Probabilistic Weighted NPE-SVDD for chemical process monitoring

Qingchao Jiang, Xuefeng Yan *

Key Laboratory of Advanced Control and Optimization for Chemical Processes of Ministry of Education, East China University of Science and Technology, Shanghai 200237, PR China

1. Introduction

Process monitoring and early fault detection have elicited increasing interest because of the increasing demand for plane safety and product quality. The multivariate statistical process monitoring (MSPM) methods have been extensively used and developed because of the rapid developments in data collection and computing technology (AlGhazzawi & Lennox, 2008; Chiang, Braatz, & Russell, 2001; Choi & Lee, 2004; Ge, Song, & Gao, 2013; Qin, 2003; Qin & Yu, 2007; Venkatasubramanian, Rengaswamy, Kavuri, & Yin, 2003; Yu, 2012b; Yu & Qin, 2008, 2009). Among the MSPM methods, the principal component analysis (PCA) (Jiang & Yan, 2012; Jiang, Yan, & Zhao, 2013; Kouri & MacGregor, 1996; Ku, Storer, & Georgakis, 1995; Lee, Yoo, Choi, Vanrolleghem, & Lee, 2004; Nomikos & MacGregor, 1995) and partial least squares (PLS) (Chiang et al., 2001; Kruger & Dimitriadis, 2008; Muradore & Fiorini, 2012; Qin, 1998) usually serve as the most fundamental techniques and have been successfully applied to monitor a wide range of chemical processes (Ge, Gao, & Song, 2011; Kresta, Macgregor, & Marlin, 1991; Lee, Yoo, & Lee, 2004; Rashid & Yu, 2012; Yu, 2011, 2012c). PCA, a classical dimensionality reduction method, can effectively process high-dimensional, highly correlated data by projecting the data onto a lower-dimensional subspace containing most variations of normal data (Chiang et al., 2001; Jiang & Yan, 2014; Kouri & MacGregor, 1996). PCA assumes that the relationship between variables is linear (Ge, Yang, & Song, 2009; Lee et al., 2004; Yu, 2011, 2012a). Numerous nonlinear PCA approaches have been developed by considering the nonlinear behavior of the chemical process (Dong & McAvoy, 1996; Kramer, 1991). The kernel PCA (KPCA) proposed by Scholkopf, Smola, and Müller (1998) is the most popular approach and has been extended to solve various monitoring problems (Elshenawy, Yin, Naik, & Ding, 2009; Ge et al., 2009; Zhang, Li, & Teng, 2012).

These PCA- and KPCA-based methods have shown advantages in high-dimensional processes. However, the usual problem is that useful information is suppressed, which can seriously affect the monitoring performance. In PCA-based process monitoring, the high-dimensional process data are reflected into the lower-dimensional dominant subspace. However, fault information has no definite mapping to a certain PC and useful information may be suppressed by irrelevant information (Jiang & Yan, 2012; Jiang et al., 2013). Moreover, the fault information may be dispersed into both the dominant subspace and the residual subspace. If the fault information is relatively limited, the dispersed information would be suppressed. The suppression of useful information results in a challenging fault detection. Jiang et al. (2013) proposed a sensitive PCA method based on the indefinite mapping of fault information to concentrate the useful information into one subspace. An adaptively weighted PCA method has also been proposed to highlight the useful information and improve process monitoring performance (Jiang & Yan, 2012).

Although the extracted principal components of the PCA (i.e., KPCA, WPCA, etc.) methods can retain most data variations, PCA can only capture the global structure of the process data.
The detailed local structure information among the process data is usually ignored (Belkin & Niyogi, 2001; Miao, Song, Wen, & Ge, 2012; Zhang, Ge, Song, & Cao, 2011; Zhang & Yang, 2010). The loss of this crucial information may have great impact on dimension reduction performance, as well as on process monitoring performance. A class of dimension reduction techniques based on the local structure of the dataset, which is known as manifold learning, has been developed in the pattern recognition area. Tenenbaum, De Silva, and Langford (2000) proposed a global geometric framework that can discover the nonlinear degrees of freedom that underlie complex natural observations. Roweis and Saul (2000) proposed the Locally Linear Embedding method to exploit the local symmetries of linear reconstructions and identify the underlying structure of the manifold. Niyogi (2004) introduced the Locality Preserving Projections (LPP) to preserve the neighborhood structure of the data set. Zhang et al. (2011) proposed a global–local structure analysis (GLSA) model to exploit the underlying geometrical manifold and simultaneously retain the global data information. Locally Linear Embedding (LLE) dimensionality reduction is a promising method for handling nonlinear dataset; thus, considerable research has been done on this method (Li & Zhang, 2011; McClure, Gopaluni, Chmelyk, Marshman, & Shah, 2012; Xu, Zhang, Xu, & Chen, 2011; Zhang & Yang, 2010). LLE does not provide an explicit mapping matrix from high-dimensional space to low-dimensional embedded space; thus, Li and Zhang (2011) proposed a local linear regression method to find the projection that best approximates the mapping from high-dimensional samples to the embedding. However, this regression requires mapping of the nearest neighbors of a sample on each point and is not very suitable for online process monitoring.

Neighborhood Preserving Embedding (NPE), a linear approximation of the LLE algorithm, is usually used for online monitoring (He, Cai, Yan, & Zhang, 2005; Hu & Yuan, 2008; Miao, Ge, Song, & Zhou, 2013). NPE has been demonstrated to have the following advantages over PCA and LLE (He et al., 2005; Hu & Yuan, 2008): (1) NPE, as a linear approximation of LLE, reveals the intrinsic structure of the observed data and finds more meaningful information than PCA; (2) NPE is more easily applied to any new data rather than only on the training data in contrast to the nonlinear dimensionality reduction techniques, such as LLE, Laplacian eigenmaps, and Isomap; and (3) NPE is derived by preserving local neighborhood information; thus, it is less sensitive to outliers than PCA and the robustness of NPE is relatively good.

