Postprint of Multi-mode Batch Process Fault Detection Based on Statistical Difference LPP

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Abstract

To address the non-Gaussian and multimodal characteristics of industrial process data, a multimodal batch process fault detection method based on statistical difference LPP is proposed. First, statistical moment analysis is applied to the batch process training dataset to compute the mean and variance of statistical process variables, transforming unequal-length batches into equal-length statistical measures to ensure that the statistical moments approximately follow a Gaussian distribution. Then, a difference algorithm is employed to convert multimodality into unimodality. Finally, the LPP algorithm is utilized for dimensionality reduction and feature extraction, the T^2 statistic of samples is calculated, and kernel density estimation is used to determine the control limit. For new test sample data after statistical difference processing, projection onto the LPP model is performed, the T^2 statistic of the new data is calculated and compared with the control limit for fault detection. Finally, simulation results on semiconductor process data demonstrate that the proposed algorithm achieves the best fault detection performance, validating the effectiveness of the proposed method.

Full Text

Fault Detection of Multi-Mode Batch Process Based on Statistics Difference LPP

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Abstract

Aiming at the non-Gaussian and multi-mode characteristics inherent in industrial process data, this paper proposes a fault detection method for multi-mode batch processes based on statistics difference locality preserving projections (SDLPP). First, the method of statistical pattern analysis is applied to the batch process training dataset to calculate the mean and variance of statistical process variables, transforming uneven-length batches into equal-length statistics to ensure the statistical pattern approximately obeys a Gaussian distribution. Then, a difference algorithm is employed to convert the multi-mode data into a single mode. Finally, the LPP algorithm is used for dimensionality reduction and feature extraction, the T^2 statistic of samples is calculated, and kernel density estimation is utilized to determine the control limit. For new test sample data, after statistical difference processing, the data are projected onto the LPP model, the T^2 statistic of the new data is calculated, and fault detection is performed by comparing it with the control limit. Simulation results from semiconductor process data demonstrate that the proposed algorithm achieves the best fault detection performance, thereby verifying its effectiveness.

Key Words: multimode batch process; statistics pattern analysis; difference algorithm; locality preserving projections algorithm; fault detection

0 Introduction

With the rapid development of modern industry, fluctuations in raw materials, adjustments in operating points, variations in product specifications, and differences between batches cause frequent changes in production process conditions. This leads to process variables that do not fully obey Gaussian distributions, with their means and covariance structures changing as modes switch. Since traditional principal component analysis (PCA) [1–3] requires data to satisfy the basic characteristic of a single distribution when applied to multi-mode processes, it cannot meet this requirement and also lacks the ability to provide features for non-Gaussian data. Therefore, directly applying the PCA algorithm to batch processes cannot achieve satisfactory detection results.

To address multi-mode problems in industrial production processes, Zhao et al. [4,5] proposed multi-model methods based on PCA and PLS. These methods establish local models for each mode separately for fault detection, but they have certain limitations. After establishing multiple sub-models, online detection requires real-time sample classification, where correct sample 归属划分 is crucial, as erroneous judgment can lead to mismatches between models and test samples, producing incorrect detection results. To overcome this limitation, Ma Hehe et al. [6] from East China University of Science and Technology proposed a local neighborhood standardization (LNS) data processing method that standardizes each sample using the mean and standard deviation of its local neighbors, making the standardized data approximately obey a unimodal distribution. Combined with PCA, they proposed a multi-mode fault detection method: local neighborhood standardization principle component analysis (LNS-PCA). This algorithm treats all modes in the process as a unified whole and establishes a unified fault detection model, which can effectively avoid the need to determine the 归属 of real-time test samples. However, the selection of the neighbor number k in this method has a significant impact on detection results, and the empirically selected k must be based on knowledge of each mode's process.

