Localized Fisher Discriminant Analysis Based Complex Chemical Process Monitoring

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DOI 10.1002/aic.12392
Published online October 11, 2010 in Wiley Online Library (wileyonlinelibrary.com).

Complex chemical process is often corrupted with various types of faults and the fault-free training data may not be available to build the normal operation model. Therefore, the supervised monitoring methods such as principal component analysis (PCA), partial least squares (PLS), and independent component analysis (ICA) are not applicable in such situations. On the other hand, the traditional unsupervised algorithms like Fisher discriminant analysis (FDA) may not take into account the multimodality within the abnormal data and thus their capability of fault detection and classification can be significantly degraded. In this study, a novel localized Fisher discriminant analysis (LFDA) based process monitoring approach is proposed to monitor the processes containing multiple types of steady-state or dynamic faults. The stationary testing and Gaussian mixture model are integrated with LFDA to remove any nonstationarity and isolate the normal and multiple faulty clusters during the preprocessing steps. Then the localized between-class and within-class scatter mattress are computed for the generalized eigenvalue decomposition to extract the localized Fisher discriminant directions that can not only separate the normal and faulty data with maximized margin but also preserve the multimodality within the multiple faulty clusters. In this way, different types of process faults can be well classified using the discriminant function index. The proposed LFDA monitoring approach is applied to the Tennessee Eastman process and compared with the traditional FDA method. The monitoring results in three different test scenarios demonstrate the superiority of the LFDA approach in detecting and classifying multiple types of faults with high accuracy and sensitivity.
 AIChE J, 57: 1817–1828, 2011
Keywords: chemical process monitoring, fault detection and classification, localized Fisher discriminant analysis, stationarity testing, Gaussian mixture model, Tennessee Eastman process

Introduction

Modern chemical industry has witnessed a dramatic increase in the plant scale and operation complexity over the past decades. With the growing number of measured variables in the precesses, the plant monitoring has become more challenging than ever due to different reasons such as (i) the complicated variable correlations, (ii) the process dynamics and nonlinearity, and (iii) the mixed operation modes and process faults. Meanwhile, the reliable and efficient process monitoring has been found to be of the critical importance to ensure the safe plant operation, stable product quality, reduced maintenance cost, and improved profit margin. Such tremendous benefits continue motivating the research activities in the process monitoring field through the past decade. The most popular methods that have been widely applied to

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process industry are the multivariate statistics based process monitoring (MSPM) techniques.[1–4] These methods are typically data driven and rely on plenty of historical data to build statistical models for fault detection and identification. Their main advantages lie in the facts that the requirements on a priori process knowledge are minimal and the traditional effort to develop the time-consuming mechanistic models for the processes is also avoided.[5–7] The well-known principal component analysis (PCA) and partial least squares (PLS) techniques are two commonly used MSPM approaches, in which a period of normal operating data are used to build the statistical model and define the normal operating region. For PCA based monitoring method, the covariance based decomposition is conducted to project the operating data onto the lower-dimensional principal component subspace (PCS) with the majority of data variability retained. Two statistical indices, Hotelling's T^2 and squared prediction error (SPE), are further derived to measure the significance of the fault within the PCS and the residual subspace, respectively.[8–10] The PLS method, on the other hand, utilizes not only the process variables but also the quality variables to construct the model and characterize the normal operation boundary.[1,10,11] Similarly, the T^2 and SPE indices are used to determine the occurrence of process faults. Both PCA and PLS based monitoring methods require the projected latent variables to follow multivariate Gaussian distribution approximately so that the second-order statistic, covariance or correlation, is adequate to contain all the faulty information.

To deal with the non-Gaussian processes, some new MSPM methods have been proposed more recently. One emerging technique is independent component analysis (ICA), which depends upon higher-order statistics such as negentropy and extracts statistically independent components from the normal operating data. Thus the latent variables are essentially non-Gaussian and can reveal more hidden features for process monitoring.[12–15] Another non-Gaussian monitoring approach is based on the Gaussian mixture model (GMM), in which the process data are assumed to follow one of the multiple Gaussian distributions with different means and covariances at a fixed prior probability. In this way, the globally non-Gaussian process data can be attributed into one of the multiple clusters and then the corresponding local Gaussian models can be selected to detect the process fault in each operation region.[16,17] Other multimodel strategies to handle non-Gaussian processes include the multiple PCA,[18] multiple PLS,[19] mixture PCA,[20] etc.

A common feature of these methods is that they all require a set of purely normal process data to build the fault-free model. In practice, such a priori condition may not be satisfied because the plant historical data are often contaminated with different kinds of process faults. In other words, the training data set are usually mixed with both normal and faulty samples. Furthermore, this type of approaches rely on normal operating data only without taking into account any inherent features of faulty data. Hence, their reliability on fault detection and diagnosis may be affected. Another popular unsupervised classification method is the *K*-means clustering technique, which can handle the fault contaminated training data and has been used for chemical process monitoring.[21,22] Nevertheless, it assumes that the number of faulty classes is known so that its practical applications are restricted. On the other hand, the supervised pattern classification methods such as the well known support vector machine (SVM) have also gained success in process fault detection and diagnosis.[23,24] SVM approach can separate two classes with maximized margin between support vector planes. However, its mathematical formulation requires user to choose appropriate kernel function, soft margin factor, and other corresponding parameters like Gaussian kernel distance, polynomial order, etc. The best selection of model parameters in SVM algorithm is not a trivial task. As a kind of linear supervised classification technique, Fisher discriminant analysis (FDA)[25] has been proposed to isolate process faults from normal operation and optimize their separability.[10,26] Unlike PCA, FDA searches for the directions with the maximized discrimination between normal and faulty data instead of the largest variability within normal data alone.[25] Such objective of FDA is achieved by maximizing the between-class scatter while minimizing the within-class scatter. The monitoring and diagnosis capability of FDA technique has been proved to excel that of PCA and discriminant PLS methods in literature.[10,26] Although the FDA method has gained some success in process monitoring, it may suffer from its fundamental limitation in dealing with the normal or faulty data that has within-class multimodality. One of the objectives in conventional FDA to minimize the within-class scatter can sacrifice the separability between classes and further affect the fault detection accuracy. In industrial practice, it is very likely that the abnormal process data include multiple types of faults, which follow different statistical distributions. Aimed at this issue, a pairwise FDA strategy has been adopted to obtain all the specific discriminant directions between the normal data and each class of faulty data.[26] However, this approach may lead to contradictory results on fault detection of new sample points because the same normal data set needs to be paired with all possible faults individually. For instance, an arbitrary test sample can be classified into normal operation during the first pair but determined as faulty one at the second pair. Moreover, this approach depends upon a preliminary *k*-means clustering step to classify different kinds of faults and a priori process knowledge is needed to determine the actual number of faults present in the training data set. Another well-established classification algorithm, namely soft independent modeling by class analogy (SIMCA), adopts the idea of examining each individual cluster in a recursive way and a measure of goodness of model is used to determine which class the observation is finally categorized into.[27] Despite its classification capability, the SIMCA method does not provide the best separating hyperplane between different classes. Moreover, its measure of model goodness may not guarantee the optimal reconciliation of potentially conflicting classification results.

