Data Density-Based Fault Detection and Diagnosis with Nonlinearities between Variables and Multimodal Data Distributions

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Abstract

Multivariate statistical process control (MSPC) is an important means of monitoring multiple process variables and their interrelationships while controlling chemical and industrial plants efficiently and stably. To consider nonlinearities between process variables and multimodal data distributions, the data density can be used as an index for fault detection. Data domains with a low data density are considered abnormal states. However, after fault detection, faulty process variables cannot be diagnosed with an MSPC model based on the data density. Therefore, we have developed a new index to diagnose the process variables that contribute to process faults using a data density-based MSPC model. The proposed index uses the partial derivative of an MSPC model with respect to each process variable. We demonstrate the effectiveness of the proposed method using numerical simulation data, Tennessee Eastman process data, and real plant data analyses.

Keywords: Process control; Fault detection; Fault diagnosis; Data density; One-class support vector machine

1 Introduction

For the safe and stable operation of industrial and chemical plants, it is necessary to monitor and control their operating conditions. Because of the huge amount of operating data in plants, data-based process control systems have received considerable attention in recent years. Controlling each process variable independently is inefficient, because there are many process variables that must be controlled. One practical solution is multivariate statistical process control (MSPC) [1,2], which monitors multiple process variables and their relationships simultaneously.

A major component of MSPC is principal component analysis (PCA) [3]-based process control [4]. After extracting the principal components (PCs) from multivariate normal data, the T^2 statistic is calculated as follows:

$$T^2 = \sum_{i=1}^d \frac{t_i^2}{s_i^2}, \quad (1)$$

where d is the number of PCs and s_i is the standard deviation of the i^{th} PC. T^2 represents the magnitude of the principal variation in a training dataset. Errors in PCA models are monitored using the Q statistic, or squared prediction error, which is calculated as:

$$Q = \sum_{i=1}^m (x_i - \hat{x}_i)^2, \quad (2)$$

where m is the number of process variables and $\hat{x}_i$ is the process variable value estimated by the PCA model. A process fault is detected when one of the T^2 and Q statistics exceeds some threshold.

After fault detection with the T^2 and Q statistics, we must diagnose the cause of the fault. Therefore, the contribution of different process variables to the fault is calculated for each statistic [5,6]. We can use the indexes $\text{Cont}T^2(x_i)$ and $\text{Cont}Q(x_i)$ to represent the magnitude of the i^{th} process variable x_i :

$$\text{Cont}T^2(x_i) = \mathbf{t}^T \mathbf{S}^{-1} \left[x_i \mathbf{p}_i (\mathbf{P}^T \mathbf{P})^{-1} \right]^T, \quad (3)$$

$$ContQ(x_i) = (x_i - \hat{x}_i)^2, \quad (4)$$

where $\mathbf{t}$ is a score vector for the training data, $\mathbf{S}$ is a variance–covariance matrix of a score matrix $\mathbf{T}$ for the training data, $\mathbf{p}_i$ is a loading vector corresponding to x_i , and $\mathbf{P}$ is a loading matrix. Process variables with large $ContT^2$ or $ContQ$ values are diagnosed to be the faulty variables. [Zhao et.al. combined PCA with rule-based reasoning approach to identify the root cause of faults in municipal solid waste incinerators \[7\].](#)

As well as PCA, partial least-squares (PLS) [8] and independent component analysis [9,10] have been applied to MSPC. When there is a nonlinear relationship between the process variables and the data distribution is multimodal, nonlinear MSPC methods [11] are more effective than linear ones. Jade *et al.* and Lee *et al.* applied kernel PCA (KPCA) [12], which is the extension of PCA to a nonlinear problem, to MSPC [13,14]. Cheng *et al.* added an adaptation mechanism to KPCA to give adaptive KPCA [15]. Godoy *et al.* applied kernel PLS to fault detection and developed a contribution plot for KPLS to identify faulty process variables [16]. A one-class support vector machine (OCSVM) can be applied to the domain description problem, enabling us to estimate domains in which the data density is high [17-19]. The k-nearest neighbors (k-NN) algorithm can also be applied to estimate the data density [20]. Data density estimation methods such as OCSVM and k-NN have been employed to distinguish process states and estimate prediction errors in soft sensors [21,22]. Such inferential models predict a difficult-to-measure process variable from easy-to-measure process variables [23].