The process monitoring problem could be considered as a one-class classification problem because the monitoring task is to separate the faulty data samples from the normal ones (Mahadevan & Shah, 2009). Several classification methods are reported for fault detection (Ghate & Dudul, 2010; Rengaswamy & Venkatasubramanian, 2000; Tax & Duin, 1999, 2004), and among them, the Support Vector Data Description (SVDD) is a relatively new method and considerable research has recently been done on it. An SVDD model can be constructed by representing all normal process data samples as one class to differentiate the abnormal from the normal data samples (Chen, Kruger, Meronk, & Leung, 2004; Ge et al., 2011). In addition, kernel density is a powerful tool for the nonparametric estimation of probability density functions (Parzen, 1962; Webb, 2003). It has been widely used to determine the distribution of process data or obtain control limits for monitoring statistics (Lee et al., 2004). Kernel density could usually reveal more process information and provide more accurate results by considering more probability density factors (Chen, Wynne, Goulding, & Sandoz, 2000; Coussement, Gicquel, & Parente, 2012).

Although NPE has been successfully used in process monitoring, the problem of suppression of useful information still remains, which requires emphasis of useful information. Considering the suppression of useful information problem, a novel probabilistic weighted NPE-SVDD method has been proposed to improve the NPE-based process monitoring performance. First, the conventional NPE is used for dimensionality reduction and the process data are projected into the lower-dimensional feature space using NPE projection. Second, given that fault has no definite mapping to a certain embedding, kernel density estimation (KDE) is employed to estimate the probability density of the current sample in feature space and evaluate the importance of each embedding. Then, different weighing values are set on the embedding to highlight the useful information and suppress the process noise. Finally, the SVDD is used to discriminate the normal and abnormal observations.

The structure of the rest of this paper follows. First, a brief introduction of NPE and basic SVDD are shown in Section 2. Second, the WNPE-SVDD for process monitoring is proposed and some details are provided in Section 3. In Section 4, the proposed method is tested in a numerical process, continuous stirred tank reactor (CSTR) process, and Tennessee Eastman (TE) process. The monitoring results and several comparisons with conventional PCA, KPCA, WPCA, GLSA, LPP, and NPE-SVDD are shown. Finally, the conclusions and discussions in this study are provided in Section 5.

2. Review of NPE and SVDD

In this section, the NPE for dimensionality reduction is reviewed. The NPE-SVDD for process monitoring is also presented.

2.1. NPE for dimensionality reduction

In contrast with PCA, which focuses on preserving global structure, NPE considers the local structure and optimally preserves the local manifold structure of the dataset. Let the dataset be \(X = \{x_1, x_2, ..., x_n\} \in \mathbb{R}^m\), with \(n\) points and \(m\) measured variables, \(W^d\) denotes the weight matrix and \(w^d_{ij}\) in \(W^d\) represents the linear combination coefficient to reconstruct \(x_i\) using its nearest neighbor \(x_j\). The following error function should be minimized in computing the weight matrix \(W^d\) (He et al., 2005; Miao et al., 2013)

\[
e(W^d) = \arg\min_{W^d} \sum_{i=1}^{n} \|x_i - \sum_{j=1}^{n} w^d_{ij} x_j\|^2
\]

The coefficients \(w^d_{ij}\) subjected to the constraints \(\sum_{j=1}^{n} w^d_{ij} = 1\) and \(w^d_{ij} = 0\) if \(x_i\) is not a neighbor of \(x_j\) (Roweis & Saul, 2000; Zhang & Yang, 2010). The following function should be optimized to find the embedding \(Y = \{y_1, y_2, ..., y_n\} \in \mathbb{R}^d (d \leq m)\) in the low-dimensional subspace, which can preserve the same local neighborhood properties (He et al., 2005; Miao et al., 2013): \(\psi(Y) = \arg\min_{Y} \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{n} w^d_{ij} y_j\|^2\)

The objective of the linear dimensionality reduction algorithm is to find a transformation matrix \(P = [p_1, p_2, ..., p_m] \in \mathbb{R}^{m×d}\) that maps each high-dimensional data \(X\) into the low-dimensional space \(Y = \{y_1, y_2, ..., y_n\} \in \mathbb{R}^d\); that is, \(y_i = P x_i\). The transformation matrix \(P\) can be represented by minimizing the following reconstruction error (He et al., 2005; Miao et al., 2013):

\[
P_{opt} = \arg\min_{P} \|Y - \sum_{j=1}^{n} w^d_{ij} y_j\|^2 = \arg\min_{P} \sum_{i=1}^{n} \|P x_i - \sum_{j=1}^{n} w^d_{ij} y_j\|^2
\]

Therefore, \(P\) can be calculated by solving the generalized eigenvalue problem, as shown in the following equation:

\[
XMX^T p = \lambda XX^T p
\]
where $M = (I - W D)(I - W D)$. The eigenvectors associated with the smallest $d$ eigenvalues form the transformation matrix $P = [p_1, p_2, \ldots, p_d] \in \mathbb{R}^m$. $T^2$ and $Q$ statistics are constructed as follows for process monitoring:

$$T^2 = (y^\text{new})^T S^{-1} y^\text{new}$$  \hspace{1cm} (5)  

$$Q = \| y^\text{new} - P^T x^\text{new} \|^2 = \| (I - BP^T)x^\text{new} \|^2$$  \hspace{1cm} (6)

where $y^\text{new}$ is the projection of the data $x^\text{new}$ in NPE space and $y^\text{new} = P^T x^\text{new}$. $S = Y^T Y/(n-1)$ is the covariance matrix of the projection $Y$ under normal conditions; $B$ is the projection of $y^\text{new}$ back to the original space by $x^\text{new} = By^\text{new}$. More details on NPE are provided in the literature (He et al., 2005; Hu & Yuan, 2008; Miao et al., 2013).