To compensate for the shortcomings of the LNS-PCA algorithm, Wang et al. [7] proposed a weighted K-neighborhood standardisation PCA (WKNS-PCA) algorithm. This method can make multi-mode process data approximately obey a Gaussian distribution without needing to determine the neighbor parameter k. Compared with LNS-PCA, this algorithm is more scientific, effective, and has superior data processing capabilities. However, both of these algorithms are global algorithms that cannot maintain the local structure of data. To preserve data locality, Hu et al. [8] successfully applied locality preserving projections (LPP) to statistical process monitoring. To better maintain local data structure, Cai et al. [9] proposed orthogonal locality preserving projections (OLPP), which adds an orthogonal constraint condition to LPP and obtains mutually orthogonal projection directions through iterative calculation. Building on this, Guo et al. [10] proposed a dynamic multi-way orthogonal locality preserving projections (DMOLPP) algorithm for batch process fault detection, which combines sliding window technology with orthogonal locality preserving projections to reduce data error reconstruction difficulty while preserving feature information from original training samples. However, these local algorithms cannot handle the multi-mode problem in data.

1 Locality Preserving Projections Algorithm

The LPP algorithm [11-14] is a dimensionality reduction method for extracting data feature information. It can effectively preserve local information by maintaining the structure among neighboring points in the data and is essentially a linear approximation of Laplacian eigenmaps. It is an extension of the LE algorithm with the same objective function but uses explicit linear mapping. The core of the algorithm is to find a transformation matrix $\mathbf{A}$ that projects a series of $\mathbf{X}$ ^{m×n} to $\mathbf{Y}$ ^{l×n}, making $\mathbf{Y}$ represent $\mathbf{X}$ as much as possible. The matrix $\mathbf{A}$ can be obtained by optimizing the following minimization problem:

$$\mathbf{Y} = \mathbf{A}^T\mathbf{X}$$

The optimization problem is:

$$\arg\min_{\mathbf{A}} \sum_{i,j} \|\mathbf{y}_i - \mathbf{y}_j\|^2 W_{ij}$$

Through appropriate transformation, this becomes:

$$\arg\min_{\mathbf{a}} \mathbf{a}^T\mathbf{X}\mathbf{L}\mathbf{X}^T\mathbf{a}$$

Subject to the constraint:

$$\mathbf{a}^T\mathbf{X}\mathbf{D}\mathbf{X}^T\mathbf{a} = 1$$

where **L** is the Laplacian matrix, **L** = **D** - **W**, **W** is the similarity matrix defined on data points, and **D** is a diagonal matrix where **D**_{ii} = Σ_j **W**_{ij}. The elements of **W** are calculated as:

$$W_{ij} = \begin{cases} \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/t) & \text{if } \mathbf{x}_i \text{ and } \mathbf{x}_j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

where the parameter t is selected empirically. Minimizing the objective function ensures that neighboring points **x**_i and **x**_j have projections **y**_i and **y**_j that are also neighbors. Seeking the optimal projection matrix **A** is converted to solving for the eigenvectors corresponding to the smallest eigenvalues of the generalized eigenvalue problem:

$$\mathbf{X}\mathbf{L}\mathbf{X}^T\mathbf{a} = \lambda\mathbf{X}\mathbf{D}\mathbf{X}^T\mathbf{a}$$

Since both **X** **L** **X**^T and **X** **D** **X**^T are symmetric and positive semi-definite, the eigenvectors corresponding to the smallest eigenvalues of the matrix (**X** **D** **X**$^{\mathrm{T})}${-1} **X** **L** **X**^T give the projection matrix **A**.

2 Multi-Mode Batch Process Fault Detection Based on Statistical Difference LPP

To address issues such as incomplete data information and non-Gaussian, multi-mode characteristics caused by multiple operating conditions, this paper attempts to convert the multi-mode problem into a single-mode problem for fault detection. To transform data from multi-mode to single-mode while approximately obeying a Gaussian distribution, improve fault detection performance for uneven-length batch processes, and reduce algorithm complexity, this paper combines statistical pattern analysis (SPA) and proposes a multi-mode batch process fault detection method based on statistics difference locality preserving projections (SDLPP). The idea is to use the SPA algorithm to ensure data approximately obeys a Gaussian distribution, then use the difference algorithm to eliminate multi-mode structure while preserving internal data structure, and finally apply the LPP algorithm to extract data features and maintain local structure, thereby improving fault detection performance for multi-mode batch processes.