Although MSPC models based on data density can handle nonlinearity between process variables and multimodal data distributions to detect fault situations, to the best of our knowledge, there is no way of diagnosing faulty process variables based on these [nonlinear](#) models after fault detection. Of course, eqs. (3) and (4) cannot deal with nonlinearity between process variables and multimodal data distribution.

Therefore, we propose [a method that diagnoses faulty variables](#) using MSPC models and the data density. In this study, OCSVM and k-NN are used to estimate the data density. The absolute values of the partial derivative of a data density-based MSPC model with respect to each process variable provide an index of the contribution of each process variable to a fault. In the transition from a high-density domain to a low-density domain, process variables with higher index values will contribute more to the change from a normal process state to a process state in which the data density is low, i.e., an abnormal state. [Once faulty process variables are diagnosed using our approach, , rules](#)

or expert knowledge is required to diagnose the root cause of faults.

The effectiveness of the proposed method is demonstrated through two numerical simulation data analyses, the Tennessee Eastman process (TEP) [24], and an industrial membrane bioreactor (MBR) process.

2 Method

Because of its theoretical background and sparseness, OCSVM models can estimate the data density more accurately than k-NN models, although k-NN algorithms are generally simpler. Thus, we develop an expression for the partial derivative of an OCSVM model in this section, and give that for a k-NN model in Appendix A.

2.1 OCSVM

An OCSVM model f can be written as:

$$f(\mathbf{x}^{(i)}) = \phi(\mathbf{x}^{(i)})\mathbf{w} - b \quad (5)$$

where $\mathbf{x}^{(i)} \in R^{1 \times m}$ (m is the number of process variables or input variables; $\mathbf{X}$ -variables) is an item of the (normally distributed) training data, ϕ is a nonlinear function, $\mathbf{w}$ is a weight vector, and b is a constant. If $f(\mathbf{x}^{(i)}) > 0$, $\mathbf{x}^{(i)}$ is within the high-density domain of the training data, and is diagnosed as a normal datum.

In OCSVM modelling, we aim to minimize

$$\frac{1}{2}\|\mathbf{w}\|^2 + \frac{1}{\nu n} \sum_{i=1}^n \xi_i - b \quad (6)$$

subject to

$$\begin{aligned} \phi(\mathbf{x}^{(i)})\mathbf{w} &\geq b - \xi_i \\ \xi_i &\geq 0 \end{aligned}, \quad (7)$$

where n is the number of training data. $\nu \in (0, 1)$ is interpreted as the fraction of outliers in the training data, i.e., data for which $f(\mathbf{x}^{(i)}) \leq 0$. ν controls the size of the normal data domains. In this study, ν is set to 0.003 in reference to the three-sigma limit.

ξ_i is a slack variable. Using the method of Lagrange multipliers, the output of a new datum $\mathbf{x} \in R^{1 \times m}$ is given as follows:

$$f(\mathbf{x}) = \sum_{i=1}^n \alpha_i K(\mathbf{x}^{(i)}, \mathbf{x}) - b \quad (8)$$

where K is the kernel function given by:

$$K(\mathbf{x}^{(i)}, \mathbf{x}) = \phi(\mathbf{x}^{(i)}) \phi(\mathbf{x})^T. \quad (9)$$

Those $\mathbf{x}^{(i)}$ given by eq. (6) for which $\alpha_i \neq 0$ are called support vectors. Only support vectors contribute to the OCSVM model f . In eq. (8), b has the form:

$$b = \sum_{i=1}^n \alpha_i K(\mathbf{x}^{(i)}, \mathbf{x}^{(S)}) \quad (10)$$

where $\mathbf{x}^{(S)}$ is a set of support vectors. The nonlinear function ϕ does not have to be explicitly defined, and the kernel function of eq. (9) is sufficient to derive f . In this study, we use the Gaussian kernel:

$$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \exp\left(-\gamma \|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|^2\right) \quad (11)$$

where γ is a hyperparameter that can be optimized to maximize the variance in K using the training data [25,26]. LIVSVM [27] has been used as an optimization program to construct OCSVM models.