### 2.2. SVDD

SVDD is a kind of one-class classifier that tries to find a sphere with minimum volume, containing all (or most of) the data objects. A nonlinear transformation function $\phi : y \rightarrow \mathbf{F}$ is introduced to model a nonlinear process and the SVDD is used to solve the following optimization problem (Tax & Duin, 2004):

$$\min R^2 + C \sum_{i=1}^{n} e_i$$

s.t. $\| \phi(y) - a \|^2 \leq R^2 + \epsilon_i$

where $a$ is the center of the hypersphere; $R$ is the radius; $C$ represents the trade-off between the volume of the hypersphere and the number of errors; and $\epsilon_i$ represents the slack variable that allows a probability that some of the training samples can be incorrectly classified. The dual form of the optimization problem can be obtained as follows (Tax & Duin, 2004):

$$\min \sum_{i=1}^{n} (\alpha_i - \alpha_i^+\alpha_i^0) - \sum_{i=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_i^+ K(y_i, y_i')$$

s.t. $0 \leq \alpha_i \leq C, \sum_{i=1}^{n} \alpha_i^+ = 1$

where $K(y_i, y_i') = \langle \phi(y_i'), \phi(y_i) \rangle$ is a kernel function that is introduced to compute the inner product in the feature space, $\alpha_i$ is a Lagrange multiplier. Solving for Eq. (7) results in a set $\alpha_i^+$ and the samples $y_i$ with $\alpha_i > 0$ are called support vectors (SVs) of the description. The distance from the center $a$ to the boundary $R^2$ for any $y_i \in \mathbb{S}$ is as follows (Tax & Duin, 1999):

$$R^2 = K(y_i, y_i) - 2 \sum_{i=1}^{n} \alpha_i^+ K(y_i, y_i') + \sum_{i=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_i^+ K(y_i, y_i')$$

The distance to the center of the sphere for a new sample $z$ can be calculated as follows (Tax & Duin, 2004):

$$D^2 = \| z - a \|^2 = K(z, z) - 2 \sum_{i=1}^{n} \alpha_i^+ K(z, y_i') + \sum_{i=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_i^+ K(y_i', y_i')$$

The index for fault detection is defined as follows:

$$\text{DIS} = \frac{D^2}{R^2}$$  \hspace{1cm} (11)

and the control limit $\text{DIS}_0 = 1$. The sample $z$ is accepted when the distance is smaller than or equal to $R^2$. Otherwise, it is rejected and regarded as a fault point. The monitoring scheme of NPE-SVDD is summarized as follows:

First, the process data are projected into the feature subspace through NPE.

Second, the SVDD monitoring model is constructed for fault detection.

The SVDD has no Gaussian assumption of the process data and only incorporates a quadratic optimization step, which facilitates practical implementation (Ge et al., 2011).

### 3. Weighted NPE-SVDD for process monitoring

In this section, a numerical process is employed as a motivational example. The probabilistic weighted NPE and SVDD for process monitoring are presented in detail.

#### 3.1. Motivational example

A simple numerical process is considered to analyze the monitoring performance of conventional NPE-SVDD and illustrate the useful information being suppressed as shown in the following equations (Dong & McAvoy, 1996):

$$x_1 = t + e_1$$ \hspace{1cm} (12)

$$x_2 = t^2 - 3t + e_2$$ \hspace{1cm} (13)

$$x_3 = -t^2 + 3t^2 + e_3$$ \hspace{1cm} (14)

where $e_1, e_2,$ and $e_3$ are the independent noise variables $N(0, 0.01)$ and $t \in [0.01, 2]$. Normal data comprising 100 samples are generated according to these equations. Two sets of test data comprising 300 samples each are also generated. The following two faults are applied separately during the generation of test data sets (Dong & McAvoy, 1996).

**Fault 1**: a step change in $x_2$ by $-0.3$ is introduced from sample 101.

**Fault 2**: $x_1$ is linearly increased from sample 101 to sample 280 by adding $0.01 \times (k - 100)$ to the $x_1$ value of each sample, where $k$ is the sample number.

Fig. 1 shows that fault 1 can be detected by the NPE-SVDD method; however, the DIS statistic does not stay above the control limit and the missed detection (Type I error) rate is rather high. Each embedding in the feature space is considered to investigate the cause of the disadvantage of NPE-SVDD monitoring, which is defined as follows:

$$y_{j\text{new}}^\text{new} = P_j^T x_{\text{new}}$$  \hspace{1cm} (15)

where $j = 1, 2$ is the number of embedding and $P_j$ is the $j$th mapping vector in $P$. Correspondingly, the $T^2$ statistic along the $j$th embedding is constructed as follows:

$$T_{j}^2 = y_{j\text{new}}^\text{new} \cdot S_j^{-1} y_{j\text{new}}^\text{new}$$  \hspace{1cm} (16)

