 98.40(0.00) | 97.90(0.63) |
| 4   | 39.12(5.00) | 0.00(24.4) | 51.15(5.00) | 81.80(7.5) | 55.80(0.63) | 96.00(0.00) | 63.03(1.25) | 5.75(0.63) |
| 5   | 73.80(6.63) | 50.32(2.25) | 70.50(5.00) | 79.30(7.5) | 73.30(0.63) | 77.90(0.00) | 75.41(1.25) | 71.11(1.88) |
| 6   | 1.00(0.00) | 0.00(10.6) | 0.88(2.50) | 2.88(3.13) | 1.00(0.00) | 1.13(0.00) | 0.50(0.00) | 0.88(0.00) |
| 7   | 0.00(0.00) | 0.00(16.3) | 0.00(0.63) | 2.00(0.63) | 0.00(0.00) | 30.01(0.63) | 0.00(0.00) | 0.00(0.18) |
| 8   | 2.50(0.63) | 1.75(17.5) | 2.50(2.50) | 4.75(3.13) | 2.50(1.88) | 4.38(0.00) | 2.75(0.00) | 2.50(2.50) |
| 9   | 96.45(0.00) | 16.92(23.8) | 89.01(5.00) | 94.12(5.63) | 96.00(5.00) | 99.38(1.88) | 97.92(3.50) | 94.03(5.63) |
| 10  | 35.84(0.00) | 12.13(15.5) | 48.93(0.00) | 81.60(6.63) | 64.30(0.63) | 77.58(0.00) | 66.00(0.63) | 72.81(1.88) |
| 11  | 37.90(0.63) | 19.20(20.0) | 36.64(3.13) | 52.40(1.88) | 49.61(2.50) | 71.90(0.00) | 52.00(0.63) | 30.10(1.33) |
| 12  | 1.25(0.63) | 1.13(22.5) | 1.00(3.13) | 10.40(0.63) | 1.00(1.88) | 2.63(0.00) | 1.00(1.25) | 5.90(7.5) |
| 13  | 4.88(0.00) | 3.75(12.5) | 4.63(1.25) | 18.00(6.63) | 5.75(0.63) | 5.88(1.25) | 5.13(1.25) | 4.88(7.5) |
| 14  | 0.13(0.63) | 0.08(23.13) | 0.00(1.25) | 9.88(0.63) | 0.38(0.63) | 4.88(0.00) | 0.38(0.63) | 0.00(5.00) |
| 15  | 95.1(0.00) | 74.4(16.9) | 86.93(3.13) | 94.1(2.50) | 94.30(6.3) | 98.10(1.00) | 97.00(0.00) | 90.93(3.75) |
| 16  | 76.8(6.88) | 30.3(22.5) | 64.20(2.0) | 86.96(2.5) | 82.15(5.0) | 91.01(1.88) | 85.61(1.88) | 76.61(2.5) |
| 17  | 19.31(2.5) | 2.50(23.6) | 13.50(0.00) | 28.00(0.00) | 20.11(3.5) | 27.40(0.00) | 15.40(0.00) | 53.30(0.00) |
| 18  | 10.20(0.00) | 9.97(7.5) | 10.20(0.00) | 14.42(5.00) | 11.04(3.5) | 11.03(0.63) | 9.30(6.3) | 12.10(0.00) |
| 19  | 92.25(0.0) | 41.86(14.4) | 82.51(1.88) | 87.30(6.0) | 91.80(0.00) | 99.80(0.00) | 100(0.00) | 99.40(0.00) |
| 20  | 62.63(0.00) | 26.91(25.6) | 52.12(5.00) | 90.04(2.50) | 64.10(0.00) | 78.10(0.00) | 69.10(0.00) | 52.00(0.00) |
| 21  | 62.3(1.25) | 33.35(31.3) | 59.5(5.63) | 71.0(4.75) | 61.61(1.25) | 79.6(6.63) | 64.80(0.00) | 78.0(0.00) |

in more fault cases indicates that nonlinear extensions can generally obtain better fault detection results than linear PCA. Although both KPCA and NCA include orthogonal constraints in their feature extraction, the performances of NCA are much better than KPCA. The reason is that NCA adaptively learns the parameters of a neural network, while KPCA uses prefixed kernel and the associated parameter. NCA obtains different parameters for different parameters with nonlinear combination through backpropagation strategy and should be much more suitable for nonlinear feature extraction and the following fault detection tasks.

Figure 9 and 10 illustrate the detailed fault detection results of Fault 2, 4 and 7. In these figures, the blue points indicate the first 160 normal samples, while the red points represent the following 800 fault samples. The black dash lines are the control limits according to the threshold $\tau$. The blue points above control limits lead to false alarm, while the red points below control limits cause missed detection.

According to Table II, all 4 methods can successfully detect Fault 2. For PCA, the FARs are 2.5% and 18.1% for $T^2$ statistic and SPE statistic respectively. The FARs of KPCA are 5% for both $T^2$ statistic and SPE statistic. Autoencoder achieves no false alarm for SPE statistic and its FAR for $T^2$ statistic is 1.88%. However, as for our proposed NCA, the FARs are zero for both two statistics. Figure 9 shows the plots of four methods on Fault 2. For each method, the subplot above is the results of $T^2$ statistic and the subplot below is the results of SPE statistic. The small overlay plots clearly show the results of the first 160 normal samples in each subplot. Based on Table II and Figure 9 for Fault 2, we can found that NCA have the lowest MDR with no false alarm.

Figure 10 illustrates the results of Fault 4. In this experiment, neither KPCA nor autoencoder can detect this fault. The MDR of PCA is 39.1% using $T^2$ statistic. It means that PCA, KPCA, and autoencoder are not suitable for the detection of Fault 4. However, using SPE statistic, NCA obtains the MDR of 5.75% and the FAR of 0.63%. Obviously NCA is much more appropriate for detecting Fault 4.
given the superior performance of NCA, the trade-off between training time and performance seems justified.

VI. CONCLUSION

In this paper, we propose a nonlinear feature extraction method, neural component analysis (NCA), for fault detection. NCA is a unified model which includes a nonlinear encoder part and a linear decoder part. Orthogonal constraints are adopted in NCA which can alleviate the overfitting problem occurred in autoencoder and improve performances for fault detection. NCA takes the advantages of the backpropogation technique and the eigenvalue-based techniques. The convergence of the iteration scheme of NCA is very fast. The idea behind NCA is general and can potentially be extended to other detection or diagnosis problems in process monitoring.

We compare NCA with other linear and nonlinear fault detection methods, such as PCA, KPCA, and autoencoder. Based on the case studies, it is clear that NCA outperforms PCA, KPCA, and autoencoder. NCA can be considered as an alternative to the prevalent data driven fault detection techniques.

Future works will be contributed to the design of new regularization terms to the optimization problem of NCA in Equation (5). Reconstruction-based feature extraction methods, such as PCA, KPCA, autoencoder, and NCA, are mainly focus on the global Euclidean structure of process data and overlook the latent local correlation of process data. In the future, we will try to design new constraints to ensure the local information is considered in nonlinear feature extraction.

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