2.2 Partial derivative of an OCSVM model

Using eq. (11), eq. (8) can be transformed to:

$$\begin{aligned}
f(\mathbf{x}) &= \sum_{i=1}^n \alpha_i K(\mathbf{x}^{(i)}, \mathbf{x}) - b \\
&= \sum_{i=1}^n \alpha_i \exp\left(-\gamma \|\mathbf{x}^{(i)} - \mathbf{x}\|^2\right) - b \\
&= \sum_{i=1}^n \alpha_i \exp\left(-\gamma \sum_{k=1}^m (x_{i,k} - x_k)^2\right) - b
\end{aligned} \tag{12}$$

The partial derivative of eq. (12) with respect to the j^{th} process variable x_j is then:

$$\frac{\partial f(\mathbf{x})}{\partial x_j} = 2\gamma \sum_{i=1}^n \alpha_i \exp\left(-\gamma \sum_{k=1}^m (x_{i,k} - x_k)^2\right) (x_{i,j} - x_j) \tag{13}$$

Although we use a Gaussian kernel function in this paper, eq. (8) can be partially differentiated for other differentiable kernel functions.

2.3 Diagnosis of faulty variables using a nonlinear MSPC model based on data density

When a datum is transiting from the domain of a normal state to that of an abnormal state, the change in data density for x_j should be large, because if the absolute value of eq. (13) is large then x_j makes a large contribution to the fault. In eq. (13), the factor of 2γ can be removed so that the absolute value is as follows:

$$ContDD(x_j) = \left| \sum_{i=1}^n \alpha_i \exp\left(-\gamma \sum_{k=1}^m (x_{i,k} - x_k)^2\right) (x_{i,j} - x_j) \right| \tag{14}$$

$ContDD(x_j)$ is the index of the magnitude to which a process variable contributes to a fault in OCSVM. The expression for $ContDD(x_j)$ in k-NN is shown in Appendix A. When a fault occurs, the process variables whose $ContDD$ values are large are contributing most to the fault.

When a new datum instantly transits from a high-density domain to the low-density domain that is very far from high-density domains, the $ContDD$ value is almost zero, as there is little change in data density domains where data density is too low. In this case, values are interpolated between the new and previous datum, and $ContDD$ is calculated using the interpolated data. The maximum $ContDD$ value then

gives the alternative value for the new datum.

3 Results and Discussion

To verify the effectiveness of the proposed method, we analyzed two sets of numerical simulation data, TEP data, and industrial MBR data. The simulation datasets exhibit a nonlinear relationship between their $\mathbf{X}$ -variables and have a multimodal data distribution.

3.1 Numerical simulation data where the relationship between $\mathbf{X}$ and $\mathbf{y}$ is nonlinear

Consider two $\mathbf{X}$ -variables whose relationship is:

$$x_1^2 + (x_2 - 1)^2 = 1 \quad (15)$$

We generate 300 uniform pseudorandom numbers $0 < x_1, x_2 < 1$, and then add random numbers from the normal distribution with a mean of 0 and a standard deviation 0.02. Figure 1 plots x_1 and x_2 . This dataset is used to investigate the domains where PCA and OCSVM models diagnose x_1 and x_2 as abnormal variables.

Figure 2 shows the diagnosis results of faulty variables using $ContT^2$ and $ContQ$ (eqs. (3) and (4), respectively) for the entire domain of Figure 1. There is one PC, whose contribution ratio is 95.6%. The thresholds of $ContT^2$ and $ContQ$ are the 99.7% values of the indexes using the 300 normal data. $ContT^2$ and $ContQ$ values exceed the thresholds in the gray domains in Figure 2, where x_1 and x_2 are diagnosed as abnormal variables. Although $ContQ(x_1)$ and $ContQ(x_2)$ could not detect the fault variables in almost all domains (see Figure 2(c) and (d)), $ContT^2(x_1)$ and $ContT^2(x_2)$ detected fault variables in domains far from the training data (see Figure 2(a) and (b)). However, there remain large domains outside that of the training data that were not diagnosed as abnormal domains for x_1 and x_2 . In addition, $ContT^2$ detected the same abnormal domains for x_1 and x_2 . That is, $ContT^2$ and $ContQ$ could not handle the nonlinearity between x_1 and x_2 .