As a new machine learning technique, the localized Fisher discriminant analysis (LFDA) has recently been proposed in literature to tackle the issue of within-class multimodality.[28] The basic idea of LFDA is to maximize the between-class separability while preserving the within-class local structure simultaneously. The data transformation in LFDA is designed such that the relative distance and positions of those data points within the same class almost remain unchanged. In this way, the within-class multimodality is well preserved and the major drawback of conventional FDA

method can be overcome. On the other hand, LFDA algorithm is similar to traditional FDA in terms of essentially conducting generalized eigenvalue decomposition, which is easy and fast to compute.[28] In this article, a novel LFDA based fault detection and classification approach is developed to monitor the complex chemical processes with multiple types of faults. First, a period of plant historical data are collected as training set, which includes both normal samples and different types of faulty data. Then, a GMM is built to classify the training data set into normal and various faulty clusters. The LFDA approach is further used to search for the characteristic direction with maximized separability between normal and faulty data while the multimodality within the faulty data set is maintained.

This article is organized as follows. Section "Review of Fisher Discriminant Analysis" briefly reviews the traditional FDA method. The novel LFDA algorithm is described in Section "Localized Fisher Discriminant Analysis". Section "LFDA Based Process Monitoring Approach" presents the novel process monitoring approach that integrates LFDA and GMM to detect and classify different types of process faults. In Section "Case Study", the new LFDA based monitoring approach is compared with the conventional FDA method in three test scenarios of the Tennessee Eastman process (TEP). Section "Conclusions" concludes this article with future directions identified.

Review of Fisher Discriminant Analysis

FDA is a kind of supervised pattern recognition method and its basic idea is to search for a series of characteristic directions that maximize the separability between different classes while minimizing the the within-class data scattering.[25] The projection of data samples onto the feature subspace composed of the first few discriminant directions can lead to the best separation among different classes with significant dimensionality reduction.

Consider a set of training samples $\{x_1,x_2,\ldots x_n\}$ from a m-dimensional space R^m. All these n samples are assumed to categorized into K classes and the kth ($1 \le k \le K$) class C_k contains n_k samples. Then the between-class and within-class scatter matrices S_b and S_w can be defined as

$$S_b = \sum_{k=1}^{K} n_k (\bar{x}_k - \bar{x})(\bar{x}_k - \bar{x})^T \tag{1}$$

and

$$S_w = \sum_{k=1}^{K} \sum_{x_i \in C_k} (x_i - \bar{x}_k)(x_i - \bar{x}_k)^T \tag{2}$$

where $\bar{x}_k = \frac{1}{n_k} \sum_{x_i \in C_k} x_i$ denotes the mean vector of the samples within the kth class and $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$ is the mean of all the n samples.

The Fisher discriminant directions, as the linear combinations of original variables, are derived by optimizing the following objective function

$$J_{\mathrm{FDA}} = \arg\max_{\substack{w \in R^m \\ w \neq 0}} \left\{ \frac{w^T S_b w}{w^T S_w w} \right\} \tag{3}$$

where w is an arbitrary vector in the m-dimensional space R^m. The above optimization problem can be equivalently solved by the generalized eigenvalue decomposition

$$S_b p = \lambda S_w p \tag{4}$$

where λ is the generalized eigenvalue and p denotes the eigenvector that corresponds to a Fisher discriminant direction. The value of λ indicates the extent of mutual separation between classes in terms of the ratio of the between-class vs. within-class distances. In process monitoring, the normal and faulty process data are separated by projecting the raw data set onto the lower dimensional feature subspace composed of the leading Fisher discriminant vectors.

Localized Fisher Discriminant Analysis

As one of the objectives of FDA is to minimize the within-class data scatter, the derived Fisher discriminant vectors may not be the optimal directions in separating different classes if either class includes multiple distinct clusters. In this case, the data from the corresponding class do not follow multivariate Gaussian distribution but show a within-class multimodality that makes the traditional FDA algorithm inappropriate. The particular drawback of FDA method lies in the fact that it ignores the localities of data class while focusing on the global features only. To overcome the deficiency of regular FDA method, a LFDA has been proposed with both between-class separation and within-class local structure preservation simultaneously.[28]

The between-class and within-class scatter matrices can be reformulated as follows:[28]

$$S_b = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} W_{i,j}^{(b)} (x_i - x_j)(x_i - x_j)^T \tag{5}$$

and

$$S_w = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} W_{i,j}^{(w)} (x_i - x_j)(x_i - x_j)^T \tag{6}$$

where the weighting matrices $W_{i,j}^{(b)}$ and $W_{i,j}^{(w)}$ are defined as

$$W_{i,j}^{(b)} = \begin{cases} \frac{1}{n} - \frac{1}{n_k} & (\text{if } x_i \in C_k,\ x_j \in C_k) \\ \frac{1}{n} & (\text{otherwise}) \end{cases} \tag{7}$$

and

$$W_{i,j}^{(w)} = \begin{cases} \frac{1}{n_k} & (\text{if } x_i \in C_k,\ x_j \in C_k) \\ 0 & (\text{otherwise}) \end{cases} \tag{8}$$

The above reformulation indicates that the distances of data pairs between distinct classes contribute positively to the between-class scatter matrix while have no impact on the within-class scatter matrix. In contrast, the larger distances of data points within the same class make the the between-class matrix decrease whereas the within-class scatter matrix increase simultaneously.

Similarly, the localized between-class and within-class scatter matrices can be defined as[28]

$$\widetilde{S}_b = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\widetilde{W}_{i,j}^{(b)}(x_i - x_j)(x_i - x_j)^T \tag{9}$$

and

$$\widetilde{S}_w = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\widetilde{W}_{i,j}^{(w)}(x_i - x_j)(x_i - x_j)^T \tag{10}$$

where the weighting matrices $\widetilde{W}_{i,j}^{(b)}$ and $\widetilde{W}_{i,j}^{(w)}$ are expressed as

$$\widetilde{W}_{i,j}^{(b)} = \begin{cases} A_{i,j}(\frac{1}{n} - \frac{1}{n_k}) & (\text{if } x_i \in C_k,\ x_j \in C_k) \\ \frac{1}{n} & (\text{otherwise}) \end{cases} \tag{11}$$

and

$$\widetilde{W}_{i,j}^{(w)} = \begin{cases} \frac{A_{i,j}}{n_k} & (\text{if } x_i \in C_k,\ x_j \in C_k) \\ 0 & (\text{otherwise}) \end{cases} \tag{12}$$

In the above weighting factors of LFDA, an affinity matrix A has been used to characterize the closeness between all pairs of samples and its (i,j)th element $A_{i,j}$ is defined to quantify how far apart the data pair x_i and x_j are.[29] One standard way of setting the $A_{i,j}$ value is as follows

$$A_{i,j} = \exp(-\frac{||x_i - x_j||^2}{\sigma^2}) \tag{13}$$

where σ is an adjustable parameter to determine the speed of exponential decreasing of each affinity matrix entry.[30] An alternate option to localize the scaling of data pair affinity is given below

$$A_{i,j} = \exp(-\frac{||x_i - x_j||^2}{\sigma_i\sigma_j}) \tag{14}$$

where $\sigma_i = \|x_i - x_i^{(K)}\|$ denotes the local scaling of data samples around x_i with $x_i^{(K)}$ being the K nearest neighbor of x_i. This strategy takes into account the density of data samples in different regions.[31] In this work, the standard definition of $A_{i,j}$ in Eq. 13 is used.