2.1 Statistical Pattern Analysis

The method based on statistical pattern analysis [15-18] redefines and measures original batch process data using a statistical pattern matrix composed of statistical eigenvalues. The statistical features used in this paper include mean and variance. Assuming each batch has mean and variance , all statistical features of one batch are combined into a row vector **SP** = [_1, _1, _2, _2, ···, _n, _n]. Thus, the final row vector **SP** formed by superimposing the selected eigenvalues is of equal length. The statistical patterns **SPs** used for modeling are training matrices constructed by superimposing **I** batches of data. Statistical patterns **SPs** can extract batch process features, including process nonlinearity and non-Gaussian characteristics.

2.2 Difference Algorithm

The difference algorithm can eliminate multi-mode structures in data. For the i-th sample **X**_{i,n} in data matrix **X** ^{m×n} (where m represents sampling times and n represents measurement variables), find its nearest neighbor **X**_{k,n} and perform difference operation as follows:

$$\mathbf{D}_i = \mathbf{X}_{i,n} - \mathbf{X}_{k,n}$$

where **D** is the difference matrix.

To verify the effectiveness of the difference algorithm in eliminating multi-mode structures, we compare the results before and after differencing using an artificially synthesized multi-mode numerical example. In this example, each sample has two variables: the first variable x_1 follows a uniform distribution on [0,1], and the second variable x_2 is linearly related to x_1, with specific data generated according to the equation x_2 = x_1 + noise. By appropriate transformation, a numerical example with two modes is obtained. [Figure 1: see original paper] shows the scatter plot of data distribution composed of 400 samples from the two modes, demonstrating that the numerical example is multi-mode. The scatter plot after applying difference operation to this example is shown in [Figure 2: see original paper]. Through comparison between [Figure 1: see original paper] and [Figure 2: see original paper], we can intuitively see that the difference algorithm can transform multi-mode structures into single-mode structures, thereby verifying its effectiveness.

Processing the aforementioned numerical example with the LPP algorithm yields the principal component plot shown in [Figure 3: see original paper]. From [Figure 3: see original paper], we can see that after LPP processing, the data still exhibits two modes, indicating that the LPP algorithm alone cannot eliminate multi-mode structures. Since the difference algorithm can eliminate multi-mode structures, combining statistical pattern analysis, difference algorithm, and locality preserving projections yields the multi-mode batch process fault detection algorithm based on statistics difference LPP. This approach ensures data approximately obeys a Gaussian distribution while using the difference algorithm to eliminate multi-mode structures, providing the data characteristics required by LPP.

The overall flowchart of the multi-mode batch process fault detection based on statistics difference LPP is shown in [Figure 4: see original paper]. The algorithm consists of two parts: model building and fault detection.

a) Model building under normal conditions 1. Collect historical dataset **X**_k(**I** × **J** × **d**) from normal operation, where **I** is the number of batches, **J** is the number of variables, and **d** is the total reflection time of a batch process. 2. Calculate the mean and variance of each batch to obtain row vector **SP**. 3. Superimpose the row vectors **SP** from **I** batches to obtain statistical patterns **SPs**. 4. For each sample in **SPs**, find its nearest neighbor, perform difference operation between the sample and its nearest neighbor to obtain statistical difference matrix **SD**. 5. Select appropriate parameters, apply LPP algorithm to obtain projection matrix **A**, calculate T^2 statistic, and establish LPP model under normal operating conditions. 6. Use kernel density estimation to determine the 95% control limit of the T^2 statistic.

b) Fault detection 1. For new batch data **X**_k^{new} at time k, calculate its mean and variance to obtain **SP**_{new}. 2. Find the nearest neighbor sample of **SP**_{new} in the modeling data, perform difference operation between **SP**_{new} and its nearest neighbor to obtain statistical difference data matrix **SD**_{new}. 3. Project the new sample' s difference matrix onto the LPP model and calculate the T^2 statistic. 4. Determine whether the current process is normal by comparing whether the T^2 statistic exceeds the control limit. If it exceeds the limit, it is a fault sample; otherwise, it is normal.