$s_j^{-1} = y_{j\text{new}}^\text{new} \cdot S_j^{-1} y_{j\text{new}}^\text{new}$ is used to scale the $T^2$ statistics to the same level. In the current study, the embedding evaluated by KDE is also scaled by $y_{j\text{new}}^\text{new} = y_{j\text{new}}^\text{new} \cdot s_j^{-1/2}$. The two $T_j^2$ in the simple process are illustrated.
The weighting matrix is designed to highlight the more useful information for fault detection; hence the more important embedding should be weighted more heavily. The determination of the weighting values is based on the fact that the embedding with relatively smaller densities more likely to indicate deviations from the normal condition and contain more fault information. According to the estimated densities, the weighting values are determined as follows:

\[
w^p_i(k) = \begin{cases} 
1 & \text{if } \frac{\hat{p}_i(y^k_0)}{\hat{p}_i(y^k_1)} > a \\
\beta & \text{if } \frac{\hat{p}_i(y^k_0)}{\hat{p}_i(y^k_1)} \leq a
\end{cases}
\]

where \(a\) is the density threshold and \(\beta\) is the weighting value to highlight the embedding. Therefore, embedding with small enough density values would be assigned with larger weights. Generally, the values of \(a\) and \(\beta\) could be determined by an empirical study based on normal training data. The determination of the values of \(a\) and \(\beta\) should guarantee that monitoring would not be violated by acceptable disturbances. Moreover, certain embedding is easily affected by noise and should be suppressed by assigning small weight. In this study, the suggested value for \(\alpha\) is from 0.01 to 0.2 and for \(\beta\) is from 10 to 100. \(\frac{\hat{p}_i(y^k_0)}{\hat{p}_i(y^k_1)}\) is the density of the \(k\)th embedding on the \((k-1)\)th sample point \((k\) is the current sample time), which can be estimated online by KDE. The mean value of the previous \((\text{window width})\) samples are used because the evaluation of the importance of embedding by only one point is relatively subjective, as shown in the following.

\[
\hat{p}_i(y) = \frac{1}{nh} \sum_{k=1}^{n} K_2 \left( \frac{y - y^k_1}{h} \right)
\]
expression:
\[ y_i^2 = \frac{1}{J} \sum_{t=k-j}^{k-1} y_i^t \]  

(21)

The detailed steps of WNPE-SVDD, consisting of offline and online monitoring, are listed below.

(1) Offline modeling

- **Step 1**: A dataset in normal condition is acquired as training data and normalized.
- **Step 2**: NPE algorithm is performed and the embedding and projecting matrix \( P \) are obtained.
- **Step 3**: The probability density value of each embedding of normal data is estimated using KDE.
- **Step 4**: Parameters, including the window width \( j \), probability density threshold \( \alpha \), and the weight \( \beta \) are specified.
- **Step 5**: The weighted embedding of normal dataset is calculated.
- **Step 6**: The SVDD model is constructed and the distance \( R^2 \) to the center \( a \) in normal condition is calculated.

(2) Online monitoring

- **Step 1**: The current sampled data \( x^k \) is normalized.
- **Step 2**: The embedding of \( x^k \) is calculated.
- **Step 3**: The density value of each embedding is estimated and the real-time and dynamic weighting matrix \( W^P \) is determined.
- **Step 4**: The weighted embedding is calculated.
- **Step 5**: The index DIS of the current sample is calculated.
- **Step 6**: If the DIS exceeds the confidence limit, detection of certain fault types is indicated; fault diagnosis tools are then used to analyze the root cause. Otherwise, Step 1 is repeated and monitoring continues.

The procedures for WNPE-SVDD-based process monitoring are illustrated in Appendix Fig. A1.

4. Case studies

In this section, the proposed WNPE-SVDD method is applied on the numerical process, the CSTR process, and the TE benchmark process. The monitoring results of the TE benchmark process are compared with some other methods, such as PCA, KPCA, WPCA, GLSA, and conventional NPE-SVDD.

4.1. Case study on the simple numerical process

The numerical nonlinear process is introduced in the section on motivational example. Fig. 3 shows the monitoring result of PCA (Fig. 3(a)) and KPCA (Fig. 3(b)). As shown in Fig. 3(a), the \( T^2 \) statistics failed to indicate the fault. In Fig. 3(b), the fault was detected; however, the \( T^2 \) statistics did not stay above threshold, which leads to high missed detection rate. The monitoring result of conventional NPE-SVDD is illustrated in Fig. 1 in the motivational example section. As shown in Fig. 1, the missed detection is

![Fig. 3. Monitoring result of fault 1 using (a) PCA, (b) KPCA, (c) density values of each embedding, and (d) WNPE-SVDD.](image-url)
also not suitable for practical use. The WNPE-SVDD is applied for performance improvement. The estimated density values of each embedding for sample points are plotted in Fig. 3(c). As shown in Fig. 3(c), the second embedding has shown larger deviation between normal status and abnormal status, which indicates that the second embedding should be highlighted. The monitoring performance of WNPE-SVDD is shown in Fig. 3(d). The fault has been timely detected and the missed detection rates have been reduced significantly. The monitoring performances of fault 2 using PCA, KPCA, NPE-SVDD, and WNPE-SVDD are shown in Fig. 4(a), (b), (c), and (e), respectively. The density values of each embedding at monitoring fault 2 are shown in Fig. 4(d). WNPE-SVDD performed best based on the comparison of monitoring performances.

The fault can be detected in time, and when the fault disappeared, the statistic came back to normal.

4.2. Case study on the CSTR process

The simulation model parameters and the simulation conditions used in the study by Yoon and MacGregor (2001) are adopted in this case study. The diagram of the process is shown in Appendix Fig. A2. This reactor is based on the three following assumptions: perfect mixing, constant physical properties, and negligible shaft work (Yoon & MacGregor, 2001).