With the affinity matrix included, the closer sample pair within the same class tends to have more contribution on both the within-class and between-class scatter matrices. On the other hand, the pair of samples within the same class that are far away from each other normally have higher probability to come from different clusters. Hence, those points should have less impact on the within-class scattering. Through the modified scattering matrices, the within-class multimodality of data can be preserved to the maximal extent.

Similar to the conventional FDA method, the localized Fisher discriminant directions can be obtained by solving the optimization problem as follows

$$J_{\text{LFDA}} = \underset{\substack{\widetilde{w}\in(R)^m \\ \widetilde{w}\neq 0}}{\arg\max}\left\{\frac{\widetilde{w}^T\widetilde{S}_b\widetilde{w}}{\widetilde{w}^T\widetilde{S}_w\widetilde{w}}\right\} \tag{15}$$

which is also equivalent to the generalized eigenvalue decomposition below

$$\widetilde{S}_b\widetilde{p} = \widetilde{\lambda}\widetilde{S}_w\widetilde{p} \tag{16}$$

with $\widetilde{\lambda}$ and $\widetilde{p}$ being the generalized eigenvalue and eigenvector, respectively. Assume that the generalized eigenvalues $\widetilde{\lambda}_1 \geq \widetilde{\lambda}_2 \geq \ldots \geq \widetilde{\lambda}_m$ are arranged in descending order, the corresponding generalized eigenvectors $\widetilde{p}_1, \widetilde{p}_1, \ldots, \widetilde{p}_m$ are the localized Fisher discriminant directions of decreasing class separability. It is noted that the LFDA method will be identical to the conventional FDA if all the entries of the affinity matrix A are set to one.

LFDA Based Process Monitoring Approach

Based on the above LFDA algorithm, a new process monitoring approach is proposed to deal with the plant operating data mixed with both normal and multiple types of faulty data. The underlying assumption is that the historical data collected as training set are composed of normal samples along with various process faults. The normal operating data can be assumed to follow multivariate Gaussian distribution. The faulty data, on the other hand, obey a non-Gaussian distribution with a mixture of different kinds of process faults. For each subset of abnormal data with a single faulty condition, it may not necessarily follow multivariate Gaussian distribution because of some types of nonstationary faults such as process drifting error, though the operation data under a single stationary fault like step change and increased random variations is still of Gaussian distribution.

In the data preprocessing steps, the training data set needs to be classified into multiple clusters and each of them corresponds to either the normal operating data or one of the various types of faulty data. First of all, the stationarity test[32] is conducted throughout the training data set to separate the dynamic trends with the nonstationary faults from the steady-state operation data. The data sequence is first divided into a series of time intervals with equal lengths. Then the mean value for each interval is computed and the number of runs of mean values above and below the median value of the series are further counted. If the number of counts is found to be significantly larger than the known probabilities of runs for random data, the sample points in the corresponding time intervals are determined to be nonstationary. For the nonstationary data segments, the first order derivative is taken as follows to remove the dynamics:

$$\widetilde{x}_i = \frac{x_{i+1} - x_{i-1}}{t_{i+1} - t_{i-1}} \tag{17}$$

where x_i is the identified nonstationary sample while $\widetilde{x}_i$ denotes its corresponding transformed point. t_{i+1} and t_{i-1} represent the sampling times of data points x_{i+1} and x_{i-1}. On the other hand, all the stationary samples remain unchanged as $\widetilde{x}_i = x_i$. In industrial practice, the first-order derivative can normally serve as good approximation of the stationarized samples. However, the second-or higher-order derivatives can also be used in the situations when the first order derivative is not adequate to remove the non-stationarity of certain sample points. The transformed data set then consists of multiple steady-state clusters, each of which an be assumed to follow a multivariate Gaussian distribution approximately. Then, the GMM[17,33,34] is built on the transformed data set to isolate

multiple process faults from the normal operation. Each Gaussian component corresponds to either the normal data set or an individual process fault. To eliminate the requirement of a priori knowledge on the exact number of process faults existing in the data set, the F-J learning algorithm is used to train the GMM with the automatically optimized number of clusters.[33]

With the isolated normal and faulty data sets, the LFDA method is further implemented on all the training samples to derive the optimal directions for classifying normal and faulty data in the test set. First, the transformed training samples are plugged into Eqs. 9 and 10 to obtain the localized between-class and within-class scatter matrices as follows:

$$\widetilde{S}_b = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\widetilde{W}_{i,j}^{(b)}(\widetilde{x}_i - \widetilde{x}_j)(\widetilde{x}_i - \widetilde{x}_j)^T \tag{18}$$

and

$$\widetilde{S}_w = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\widetilde{W}_{i,j}^{(w)}(\widetilde{x}_i - \widetilde{x}_j)(\widetilde{x}_i - \widetilde{x}_j)^T \tag{19}$$

where one class corresponds to normal operating data set following Gaussian distribution while the other class represents multiple types of process faults.

Then, the generalized eigenvalue decomposition as Eq. 16 on the above scatter matrices can lead to the localized Fisher discriminant directions $\widetilde{p}_1, \widetilde{p}_2, \ldots, \widetilde{p}_m$ with the corresponding eigenvalues in descending order. The first r eigenvectors are extracted to form a reduced dimensional Fisher discriminant subspace and then the localized Fisher discriminant function can be defined as

$$g_k(\widetilde{x}) = -\frac{1}{2}(\widetilde{x} - \overline{\widetilde{x}_k})^T\widetilde{P}_r \times \left(\frac{1}{n_k - 1}\widetilde{P}_r^T\left(\sum_{\widetilde{x}_i \in C_k}(\widetilde{x}_i - \overline{\widetilde{x}_k})(\widetilde{x}_i - \overline{\widetilde{x}_k})^T\right)\widetilde{P}_r\right)^{-1}\widetilde{P}_r^T(\widetilde{x} - \overline{\widetilde{x}_k}) + \ln K - \frac{1}{2}\ln\left[\det\left(\frac{1}{n_k - 1}\widetilde{P}_r^T\left(\sum_{\widetilde{x}_i \in C_k}(\widetilde{x}_i - \overline{\widetilde{x}_k})(\widetilde{x}_i - \overline{\widetilde{x}_k})^T\right)\widetilde{P}_r\right)\right] \tag{20}$$

where $\widetilde{P}_r = [\widetilde{p}_1\ \widetilde{p}_2 \ldots \widetilde{p}_r]$ spans the r-dimensional Fisher discriminant subspace and $g_k(\widetilde{x})$ represents the discriminant function value of an arbitrary sample point $\widetilde{x}$ belonging to the kth class in the training data set. The above discriminant function is analogous to the one used in the conventional FDA[25] but has been modified to accommodate the localized feature in LFDA method.