The diagnosis results of faulty variables using the proposed method are shown in Figure 3. The threshold of $ContDD$ was the 99.7% value of the index using the 300 normal data. Using $ContDD$, x_1 and x_2 were diagnosed as abnormal variables in the right and left domains of the training data domain for x_1 (see Figure 3(a)), and in the upper and lower domains of the training data domain for x_2 (see Figure 3(b)). For example, when a datum is transiting to the left from coordinates (0, 0), and either left or

right from (1, 0.9), it will encounter low-density domains, and only x_1 is diagnosed as the abnormal variable. When a datum is transiting up from (1, 0.9), and either up or down from (0, 0), low-density domains are encountered, and only x_2 is diagnosed as the abnormal variable.

When a datum is transiting diagonally from (0.7, 0.2), both x_1 and x_2 are diagnosed as the abnormal variables, that is, the gray domains of $ContDD(x_1)$ and $ContDD(x_2)$ overlap (see Figure 3(c)). In addition, Figure 3(c) indicates that $ContDD(x_1)$ and $ContDD(x_2)$ can deal with nonlinearity in the relationship between x_1 and x_2 . Thus, the proposed index can appropriately diagnose abnormal variables that have a nonlinear relationship.

Figure 3(c) contains white domains that are far from the training data domain, which means that the proposed index cannot diagnose abnormal variables in these domains. This is because the data density around these domains is almost zero and exhibits little change. However, our aim is not to diagnose faults in domains that are very far from the normal data domains, but to form a diagnosis in domains close to normal data domains, i.e., immediately after the transition to faulty status. Of course, we can interpolate data between a new datum and the previous datum after a sudden transition, and can calculate $ContDD$ using the interpolated data. Some of the $ContDD$ values will be high, indicating that there exist abnormal variables in the transition.

3.2 Numerical simulation data including multimodal data distribution

We consider two $\mathbf{X}$ -variables and generate 300 data at random from three normal distributions. Table 1 shows the averages of these distributions. The standard deviation of each distribution is 0.02, and there is no correlation between x_1 and x_2 . The number of data in each distribution is 100. Figure 4 plots x_1 and x_2 . This dataset is used to investigate the domains where PCA and OCSVM models diagnose x_1 and x_2 as abnormal variables.

Figure 5 shows [the diagnosis results of faulty variables](#) using only $ContT^2$ in the entire domain shown in Figure 4. As there are two PCs, which is equal to the number of $\mathbf{X}$ -variables, the Q statistic has no meaning. The threshold of $ContT^2$ is set to the 99.7% value of the index using the 300 normal data. $ContT^2$ values exceed the thresholds in the gray domains in Figure 5, in which x_1 and x_2 were diagnosed as abnormal variables. Although $ContT^2(x_1)$ and $ContT^2(x_2)$ could detect fault variables in domains outside the training data, there remain large domains that are outside the domain of the training data, but are not diagnosed as abnormal domains for x_1 and x_2 . Thus, $ContT^2$ could not handle a multimodal data distribution.

The diagnosis results of faulty variables using the proposed method are shown in Figure 6. The threshold of *ContDD* was the 99.7% value of the indexes using the 300 normal data. Using *ContDD*, x_1 and x_2 were diagnosed as abnormal variables in the right and left domains of the training data domain for x_1 (see Figure 6(a)) and in the upper and lower domains of the training data domain for x_2 (see Figure 6(b)). For example, when a datum is transiting left or right from (1, 1), (3, 5), or (5, 1), low-density data domains are encountered, and only x_1 is diagnosed as the abnormal variable. When a datum is transiting up or down from (1, 1), (3, 5), or (5, 1), it encounters low-density domains, and only x_2 is diagnosed as the abnormal variable.

When a datum is transiting diagonally from (1, 1), (3, 5), or (5, 1), both x_1 and x_2 are diagnosed as the abnormal variables, that is, the gray domains of *ContDD*(x_1) and *ContDD*(x_2) overlap (see Figure 6(c)). In addition, Figure 6(c) indicates that *ContDD*(x_1) and *ContDD*(x_2) could handle a multimodal data distribution. Therefore, the proposed index can appropriately diagnose abnormal variables when the data distribution is multimodal.