The process is monitored by measuring the cooling water temperature $T_C$, inlet temperature $T_0$, inlet concentrations $C_{A/2}$.
and $C_{AS}$, solvent flow $F_S$, cooling water flow $F_C$, outlet concentration $C_A$, temperature $T$, and reactant flow $F_A$. These nine variables form the following measurement vector (Yoon & MacGregor, 2001; Yue & Qin, 2001):

$$\mathbf{x} = [T_C, T_D, C_{AS}, F_S, F_C, C_A, T_F, A]^T$$

(22)

The variables are sampled every minute and 500 samples obtained under normal conditions are used as the training set. Five different faults are introduced into the system and for each of the five scenarios, 1000 observations are simulated. The faults are introduced at the 501st measurement. The first simulated fault, fault 1, is a bias in the sensor of the output temperature $T$ and the bias magnitude is 0.2k (the bias magnitude is 1k in the reference and the magnitude has been reduced by 80% for acid testing). This fault is considered as a complex fault because it affects several variables (Yoon & MacGregor, 2001; Yue & Qin, 2001). The monitoring results of the fault using KPCA, NPE-SVDD, and WNPE-SVDD are shown in Fig. 5. Fig. 5(a) shows the monitoring performance of KPCA, wherein the false alarm rate is high. Fig. 5(b) shows the monitoring performance of NPE-SVDD, wherein the number of missed detections is high. Fig. 5(c) shows the monitoring performance of WNPE-SVDD. Both missed detection rate and false alarm (Type II error) rate have been reduced significantly because the useful information has been highlighted and irrelevant information has been suppressed.

Fig. 5. Monitoring performances of CSTR fault 1 using (a) KPCA, (b) NPE-SVDD, and (c) WNPE-SVDD.

Fig. 6. Monitoring performances of CSTR fault 2 using (a) KPCA, (b) NPE-SVDD, and (c) WNPE-SVDD.
The second and third faults, faults 2 and 3, are biases in the sensors of the inlet temperature $T_0$ and inlet reactant concentration $C_{AA}$, respectively. The bias magnitude for $T_0$ is $0.3k$ (reduced by 80% compared with the reference) and for $C_{AA}$ is $0.2$ kmol/m$^3$ (reduced by 80% compared with the reference). These faults are considered simple faults because they only affect one variable. The monitoring performances of fault 2 using KPCA, NPE-SVDD, and WNPE-SVDD are shown in Fig. 6. The false alarm rate and missed detection rate of KPCA (Fig. 6(a)) are high. The NPE-SVDD and WNPE-SVDD can detect the fault successfully, with low missed detection rate and false alarm rate. When the fault occurs, the embedding $y$ deviates significantly from its normal value. After mapping by kernel function in SVDD, the distance $D^2$ became a constant value. The monitoring performances of fault 3 using KPCA, NPE-SVDD, and WNPE-SVDD are shown in Fig. 7. As shown in Fig. 7(a), the $T^2$ statistic totally failed to detect the fault, as well as the $Q$ statistic. The NPE-SVDD and WNPE-SVDD have detected the fault successfully, with no missed detection and false alarms. The fourth fault, fault 4, is a drift in the sensor of $C_{AA}$ and its magnitude is $\frac{dC_{AA}}{dt} = 0.04$ (kmol/(m$^3$ min)) (reduced by 80% compared with the reference), which is also a simple fault. The monitoring performances of fault 4 using KPCA, NPE-SVDD, and WNPE-SVDD are shown in Fig. 8. NPE-SVDD and WNPE-SVDD accurately detected the fault. The last fault, fault 5, is a slow drift in the reaction kinetics. The fault has the form of an exponential degradation of the reaction rate caused by catalyst poisoning.

![Fig. 7. Monitoring performances of CSTR fault 3 using (a) KPCA, (b) NPE-SVDD, and (c) WNPE-SVDD.](image)

![Fig. 8. Monitoring performances of CSTR fault 4 using (a) KPCA, (b) NPE-SVDD, and (c) WNPE-SVDD.](image)
In this case, the reaction rate coefficient changes with time as 
\[ k_0(t+1) = 0.996 \times k_0(t) \] 
(Yoon & MacGregor, 2001; Yue & Qin, 2001). The monitoring results of the faults using KPCA, NPE-SVDD, WNPE-SVDD are shown in Fig. 9. The false alarm rate in KPCA is high. NPE-SVDD (Fig. 9(b)) and WNPE-SVDD (Fig. 9(c)) can detect the fault successfully.

Fig. 9. Monitoring performances of CSTR fault 5 using (a) KPCA, (b) NPE-SVDD, and (c) WNPE-SVDD.

Fig. 10. Monitoring performances of TE fault 4 using (a) PCA, (b) KPCA, (c) NPE-SVDD, and (d) WNPE-SVDD.
4.3. Case study on the TE benchmark process

The TE process is a benchmark case in process engineering, which was developed by Downs and Vogel (1993). This case consists of the following five major unit operations: reactor, product condenser, vapor–liquid separator, recycle compressor, and product stripper. Two products are produced by two simultaneous gas–liquid exothermic reactions and a byproduct is generated by two additional exothermic reactions. The process includes 12 manipulated variables, 22 continuous process measurements, and 19 compositions, as shown in Appendix Tables A1–A3. The fault simulator can generate 20 different types of faults, as shown in Appendix Table A4. All process measurements are contaminated by Gaussian noise. Once a fault enters the process, it affects almost all state variables in the process.

The base control scheme for the TE process is shown in Appendix Fig. A3 and the simulation code for the open loop can be downloaded from http://brahms.scs.uiuc.edu (Chiang et al., 2001; McAvoy & Ye, 1994). The second plant-wide control structure described in the study by Lyman and Georgakis (1995) is implemented to simulate the realistic conditions (closed-loop). A normal process dataset (500 samples) has been collected under the base operation to develop the monitoring models. A set of 20 programmed faults (default values) are simulated and the corresponding process data are collected for testing.

A total of 52 variables of the TE process are monitored in this case study without the stirring rate because it is not controlled.