Similarly, the stationarity test needs to be performed through the test data set and the identified non-stationarity should be removed in the data preprocessing step. Then the discriminant functions for each transformed test point $\widetilde{x}_t$ with respect to all the K classes are computed using Eq. 20, and the monitored sample is categorized into either the normal or one of the faulty clusters by the following criterion:

$$C(\widetilde{x}_t) = \arg\max_{1 \le k \le K}\{g_k(\widetilde{x}_t)\} \tag{21}$$

The flow chart of the LFDA based process monitoring approach is illustrated in Figure 1 and the step-by-step procedures are outlined below:

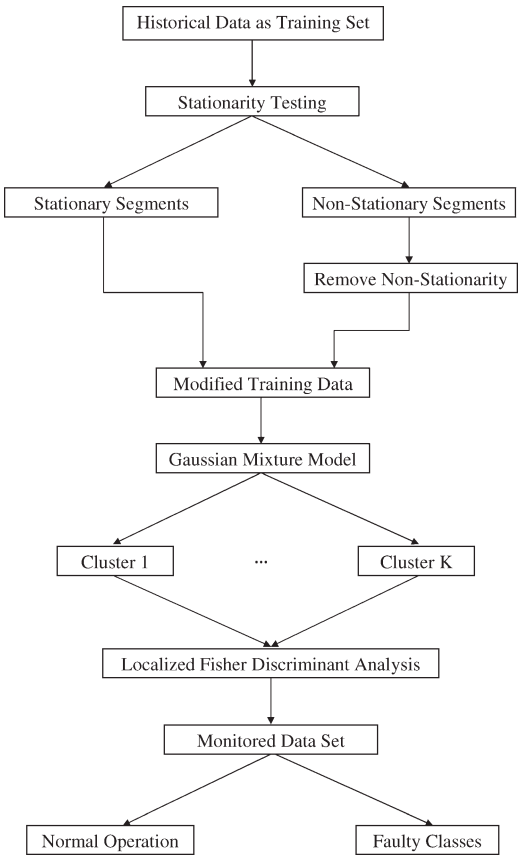

Figure 1. Schematic diagram of the LFDA based process monitoring approach.

(i) Use historical data as training set that includes both normal and different types of faulty samples.

(ii) Conduct stationarity testing on the entire training set to detect any non-stationarity.

(iii) For the nonstationary data points, take the first-order derivative to remove the non-stationarity.

(iv) For the preprocessed training set, build GMM to categorize the normal and multiple types of faulty data.

(v) The localized between-class and within-class scatter matrices are further calculated from Eqs. 9 and 10.

(vi) The generalized eigenvalue analysis is performed on the pair of scatter matrices to derive the localized Fisher discriminant directions.

(vii) For the monitored data set, the stationarity testing is carried out and the non-stationarity is removed by the first-order derivative.

(viii) The discriminant function within the reduced-dimensional Fisher subspace is then computed on the monitored samples to determine if they are from normal or any type of faulty operation.

Case Study

Tennessee Eastman process

In this study, the TEP is simulated under normal or various types of faulty operations and the data set is used to assess the performance of the new LFDA based process

Table 1. Manipulated Variables in the Tennessee Eastman Process

Variable No.	Manipulated Variables
1	D Feed flow valve
2	E Feed flow valve
3	A Feed flow valve
4	A+C Feed flow valve
5	Recycle valve
6	Purge valve
7	Separator valve
8	Stripper valve
9	Steam valve
10	Reactor coolant flow
11	Condenser coolant flow
12	Agitator speed

Table 2. Measurement Variables in the Tennessee Eastman Process

Variable No.	Measurement Variables
1	A Feed rate
2	D Feed rate
3	E Feed rate
4	A+C Feed rate
5	Recycle flow rate
6	Reactor feed rate
7	Reactor pressure
8	Reactor level
9	Reactor temperature
10	Purge rate
11	Separator temperature
12	Separator level
13	Separator pressure
14	Separator underflow
15	Stripper level
16	Stripper pressure
17	Stripper underflow
18	Stripper temperature
19	Stem flow rate
20	Compressor work
21	Reactor coolant temperature
22	Condenser coolant temperature
23	Feed % A
24	Feed % B
25	Feed % C
26	Feed % D
27	Feed % E
28	Feed % F
29	Purge % A
30	Purge % B
31	Purge % C
32	Purge % D
33	Purge % E
34	Purge % F
35	Purge % G
36	Purge % H
37	Product % D
38	Product % E
39	Product % F
40	Product % G
41	Product % H

monitoring approach against the conventional multi-class FDA method. The TEP is composed of four operation units, including an exothermic two-phase reactor, a flash separator, a reboiled stripper and a recycle compressor.[35,36] There are four reactants A, C, D, and E involved in two main reactions to produce two products G and H. Meanwhile, a byproduct F is produced from two additional reactions including the reactants A, D, and E. As shown in Tables 1 and 2, there are total 12 manipulated variables as process inputs and 41 measured variables as outputs, among which the first 22 variables are continuous measurements while the other 19 are composition measurements from gas chromatography with two different sampling rates and pure delay. The decentralized control strategy has been implemented in this TEP with all the control loops operating under closed-loop conditions.[36] The process flow sheet is shown in Figure 2 and fifteen types of predefined process faults are listed in Table 3. As the proposed monitoring approach is designed for continuous process, only the 22 continuous output measurements are selected as monitored variables. Several types of predefined process faults are mixed in different simulation scenarios so that the LFDA based monitoring approach can be