3 Simulation Example

To verify the effectiveness of the proposed algorithm, eight algorithms—PCA, LPP, DPCA, DLPP, SPCA, SLPP, SDPCA, and SDLPP—were applied to fault detection in semiconductor production process data for comparison, further demonstrating the superiority of the SDLPP algorithm for multi-mode batch process fault detection.

As a well-established industrial process simulation platform, semiconductor production processes have been widely applied in data-driven fault detection research. This paper uses a semiconductor industrial example—the A1 etch process [19-22]—to compare the performance of different fault detection methods. Semiconductor production processes are typical non-linear, time-varying, multi-stage, and multi-mode batch processes. One example (variable EndPt A) demonstrates these characteristics, as shown in [Figure 5: see original paper].

To verify that the SPA algorithm can solve non-Gaussian problems in production processes, the SPA algorithm is applied to the second variable of all batches in the semiconductor uneven-length multi-mode batch process, as shown in [Figure

6: see original paper]. [Figure 6: see original paper] clearly shows that the original variable does not obey a Gaussian distribution, but both the mean and variance of the processed variable approximately obey a Gaussian distribution after SPA processing, thereby verifying the effectiveness of the algorithm.

The semiconductor production process data consists of 108 normal wafers and 20 fault batches. Due to one normal batch (the 12th fault batch) losing a large amount of data, the actual dataset comprises 107 normal batches and 20 fault batches. In this simulation experiment, 96 normal batches were randomly selected as modeling data, the remaining 11 normal batches as validation data, and the 20 fault batches as test data. Seventeen variables were selected from 21 measurement variables as detection variables, as shown in . Each batch has uneven length, with duration between 95-112 seconds.

The 96 uneven-length normal batch data were modeled using PCA, LPP, DPCA, DLPP, SPCA, SLPP, SDPCA, and SDLPP methods, and fault detection was performed on 11 validation batches and 20 fault batches. The number of principal components for all eight algorithms was set to 16. The T^2 detection results of the eight methods are shown in [Figure 7: see original paper], where the dashed lines represent the 95% control limits of the T^2 statistics.

From [Figure 7: see original paper], we can see that under the same condition of principal component selection: - PCA detects all validation data but misses 15 fault data points. - LPP detects all validation data but misses 15 fault data points. - DPCA detects all validation data but misses 13 fault data points. - DLPP detects all validation data but misses 16 fault data points. - SPCA misses 3 validation data points and 13 fault data points. - SLPP misses 3 validation data points and 5 fault data points. - SDPCA detects all validation data but misses 6 fault data points. - SDLPP misses only 1 validation data point and 1 fault data point.

Compared with the traditional LPP algorithm, the detection performance of SLPP is significantly better, verifying the effectiveness of the statistical pattern analysis algorithm. Compared with SPCA and SDPCA, SLPP and SDLPP have better fault detection performance, respectively. This is because SPCA and SDPCA extract global data features, while SLPP and SDLPP extract local data features, improving fault detection performance. Compared with the other seven algorithms, SDLPP achieves the best detection performance, verifying its effectiveness for multi-mode batch process fault detection.

presents the detailed detection result statistics of the eight algorithms for semiconductor process data. As shown in , for multi-mode process fault detection, the SDLPP algorithm can ensure the lowest missed alarm rate while maintaining a relatively low false alarm rate. Compared with the other seven algorithms, SDLPP achieves the best fault detection performance, thereby verifying the algorithm’ s effectiveness.

4 Conclusion

This paper proposes a multi-mode batch process fault detection method based on statistics difference LPP and applies it to process monitoring and fault detection in semiconductor production. The method first uses the statistical pattern of multi-mode batch processes as the training set, then performs difference processing on the training set for multi-mode feature analysis, and finally applies the LPP algorithm for fault detection on the differenced training set. This effectively solves problems of incomplete data information and non-Gaussian, multi-mode characteristics caused by multiple operating conditions. The semiconductor production process is a typical multi-mode batch process. Through comparative simulation studies with PCA, LPP, DPCA, DLPP, SPCA, SLPP, and SDPCA methods, the superiority of the proposed method for multi-mode batch process fault detection is verified.

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Note: Figure translations are in progress. See original paper for figures.