Fig. 11. Monitoring performances of TE fault 4 using (a) embedding in the feature space and (b) estimated density values of the embedding.
All faults are introduced into the process on the 161st time point. Four typical testing sets and faults 4, 5, and 10 are employed. Fault 4 involves a sudden temperature increase in the reactor and the change is compensated by the control loops (Chiang et al., 2001; Lyman & Georgakis, 1995). The monitoring results of fault 4 using PCA, KPCA, NPE-SVDD, and WNPE-SVDD are shown in Fig. 10. The monitoring performance of WNPE-SVDD is the best compared with PCA, KPCA, and NPE-SVDD methods. Both missed detections and false alarms are affordable in practical use. All the squared embedding in feature space are plotted in Fig. 11(a) to investigate the cause of poor monitoring performance of NPE-SVDD. The estimated density values of all embedding are plotted in Fig. 11(b). The 16th, 22th, and 25th embedding (the real line) markedly change and the corresponding density values show larger deviation when the fault occurs. These embedding values are weighted heavily in the WNPE-SVDD monitoring.

Fault 5 involves a step change in the condenser cooling water temperature (Chiang et al., 2001; Lyman & Georgakis, 1995). When the fault occurs, the flow rate of the outlet stream from the condenser to the vapor increases, which results in an increase in temperature. The monitoring results of the fault using PCA, KPCA, NPE-SVDD, and WNPE-SVDD are shown in Fig. 12. NPE-SVDD and WNPE-SVDD have significantly reduced the missed detections in KPCA monitoring. Furthermore, the WNPE-SVDD also reduced the false alarming rates in KPCA and NPE-SVDD monitoring, which exhibited the best performance. Fault 10 is a random change in the temperature of stream 4 (C feed) in the TE process, which has been used considerably for algorithm testing (Chiang et al., 2001; Lyman & Georgakis, 1995). The monitoring results of this fault using KPCA, NPE-SVDD, and WNPE-SVDD are shown in Fig. 13. NPE-SVDD and WNPE-SVDD showed better monitoring performance than PCA and KPCA. In particular, WNPE-SVDD performs the best among them.

The missed detection rates for each fault in the TE process using PCA (Chiang et al., 2001), KPCA (Scholkopf et al., 1998), WPCA (Jiang & Yan, 2012), GLSA (Zhang et al., 2011), LPP (Niyogi, 2004), NPE-SVDD, and WNPE-SVDD are summarized in Table 1. Faults 3, 9, and 15 are not used for comparison because no observable change in the mean or variance can be detected by visually comparing the plots of each observation variable associated with faults 3, 9, and 15 with plots associated with the normal condition. As shown in Table 1, WNPE-SVDD is a useful method for chemical process monitoring. In some cases, the monitoring performances have been improved significantly compared with the conventional methods.

5. Conclusions

A probabilistic weighted NPE-SVDD method is proposed to improve NPE-based chemical process monitoring performance. First, the measured data are mapped into the feature space by NPE, which reveals the underlying data manifold of process data. Second, the importance of each embedding is evaluated by kernel density estimation in online monitoring. Then, different weighting values are assigned on the embedding to highlight the main deviation information. Finally, the SVDD is employed to judge the process status. The proposed method has been applied on a
numerical process, CSTR process, and TE benchmark process. WNPE-SVDD showed better performances in some cases compared with the conventional methods, such as PCA, KPAC, WPCA, GLSA, LPP, and NPE-SVDD.

Nonetheless, some issues should be addressed in using WNPE-SVDD. First, the KDE along each embedding reveals more process information but also increases the computation complexity. However, the estimation is performed in lower-dimensional feature space and with the modern computer. Thus, the computation speed could easily satisfy the practical application requirement. Second, the introduction of weighting could change the data structure; however, the aim of fault detection is to discriminate the abnormal status from the normal condition. Thus, weighting of the embedding should be performed. Third, the weighting strategy could also be introduced to some other manifold learning algorithm, such as the recently developed LPP and GLSA to further improve the monitoring performance.

### Table 1
False alarm/missed detection rates of PCA (Chiang et al., 2001), KPCA (Scholkopf et al., 1998), WPCA (Jiang & Yan, 2012), GLSA (Zhang et al., 2011), LPP (Niyogi, 2004), NPE-SVDD, and WNPE-SVDD.