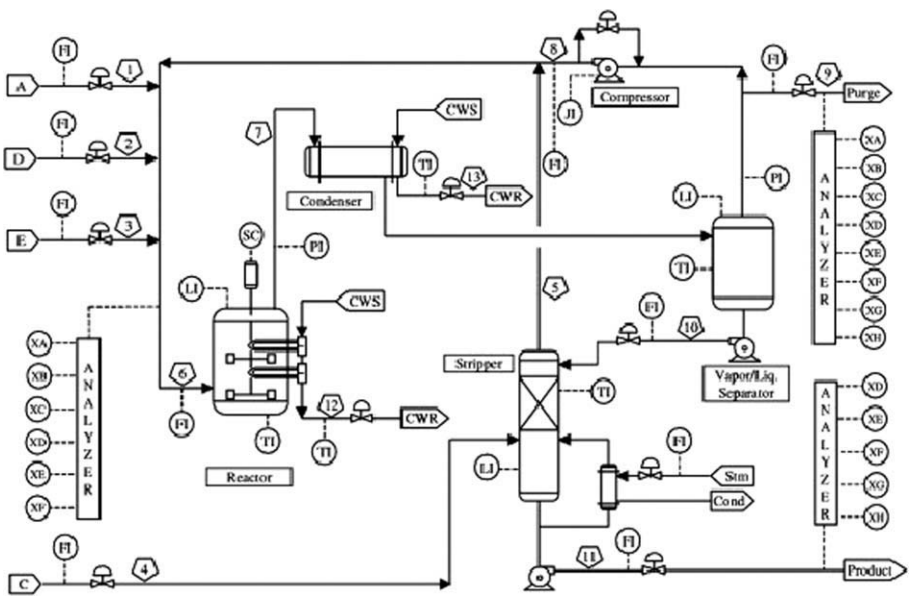

Figure 2. Process flowsheet of Tennessee Eastman chemical process.[35]

Table 3. Pre-defined Process Faults in the Tennessee Eastman Process

Fault No.	Fault Description
1	Step change in A/C feed ratio in Stream 4
2	Step change in B composition in Stream 4
3	Step change in D feed temperature (Stream 3)
4	Step change in reactor cooling water inlet temperature
5	Step change in condenser cooling water inlet temperature
6	Sudden loss of A feed (Stream 1)
7	Stream 4 header pressure loss
8	Random variations in A,B,C compositions in Stream 4
9	Random variations in D feed temperature
10	Random variations in C feed temperature
11	Random variations in reactor cooling water inlet temperature
12	Random variations in condenser cooling water inlet temperature
13	Slow drift in reaction kinetics
14	Reactor cooling water valve sticking
15	Condenser cooling water valve sticking

Table 4. Three Test Cases in the Simulated Tennessee Eastman Process

Case No.	Faulty Scenarios
1	Training data set: Step change in D feed temperature (600th–900th min) Random variations in A,B,C compositions (1200th–1800th min) Test data set: Step change in D feed temperature (420th-600th min)
2	Training data set: Step change in reactor coolant temperature (480th–660th min) Slow drift in reactor kinetics (900th–1350th min) Test data set: Slow drift in reactor kinetics (270th–450th min) Step change in reactor coolant temperature (510th–660th min)
3	Training data set: Sudden loss of A feed (750th–900th min) Random variations in condenser coolant temperature (1050th–1170th min) Slow drift in reactor kinetics (1350th–1650th min) Test data set: Random variations in condenser coolant temperature (540th–690th min) Slow drift in reactor kinetics (840th–1020th min) Sudden loss of A feed (1110th–1260th min)

tested on its capability of detecting and classifying multiple faults concurrent in a process.

Multi-fault process monitoring results

All the three test scenarios are listed in Table 4. In the first simulation scenario, the training data set is composed of both normal and faulty samples. The normal data are generated under the steady-state condition as given in[37] with sampling time of 0.05 h for continuous 10 h. Then a step change in D feed temperature occurs from the 600th min until the 900th min. From the 1200th min, the random variations in A, B, C compositions start and last for 600 min. The test data set includes the first 420 min worth of normal operation data followed by 180 min of faulty data with the step change in D feed temperature. It is noted that the training data set is composed of both normal and faulty

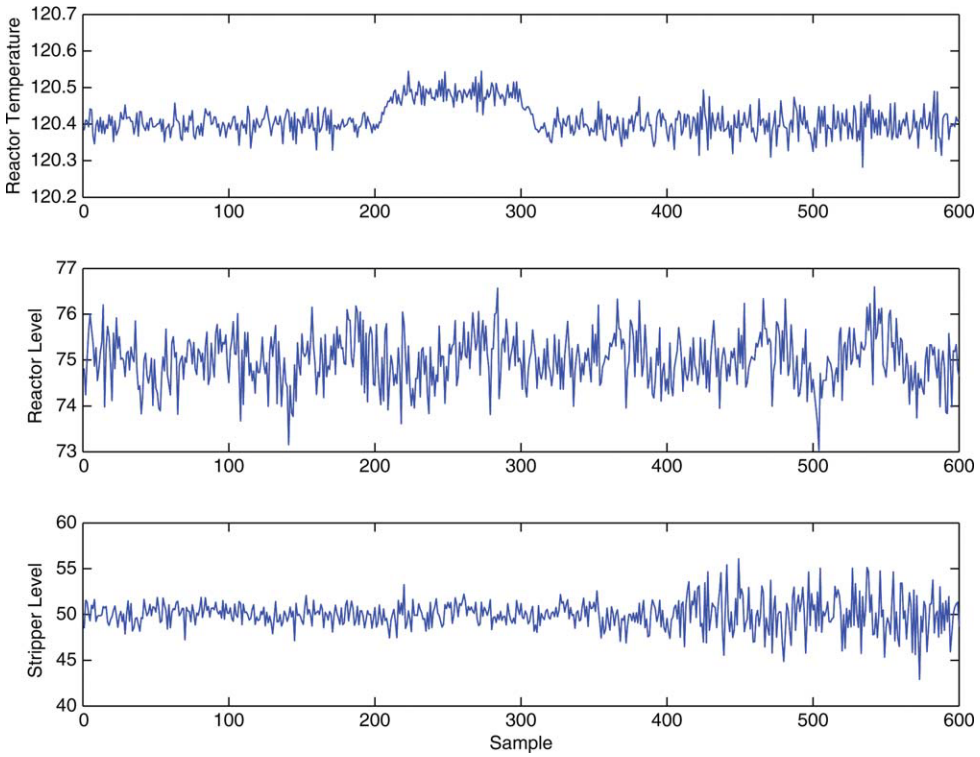

Figure 3. Training data trends of three monitored variables in the first test scenario.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