Although Figure 6(c) contains white domains in which no variables are detected as being abnormal, these domains are very far from the training data. The important thing is to diagnose domains close to the normal data domains, which represent the transition from a normal state to an abnormal state. In addition, interpolating between a new datum and the previous datum after a sudden transition and calculating *ContDD*, we can identify large maximum values indicating faulty variables in the transition.

3.3 Diagnosis of faulty process variables in TEP

TEP was developed by the Eastman Chemical Company to simulate a real industrial process, and has been used to compare the performance of process control and monitoring methods. A TEP diagram has been published by Downs and Vogel [24]. TEP consists of a reactor, condenser, compressor, separator, and stripper, as well as eight components A, B, C, D, E, F, G, and H. The liquid products G and H and the by-product F are produced from the gaseous reactants A, C, D, and E through some chemical reactions. Twenty-two easy-to-measure process variables without composition measurements were used as **X**-variables (see Table 2). The **X**-variables were measured online every 3 min. It is important to control these variables for safe and effective plant operations.

There are 21 preprogrammed faults, including five unknown faults, in TEP. In this study, we target and discuss the process faults of B composition, A/C feed ratio

constant and reaction kinetics, because only minor differences were confirmed between the traditional results and those of the proposed method in the other process faults. The training and test data were obtained from the literature [28]. Thus, the control scheme is exactly the same as that used by Russell et al. [28]. The training data for the normal condition and each fault consisted of 500 (1,500 min) and 480 (1,440 min) observations, respectively. The test data for each fault consisted of 960 (2,880 min) observations, including 160 (480 min) normal data.

The thresholds of $ContT^2$, $ContQ$, and $ContDD$ were determined as in the numerical simulation data analyses. Since $ContT^2$, $ContQ$, and $ContDD$ were divided by each threshold and normalized, the thresholds of normalized $ContT^2$, $ContQ$, and $ContDD$ are one. The fault detection results and the diagnosis results of faulty variables are shown in Table 3 and Figures 7 and 8 for the process fault of B composition, A/C feed ratio constant. Faulty process variables could be detected at 540 min by both $ContT^2$ and $ContQ$, but at 513 min by $ContDD$. The proposed index achieved earlier fault detection than $ContT^2$ and $ContQ$. Some of the process variables diagnosed with $ContT^2$ and $ContQ$ were also diagnosed with $ContDD$.

Table 4 and Figures 9 and 10 show the fault detection results and the diagnosis results of faulty variables for the process fault of reaction kinetics. Faulty process variables could be detected at 600 min by $ContT^2$ and at 639 min by $ContQ$, but at 567 min by $ContDD$, which means the proposed index again achieved earlier fault detection. In fact, variable values diagnosed by $ContDD$ generally change after the fault.

In the B composition, A/C feed ratio constant, and reaction kinetics process faults, the process variables diagnosed with $ContDD$ include the reactor temperature. Although the closed-loop feedback control means it is difficult to discuss the actual faulty process variables in TEP, the proposed index diagnosed appropriate process variables because the faults are related to materials and reaction rate. Results for only two faults are presented in this paper, but the proposed index could diagnose faulty process variables for other faults. We have confirmed that early and accurate fault detection and diagnosis of faulty variables is possible using the proposed method.

3.4 Diagnosis of faulty variables in an industrial MBR plant

To verify the diagnosis performance of the proposed method for faulty water quality process variables, we used data obtained from an MBR plant whose system comprises anoxic, aerobic, and membrane tanks. A membrane module is immersed in the membrane tank. Further details of the target MBR plant and water quality variables are given in Tables 5 and 6, respectively. In this case study, we used the first 327 (days)

data as a normal training dataset and the next 64 (days) data as a test dataset. In the test data, the abnormal event occurs in the viscometer after the 21st day, but viscosity values remain within the normal range, making it difficult to diagnose the fault. However, the relationship between viscosity and other variables would change.