<table>
<thead>
<tr>
<th>Fault no.</th>
<th>PCA $T^2$</th>
<th>KPCA $T^2$</th>
<th>WPCA $T^2$</th>
<th>GLSA $T^2$</th>
<th>LPP $T^2$</th>
<th>NPE-SVDD</th>
<th>WNPE-SVDD</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.04/0.01</td>
<td>0.01/0</td>
<td>0.04/0.01</td>
<td>0.04/0</td>
<td>0.01/0</td>
<td>0.08/0</td>
<td>0.02/0.01</td>
</tr>
<tr>
<td>2</td>
<td>0.03/0.02</td>
<td>0/0.01</td>
<td>0.03/0.02</td>
<td>0.06/0.01</td>
<td>0.01/0.02</td>
<td>0.04/0.01</td>
<td>0.04/0.01</td>
</tr>
<tr>
<td>4</td>
<td>0.03/0.4</td>
<td>0.01/0</td>
<td>0.03/0.08</td>
<td>0.11/0</td>
<td>0.01/0.06</td>
<td>0.08/0.05</td>
<td>0.05/0</td>
</tr>
<tr>
<td>5</td>
<td>0.03/0.7</td>
<td>0.01/0.72</td>
<td>0.03/0.72</td>
<td>0.11/0</td>
<td>0.01/0</td>
<td>0.07/0</td>
<td>0.05/0</td>
</tr>
<tr>
<td>6</td>
<td>0.01/0.01</td>
<td>0/0</td>
<td>0.01/0.01</td>
<td>0.02/0</td>
<td>0/0</td>
<td>0.04/0</td>
<td>0.01/0</td>
</tr>
<tr>
<td>7</td>
<td>0.01/0</td>
<td>0/0</td>
<td>0.01/0</td>
<td>0.03/0</td>
<td>0/0</td>
<td>0.03/0</td>
<td>0.01/0</td>
</tr>
<tr>
<td>8</td>
<td>0.03/0.03</td>
<td>0.01/0.01</td>
<td>0.03/0.03</td>
<td>0.1/0.01</td>
<td>0.01/0.02</td>
<td>0.04/0.02</td>
<td>0.03/0.02</td>
</tr>
<tr>
<td>10</td>
<td>0.01/0.5</td>
<td>0.02/0.57</td>
<td>0.01/0.49</td>
<td>0.07/0.06</td>
<td>0.01/0.38</td>
<td>0.04/0.21</td>
<td>0.03/0.2</td>
</tr>
<tr>
<td>11</td>
<td>0.04/0.41</td>
<td>0.02/0.24</td>
<td>0.04/0.35</td>
<td>0.07/0.26</td>
<td>0.01/0.5</td>
<td>0.06/0.28</td>
<td>0.04/0.24</td>
</tr>
<tr>
<td>12</td>
<td>0.03/0.01</td>
<td>0.01/0</td>
<td>0.03/0.01</td>
<td>0.13/0</td>
<td>0.01/0</td>
<td>0.08/0</td>
<td>0.04/0</td>
</tr>
<tr>
<td>13</td>
<td>0.01/0.05</td>
<td>0/0.05</td>
<td>0.01/0.05</td>
<td>0.05/0.04</td>
<td>0/0.05</td>
<td>0.01/0.04</td>
<td>0.02/0.05</td>
</tr>
<tr>
<td>14</td>
<td>0.01/0</td>
<td>0.01/0</td>
<td>0.09/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0.04/0</td>
<td>0.03/0</td>
</tr>
<tr>
<td>16</td>
<td>0.15/0.67</td>
<td>0.1/0.75</td>
<td>0.15/0.62</td>
<td>0.24/0.03</td>
<td>0.07/0.52</td>
<td>0.23/0.27</td>
<td>0.19/0.22</td>
</tr>
<tr>
<td>17</td>
<td>0.01/0.18</td>
<td>0/0.04</td>
<td>0.01/0.16</td>
<td>0.14/0.03</td>
<td>0.01/0.19</td>
<td>0.04/0.09</td>
<td>0.03/0.05</td>
</tr>
<tr>
<td>18</td>
<td>0.01/0.1</td>
<td>0/0.1</td>
<td>0.01/0.1</td>
<td>0.06/0.08</td>
<td>0.01/0.11</td>
<td>0.07/0.09</td>
<td>0.03/0.09</td>
</tr>
<tr>
<td>19</td>
<td>0.02/0.87</td>
<td>0/0.9</td>
<td>0.02/0.86</td>
<td>0.11/0.08</td>
<td>0/0.91</td>
<td>0.04/0.58</td>
<td>0.03/0.66</td>
</tr>
<tr>
<td>20</td>
<td>0.01/0.54</td>
<td>0.0/0.42</td>
<td>0.01/0.48</td>
<td>0.04/0.08</td>
<td>0/0.41</td>
<td>0/0.17</td>
<td>0.01/0.15</td>
</tr>
</tbody>
</table>

Fig. 13. Monitoring performances of TE fault 10 using (a) PCA, (b) KPCA, (c) NPE-SVDD, and (d) WNPE-SVDD.
studies could be focused on the fault diagnosis based on WNPE-SVDD. Improved diagnosis performance is more likely to be achieved because more useful information has been highlighted.

Acknowledgments

The authors gratefully acknowledge the support from the following foundations: 973 Project of China (2013CB733600), National Natural Science Foundation of China (21176073), Program for New Century Excellent Talents in University (NCET-09-0346) and the Fundamental Research Funds for the Central Universities.

Appendix A


Table A1
The control variable of TE process (Chiang et al., 2001; Lyman & Georgakis, 1995).

<table>
<thead>
<tr>
<th>Variables no.</th>
<th>State</th>
<th>Variables no.</th>
<th>State</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMV(1)</td>
<td>D feed flow (stream 2)</td>
<td>XMV(7)</td>
<td>Separator pot liquid flow (stream 10)</td>
</tr>
<tr>
<td>XMV(2)</td>
<td>E feed flow (stream 3)</td>
<td>XMV(8)</td>
<td>Stripper liquid product flow (stream 11)</td>
</tr>
<tr>
<td>XMV(3)</td>
<td>A feed flow (stream 1)</td>
<td>XMV(9)</td>
<td>Stripper steam valve</td>
</tr>
<tr>
<td>XMV(4)</td>
<td>A and C feed flow (stream 4)</td>
<td>XMV(10)</td>
<td>Reactor cooling water valve</td>
</tr>
<tr>
<td>XMV(5)</td>
<td>Compressor recycle valve</td>
<td>XMV(11)</td>
<td>Condenser cooling water flow</td>
</tr>
<tr>
<td>XMV(6)</td>
<td>Purge valve (stream 9)</td>
<td>XMV(12)</td>
<td>Stirring rate</td>
</tr>
</tbody>
</table>

Table A2
The process variable of TE process (Chiang et al., 2001; Lyman & Georgakis, 1995).