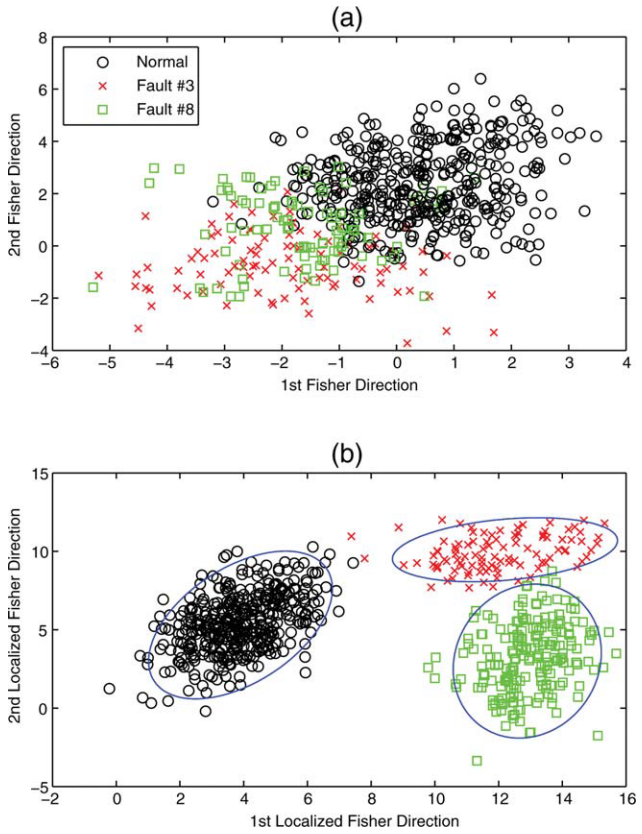

Figure 4. First test scenario: projected training data in (a) Fisher discriminant subspace and (b) localized Fisher discriminant subspace, respectively.

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samples. Therefore, the unsupervised process monitoring methods like PCA and PLS do not apply to such a situation. The training data trends of three monitored variables (reactor temperature, reactor level, and stripper level) are plotted in Figure 3, where the step error or increased variation can be seen in different variables.

As supervised monitoring techniques instead, both FDA and LFDA are able to handle the training data set contaminated with faulty samples. First, the preliminary step of data clustering is utilized to classify the normal and various types of faulty samples in the training set. Then the FDA or LFDA method is implemented on the training set to extract the Fisher or localized Fisher directions for the separation between the normal and multiple faulty clusters. The projected training samples in the two-dimensional Fisher and localized Fisher discriminant subspaces are shown in Figure 4a,b, respectively. It can be seen that the conventional FDA algorithm performs poorly in separating normal and two types of faulty samples. First of all, the normal data cluster has partial overlap with the faulty classes, which can result in significant Type-I and Type-II errors in detecting process faults from normal operation data. Secondly, the two types of process faults are mixed together without any observable separation between them and thereby the fault classification becomes unapproachable. In contrast, the LFDA approach works well to isolate the normal and two types of faulty data within the two-dimensional subspace composed of the first and the second localized Fisher discriminant components. As shown in Figure 4b, not only the normal samples are well separated from the faulty data along the first localized Fisher discriminant direction but also the two faulty classes are isolated from each other with clear boundary in the second localized Fisher discriminant component. Because the abnormal data set contains two different kinds of faults, the within-class multimodality makes the Fisher discriminant directions nonoptimal in separating normal and faulty clusters. On the contrary, the LFDA preserves the multi-Gaussianity within the faulty data while maximizing the separation between the normal and faulty classes. Hence, the normal and multiple faulty clusters can be separated with maximized margin along the leading localized Fisher discriminant directions.

The built FDA and LFDA models are further applied to the test data set to detect the single fault of step change in D feed temperature. The fault detection results of those two methods are compared in Figures 5a,b and the performance indices are summarized in Table 5. As shown in Figure 5a, the FDA method generates significant number of false alarms when the process is actually running at normal state, and total 33 samples are misclassified as faulty ones with the Type-I error of 23.6%. On the other hand, 15 out of the total 60 abnormal points are missed in fault detection and thus

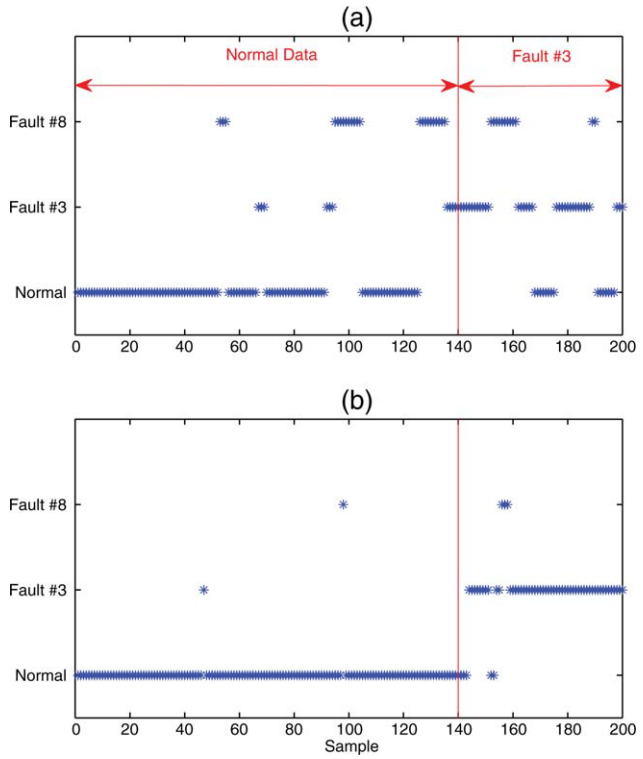

Figure 5. First test scenario: fault detection and classification results using (a) FDA and (b) LFDA methods.

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Table 5. Comparison of Fault Detection and Classification Indices Between FDA and LFDA Methods

	Type-I Error		Type-II Error		Fault Misclassification Rate	
	FDA	LFDA	FDA	LFDA	FDA	LFDA
Case 1	23.6%	1.4%	25%	3.3%	N/A	N/A
Case 2	44.4%	6.7%	10%	6.2%	31.8%	9.8%
Case 3	31.5%	3.1%	12.5%	8.1%	38.6%	2.0%

lead to 25% Type-II error. Furthermore, among the 45 alarmed faulty samples, 12 observations are classified into Fault No. 8 of random variation errors incorrectly. The above poor results indicate that the conventional FDA method is unable to detect even a single type of process fault when the training data set includes multiple kinds of faults. The LFDA based monitoring approach, however, is far superior to the FDA algorithm in predicting the process fault through the multi-fault training model. The Type-I error is as low as 1.4% with only two false alarms among the total 140 normal samples. When the process fault starts at the 141 st sample, the alarm is triggered from the 144 th sample with only 9-min delay. Since then the vast majority of faulty points are correctly classified into Fault No. 3 with only two observations misidentified as normal data and another three points as Fault No. 8. The Type-II error of LFDA approach is 3.3% and far less than that of FDA method. The low Type-I and Type-II detection errors demonstrate that the LFDA based monitoring approach has significantly enhanced fault identification capability.