The thresholds of $ContT^2$, $ContQ$, and $ContDD$ are set to the 99.7% values of the index using the normal data as in the numerical simulation data analyses. Since $ContT^2$, $ContQ$, and $ContDD$ were divided by each threshold and normalized, the thresholds of normalized $ContT^2$, $ContQ$, and $ContDD$ are one. The fault detection results and [the diagnosis results of faulty variables](#) are shown in Table 7 and Figures 11 and 12. For the T^2 and Q statistics, fault detection occurs on the 37th day, some time after the actual fault. $ContT^2$ and $ContQ$ diagnosed the mixed liquor suspended solids (MLSS) concentration in the membrane tank, water temperature in the membrane tank, and influent MLSS concentration as well as the viscosity in the aerobic tank. This is too many fault options. In contrast, the proposed $ContDD$ detected the fault time accurately, and diagnosed only the viscosity in the aerobic tank as the faulty process variable. Thus, the faulty process variable can be diagnosed accurately using the proposed method.

4 Conclusions

We have developed a new index to diagnose faulty process variables by partially differentiating an MSPC model based on the data density. We demonstrated that the proposed index could handle nonlinearity between process variables and multimodal data distributions through numerical simulation data analyses. TEP data and real MBR data were then used to show that our approach can achieve earlier and more accurate fault detection and diagnosis than traditional indexes. In fact, process faults are diagnosed by combining candidate process variables with expert knowledge about the process. By applying our proposed method to process control in industrial plants, the plants can be operated stably and safely.

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Appendix A: Partial derivative of a k-NN model

k-NN is a well-known classification method. For domain description problems, the sum of the squared Euclidian distances from the k nearest data is employed as an index of data density. This is computed as follows:

$$g(\mathbf{x}) = -\sum_{i=1}^k \sum_{l=1}^m (x_{i,l} - x_l)^2 \quad .$$

(A.1)

High values of $g(\mathbf{x})$ imply high data density. The partial derivative of eq. (A.1) with respect to a process variable x_j is as follows:

$$\frac{\partial g(\mathbf{x})}{\partial x_j} = 2 \sum_{i=1}^k (x_{i,j} - x_j) \quad .$$

(A.2)

$ContDD(x_i)$ for k-NN is then as follows:

$$ContDD(x_j) = \left| \sum_{i=1}^k (x_{i,j} - x_j) \right| \quad .$$

(A.3)

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Figure 1. Plot of x_1 and x_2 for numerical simulation data where the relationship between X and y is nonlinear.

Figure 2. Fault diagnosis using $ContT^2$ and $ContQ$ for the numerical simulation data where the relationship between X and y is nonlinear. In the gray domains, x_1 and x_2 are diagnosed as abnormal variables.

Figure 3. Fault diagnosis using the proposed method for the numerical simulation data where the relationship between X and y is nonlinear. In the gray domains, x_1 and x_2 are diagnosed as abnormal variables.

Figure 4. Plot of x_1 and x_2 for numerical simulation data where the data distribution is multimodal.

Figure 5. Fault diagnosis using $ContT^2$ for numerical simulation data where the data distribution is multimodal. In the gray domains, x_1 and x_2 are diagnosed as abnormal variables.

Figure 6. Fault diagnosis using the proposed method for numerical simulation data where the data distribution is multimodal. In the gray domains, x_1 and x_2 are diagnosed as abnormal variables.

Figure 7. Fault diagnosis results using $ContT^2$ and $ContQ$ at 540 min in a B composition, A/C feed ratio constant fault for the TEP data analysis. Each index value is normalized by dividing by each threshold.

Figure 8. Fault diagnosis result using the proposed method at 513 min in a B composition, A/C feed ratio constant fault for the TEP data analysis. Each index value is normalized by dividing by each threshold.

Figure 9. Fault diagnosis results at 600 min for $ContT^2$ and at 639 min for $ContQ$ in a reaction kinetics fault for the TEP data analysis. Each index value is normalized by dividing by each threshold.

Figure 10. Fault diagnosis result using the proposed method at 567 min in a reaction

kinetics fault for the TEP data analysis. Each index value is normalized by dividing by each threshold.

Figure 11. Fault diagnosis results using $ContI^2$ and $ContQ$ at the 37th day in the test data from an MBR plant. Each index value is normalized by dividing by each threshold.