<table>
<thead>
<tr>
<th>Variables no.</th>
<th>Process measurements</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMEAS(1)</td>
<td>A feed (stream 1)</td>
<td>km³/h</td>
</tr>
<tr>
<td>XMEAS(2)</td>
<td>D feed (stream 2)</td>
<td>kg/h</td>
</tr>
<tr>
<td>XMEAS(3)</td>
<td>E feed (stream 3)</td>
<td>kg/h</td>
</tr>
<tr>
<td>XMEAS(4)</td>
<td>A and C feed (stream 4)</td>
<td>km³/h</td>
</tr>
<tr>
<td>XMEAS(5)</td>
<td>Recycle flow (stream 8)</td>
<td>km³/h</td>
</tr>
<tr>
<td>XMEAS(6)</td>
<td>Reactor feed rate (stream 6)</td>
<td>km³/h</td>
</tr>
<tr>
<td>XMEAS(7)</td>
<td>Reactor pressure</td>
<td>kPa</td>
</tr>
<tr>
<td>XMEAS(8)</td>
<td>Reactor level</td>
<td>%</td>
</tr>
<tr>
<td>XMEAS(9)</td>
<td>Reactor temperature</td>
<td>ºC</td>
</tr>
<tr>
<td>XMEAS(10)</td>
<td>Purge rate (stream 9)</td>
<td>km³/h</td>
</tr>
<tr>
<td>XMEAS(11)</td>
<td>Product separator temperature</td>
<td>ºC</td>
</tr>
<tr>
<td>XMEAS(12)</td>
<td>Product separator level</td>
<td>%</td>
</tr>
<tr>
<td>XMEAS(13)</td>
<td>Product separator pressure</td>
<td>kPa</td>
</tr>
<tr>
<td>XMEAS(14)</td>
<td>Product separator underflow</td>
<td>m³/h</td>
</tr>
<tr>
<td>XMEAS(15)</td>
<td>Stripper level</td>
<td>%</td>
</tr>
<tr>
<td>XMEAS(16)</td>
<td>Stripper pressure</td>
<td>kPa</td>
</tr>
<tr>
<td>XMEAS(17)</td>
<td>Stripper underflow (stream 11)</td>
<td>m³/h</td>
</tr>
<tr>
<td>XMEAS(18)</td>
<td>Stripper temperature</td>
<td>ºC</td>
</tr>
<tr>
<td>XMEAS(19)</td>
<td>Stripper steam flow</td>
<td>kg/h</td>
</tr>
<tr>
<td>XMEAS(20)</td>
<td>Compress work</td>
<td>kW</td>
</tr>
<tr>
<td>XMEAS(21)</td>
<td>Reactor cooling water outlet temp</td>
<td>ºC</td>
</tr>
<tr>
<td>XMEAS(22)</td>
<td>Separator cooling water outlet temp</td>
<td>ºC</td>
</tr>
</tbody>
</table>

Table A3
The process variable of TE process-2 (Chiang et al., 2001; Lyman & Georgakis, 1995).

<table>
<thead>
<tr>
<th>Variables</th>
<th>State</th>
<th>Stream no.</th>
<th>Sample (time/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMEAS(23)</td>
<td>Composition A</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(24)</td>
<td>Composition B</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(25)</td>
<td>Composition C</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(26)</td>
<td>Composition D</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(27)</td>
<td>Composition E</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(28)</td>
<td>Composition F</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(29)</td>
<td>Composition A</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(30)</td>
<td>Composition B</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(31)</td>
<td>Composition C</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(32)</td>
<td>Composition D</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(33)</td>
<td>Composition E</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(34)</td>
<td>Composition F</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(35)</td>
<td>Composition G</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>XMEAS(36)</td>
<td>Composition H</td>
<td>9</td>
<td>6</td>
</tr>
</tbody>
</table>
Table A4
Process faults for the Tennessee Eastman process (Chiang et al., 2001; Lyman & Georgakis, 1995).

<table>
<thead>
<tr>
<th>Faults no.</th>
<th>Disturbance state</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>IDV (1)</td>
<td>A/C feed ratio, B composition constant (stream 4)</td>
<td>Step</td>
</tr>
<tr>
<td>IDV (2)</td>
<td>B composition, A/C ratio constant (stream 4)</td>
<td>Step</td>
</tr>
<tr>
<td>IDV (3)</td>
<td>D feed temperature (stream 2)</td>
<td>Step</td>
</tr>
<tr>
<td>IDV (4)</td>
<td>Reactor cooling water inlet temperature</td>
<td>Step</td>
</tr>
<tr>
<td>IDV (5)</td>
<td>Condenser cooling water inlet temperature</td>
<td>Step</td>
</tr>
<tr>
<td>IDV (6)</td>
<td>A feed loss (stream 1)</td>
<td>Step</td>
</tr>
<tr>
<td>IDV (7)</td>
<td>C header pressure loss – reduced availability (stream 4)</td>
<td>Step</td>
</tr>
<tr>
<td>IDV (8)</td>
<td>A, B, C feed composition (stream 4)</td>
<td>Random variation</td>
</tr>
<tr>
<td>IDV (9)</td>
<td>D feed temperature (stream 2)</td>
<td>Random variation</td>
</tr>
<tr>
<td>IDV (10)</td>
<td>C feed temperature (stream 4)</td>
<td>Random variation</td>
</tr>
<tr>
<td>IDV (11)</td>
<td>Reactor cooling water inlet temperature</td>
<td>Random variation</td>
</tr>
<tr>
<td>IDV (12)</td>
<td>Condenser cooling water inlet temperature</td>
<td>Random variation</td>
</tr>
<tr>
<td>IDV (13)</td>
<td>Reaction kinetics</td>
<td>Slow drift</td>
</tr>
<tr>
<td>IDV (14)</td>
<td>Reactor cooling water valve</td>
<td>Sticking</td>
</tr>
<tr>
<td>IDV (15)</td>
<td>Condenser cooling water valve</td>
<td>Sticking</td>
</tr>
<tr>
<td>IDV (16)</td>
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</tr>
<tr>
<td>IDV (17)</td>
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<td>Unknown</td>
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<tr>
<td>IDV (20)</td>
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<td>Unknown</td>
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</tbody>
</table>

Fig. A1. The steps of WNPE-SVDD for process monitoring.

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Fig. A2. Diagram of the CSTR process (Yoon & MacGregor, 2001).

Fig. A3. Control scheme for the Tennessee Eastman process (Chiang et al., 2001; Lyman & Georgakis, 1995).

References