In the second test case, the 1350-min worth of training set is mingled with normal operating data and two types of process faults, which are step change in reactor coolant temperature and drifting error in reaction kinetics. The faulty data cluster is not only multimodal but also nonstationary due to the dynamic drifting error. Figure 6a shows the projected training data along the first and second Fisher discriminant directions. The two faulty clusters can hardly be separated in the Fisher subspace as most of the samples in those two classes are mixed together. Moreover, the normal data set has significant percentage of samples overlapped by some of the faulty points. As a comparison, the projected points of the three clusters in the localized Fisher subspace occupy fairly isolated areas with only few points crossing the boundary of their own covariance ellipses. It needs to be pointed out that during the preliminary step the non-stationarity of the data segment from Fault No. 13 is detected and then removed by taking the first-order derivative. Further the LFDA algorithm can be utilized to capture the multimodality within the faulty classes while separating the two process faults from the normal cluster. It is obvious from Figure 6b that the LFDA approach leads to a multi-cluster model with high classifiability.

In the test data set, the reaction kinetics starts the slow drifting after the initial 270-min normal operation, and this fault continues for 180 min. Then the process operation returns to the normal condition and remains for another 60 min before a step error is imposed to the reactor coolant temperature. The fault detection and classification results using the FDA and LFDA methods are illustrated in Figures 7a,b. Apparently, the FDA model is unable to identify the faulty classes or even detect the abnormal operation. As given in Table 5, the Type-I error is 44.4% and represents an extremely high false alarm rate. It is unacceptable to encounter such frequent fault alerts during normal process operation as they will cause unnecessary engineer intervention and trouble shooting. The 10% Type-II error, on the other hand, indicates that the fault detection rate reaches 90% and only one-tenth of the faulty samples are missed without triggering any fault alarms. However, the fault classification results further reveals that overall 31.8% of the detected faulty points are categorized into the wrong types of faults. For instance, during the second operation stage when the drifting error is occurring, total 60 faulty samples are captured while 24 of them are misclassified as step error. As opposed to the poor performance of FDA method, the LDFA based monitoring approach successfully detects most of the faulty samples as well as classify the fault types with quite low false alarm rate. The Type-I and Type-II errors are 6.7% and 6.2% , respectively, which are much lower than those of regular FDA method. Among the eight undetected faulty points, five of them are due to the fault detection delay when the operation is shifted from normal condition to Fault No. 13 of drifting error. For the identified faulty points, on the other hand, the fault classification accuracy is

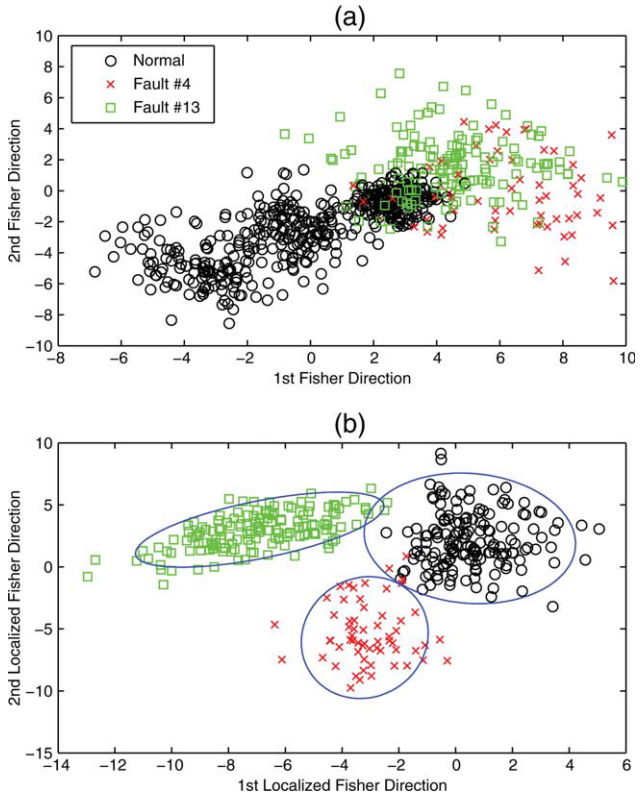

Figure 6. Second test scenario: projected training data in (a) Fisher discriminant subspace and (b) localized Fisher discriminant subspace, respectively.

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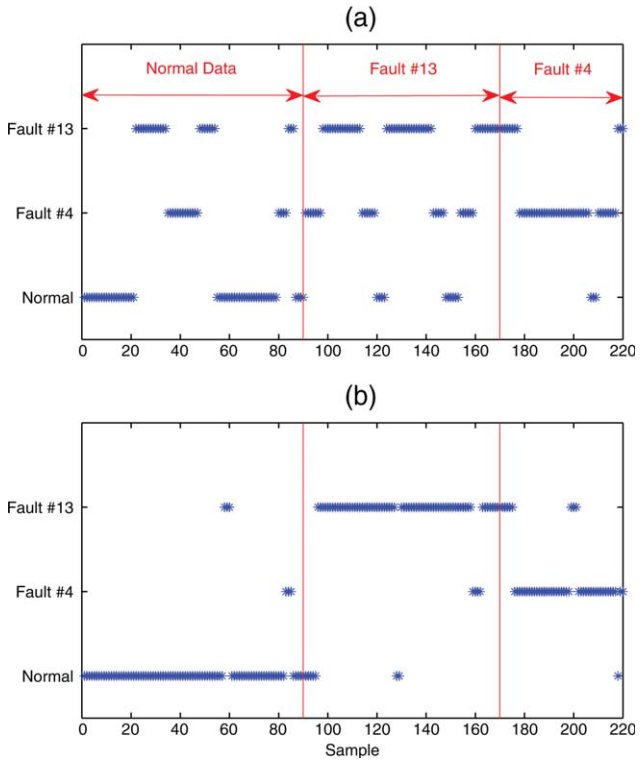

Figure 7. Second test scenario: fault detection and classification results using (a) FDA and (b) LFDA methods.

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as high as 90.2% . The results of this test scenario confirms that the LFDA based monitoring approach can classify the stationary and nonstationary types of faults in addition to its strong fault detection capacity.

The third scenario is designed to further examine the performance of LFDA approach in identifying multiple kinds of faults. In the training set, Fault No. 6 first occurs from the 750th min until the 900th min causing the sudden loss of A feed. Then there is a random variation error in condenser coolant temperature (Fault No. 12) between the 1050th and the 1170th min. In the end, the slow drifting of reaction kinetics (Fault No. 13) starts at the 1350th min and remains for 300 min. During the rest of the time period, the process runs at steady state under normal operating condition. As seen in Figure 8a, the data clusters of normal operation, Faults No. 12 and 13 are heavily mixed with each other in the Fisher subspace so that they can hardly be separated. In the LFDA based classification result instead (see Figure 8b), all the four clusters are nicely classified with substantial margin. The covariance ellipses at 95% confidence level corresponding to the four clusters do not have any overlap with each other, which infers the classification accuracy can be more than 95% by using the LFDA model.