Figure 12. Fault diagnosis result using the proposed method at the 21st day in the test data from an MBR plant. Each index value is normalized by dividing by each threshold.

Table 1. Averages of x_1 and x_2 for each normal distribution in numerical simulation data including a multimodal data distribution.

	x_1	x_2
Distribution 1	1	1
Distribution 2	3	5
Distribution 3	5	1

Table 2. Process variables in TEP.

1	A feed
2	D feed
3	E feed
4	Total feed
5	Recycle flow
6	Reactor feed rate
7	Reactor pressure
8	Reactor level
9	Reactor temperature
10	Purge rate
11	Product separator temperature
12	Product separator level
13	Product separator pressure
14	Product separator underflow
15	Stripper level
16	Stripper pressure
17	Stripper underflow
18	Stripper temperature
19	Stripper steam flow
20	Compressor work
21	Reactor cooling water outlet temperature
22	Separator cooling water outlet temperature

Table 3. Fault detection and diagnosis in a B composition, A/C feed ratio constant fault for the TEP data analysis.

	Fault detection time [min]	Diagnosed X -variable as abnormal
<i>ContT²</i>	540	Product separator pressure
		Stripper steam flow
		D feed
<i>ContQ</i>	540	Recycle flow
		Reactor temperature
		Product separator temperature
<i>ContDD</i>	513	Reactor temperature
		Product separator pressure
		Stripper steam flow

Table 4. Fault detection and diagnosis in a reaction kinetics fault for the TEP data analysis.

	Fault detection time [min]	Diagnosed X -variable as abnormal
<i>ContT</i> ²	600	Recycle flow Reactor cooling water outlet temperature
<i>ContQ</i>	639	Product separator pressure
<i>ContDD</i>	567	Reactor temperature

Table 5. Brief summary of an MBR plant.

Operation	Constant-rate filtration
Treatment object	Urban wastewater
Treatment scale	40 m ³ /day
Membrane	Immersion type flat sheet membrane (MF)
Material	Polyvinylidene fluoride

Table 6. Process variables of an MBR plant.

1	pH
2	Water temperature in the membrane tank
3	Influent MLSS ^a concentration
4	MLSS ^a concentration in the membrane tank
5	Viscosity in the aerobic tank
6	Ammoniacal nitrogen in treated wastewater
7	Nitrate nitrogen in treated wastewater
8	Phosphate-phosphorus in treated wastewater

^a mixed liquor suspended solids

Table 7. Fault detection and diagnosis in an MBR plant.

	Fault detection time [day]	Diagnosed X -variable as abnormal
<i>ContT</i> ²	37	MLSS ^a concentration in the membrane tank Viscosity in the aerobic tank
<i>ContQ</i>	37	Water temperature in the membrane tank Influent MLSS ^a concentration Viscosity in the aerobic tank
<i>ContDD</i>	21	Viscosity in the aerobic tank

^a mixed liquor suspended solids

Figure(s)

Figure 1. Plot of x_1 and x_2 for numerical simulation data where the relationship between X and y is nonlinear.

(a) $ContT^2(x_1)$

(b) $ContT^2(x_2)$

(c) $ContQ(x_1)$

(d) $ContQ(x_2)$

Figure 2. Fault diagnosis using $ContT^2$ and $ContQ$ for the numerical simulation data where the relationship between X and y is nonlinear. In the gray domains, x_1 and x_2 are diagnosed as abnormal variables.

(a) *ContDD*(x_1)

(b) *ContDD*(x_2)

(c) Overlap of *ContDD*(x_1) and *ContDD*(x_2)

Figure 3. Fault diagnosis using the proposed method for the numerical simulation data where the relationship between X and y is nonlinear. In the gray domains, x_1 and x_2 are diagnosed as abnormal variables.

Figure 4. Plot of x_1 and x_2 for numerical simulation data where the data distribution is multimodal.

Figure 5. Fault diagnosis using $ContT^2$ for numerical simulation data where the data distribution is multimodal. In the gray domains, x_1 and x_2 are diagnosed as abnormal variables.

(a) $ContDD(x_1)$

(b) $ContDD(x_2)$

(c) Overlap of $ContDD(x_1)$ and $ContDD(x_2)$

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