The comparison of the monitoring results on the test data set in Figure 9a,b further verifies the enhanced capability of LFDA approach to detect and classify multiple kinds of process faults. In the first test period with normal operating data, the fault alarms are triggered 56 times leading to a Type-II error of 31.1%. When the process operation is shifted to the second segment with Fault No. 12 of increased random variations in condenser coolant temperature, three faulty samples are not detected at all and another 14 faulty ones are misclassified as Fault No. 6 (sudden loss of A feed) with classification accuracy of only 70.2%. The fault classification is even worse during the fourth test segment when the slow drifting error occurs on the reaction kinetics. There are 26 samples miscategorized into Fault No. 12 and another two points into Fault No. 6 with the total misclassification rate of 51.9%. The high misclassification particularly between Faults No. 12 and 13 is relevant to the fact that the training samples from those two faulty clusters are mostly overlapped in the Fisher subspace. In contrast, the LFDA model causes only three false alarms during the initial normal operation segment with much lower Type-II error of 1.7%. In the second segment, the fault detection rate of LFDA approach reaches 96% with only two faulty points undetected and the remaining faulty samples in this segment are all classified into Fault No. 6 correctly with zero misclassification. The fault classification accuracy during the fourth segment is dramatically improved to 96.3%. For the rest of the test segments, the performance of the LFDA approach excels that of the FDA method in both fault detection and classification. The overall Type-I, Type-II, and fault misclassification errors of LFDA approach are as low as 3.1, 8.1,

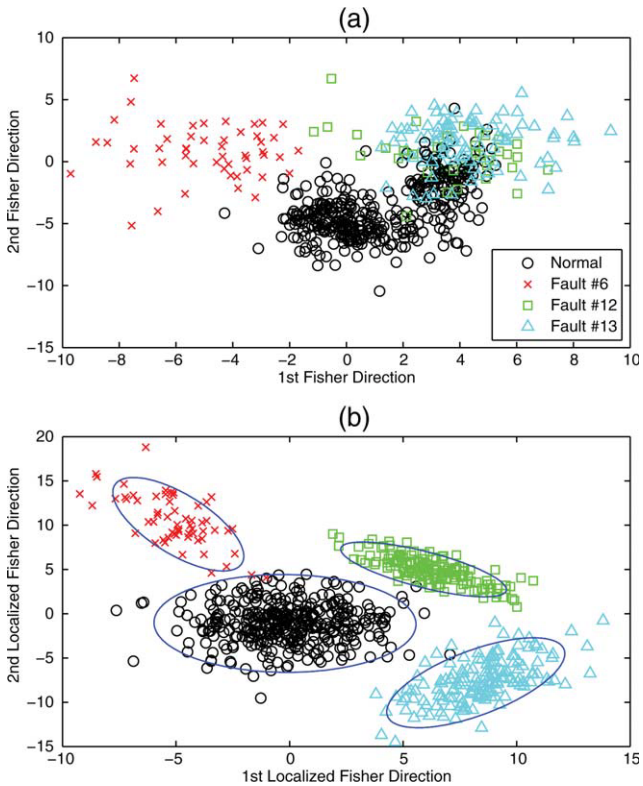

Figure 8. Third test scenario: projected training data in (a) Fisher discriminant subspace and (b) localized Fisher discriminant subspace, respectively.

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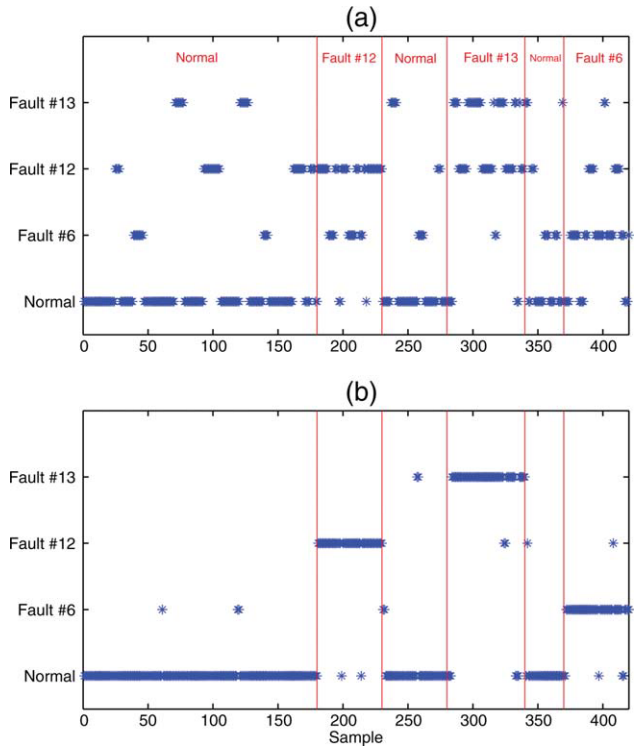

Figure 9. Third test scenario: fault detection and classification results using (a) FDA and (b) LFDA methods.

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and 2.0, whereas the corresponding performance indices of conventional FDA method are 31.5, 12.5, and 38.6. The comparison of these performance indices evidently demonstrates that the LFDA based monitoring approach has strong capability to detect multiple types of process faults as well as classify different faulty clusters with high accuracy that the traditional FDA method is unable to achieve.

Conclusions

A new LFDA based monitoring approach has been proposed in this article to handle the complex processes that contain different kinds of faults. The basic idea is to first conduct the stationarity testing along the operation data and thus remove any identified non-stationarity. Then the GMM is built to isolate the normal and multiple types of faulty clusters. The localized within-class and between-class scatter matrices are further computed to maximize the separation between the normal and faulty classes while preserving the multimodality within the faulty data alone. Therefore, the localized Fisher discriminant function can be used to not only detect the abnormal operation but also classify the various types of faults. Compared with the conventional FDA method, the LFDA based monitoring approach has the following advantages: (i) The multiple faults are considered as a single class to be separated from the normal operation and thus the pairwise strategy is avoided with the higher accuracy of fault detection; (ii) the local structure within the multimodal faulty class is retained so that the classification among different kinds of process faults is significantly enhanced; (iii) both the stationary and nonstationary faults can be handled because the non-stationarity of faulty data is detected and removed during the preprocessing step; (iv) a priori process knowledge is not required on the total number of process faults since the adopted GMM can search for the optimal number of clusters.

The LFDA based monitoring approach is applied to the TEP for fault detection and classification. The result comparison in the three test scenarios indicates that the LFDA approach is far superior to the conventional FDA method in terms of different performance indices including false alarm rate (Type-I error), fault detection rate (Type-II error) and fault misclassification rate. First of all, the LFDA approach can detect the process faults with much higher sensitivity but even fewer false alarms triggered. Secondly, the multiple types of faults are classified with quite high accuracy by using the LFDA approach whereas the FDA algorithm leads to fault misclassification most of the time. Future work may integrate the LFDA approach with the multiway analysis to address the challenging multi-fault detection and classification issues in batch and semibatch processes.

Acknowledgments

The author appreciates the valuable comments and suggestions of the anonymous reviewers.

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Manuscript received Mar. 8, 2010, and revision received Jun. 17, 2010.