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BATCH/SEMI-BATCH PROCESS FAULT DETECTION AND DIAGNOSIS USING ORTHOGONAL NONLINEAR MULTI-WAY PCA: Application to an emulsion co-polymerization process

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Abstract: In this paper, a fault detection and diagnosis for batch/semi-batch processes by utilizing the PCA scores subspace is proposed. To develop the diagnosis model, first the multi-way unfolding is utilised to transform 3-dimensional batches data onto 2-dimensional data. The process of extracting linear and nonlinear correlations from process data is performed by sequentially applying a linear PCA and an orthogonal nonlinear PCA. As a result the nonlinear structures become more apparent. In addition, the sequential approach reduces the complexity of nonlinear PCA development and compact the information to a very low dimension. The trajectory-boundary-limit crossing point discriminant analysis is proposed to diagnose the fault at the instance of being detected and to improve the diagnostic performance. The validity of the proposed strategy is demonstrated by application to the emulsion copolymerization of styrene/MMA semi-batch process.

Keywords: Fault detection and diagnosis, nonlinear systems, batch processes.

1. INTRODUCTION

Principal component analysis (PCA) has been recognized as important approach in multivariate statistical process monitoring. Its extension called a multi-way PCA (MPCA) has been successfully applied to monitor the batch/semi-batch processes (Nomikos and MacGregor 1994). MPCA allows detecting any deviation in current batch run by comparing to the reference model that has been developed from successful past batch runs. Although the approach is considerably simple, but it is powerful enough as many of its application in industrial batch monitoring had been reported (Kosanovich, Dahl et al. 1996; Lennox, Montague et al. 2001).

Batch/semi-batch processes are highly nonlinear in characteristic. The nonlinearity reduces the efficiency of the data compression which results more principal components are required to explain a certain percentage of the variance. This becomes a major disadvantage for a low-dimension process monitoring. For example, a single bi-variate plot of the first few principal components may not adequate to detect the fault. Despite multi-way unfolding is capable to remove major portion of nonlinearity among batch variables by subtracting the average trajectory from each variable (Nomikos and MacGregor 1994), some nonlinearity remains a problem (Dong and McAvoy 1996). In view this situation, incorporation of nonlinear PCA (NLPCA) into multi-way approach have been proposed (Dong and McAvoy 1996; Lee, Yoo et al. 2004). In the approaches, the nonlinear PCA is directly applied on unfolded data. This strategy requires extensive optimisation computation as the data is unfolded in multi-way approach, it results a very huge input dimension. Especially in neural network based model, if the ratio between the numbers of batches to variables (input dimension) is very low, to construct an optimal neural network model will be very difficult and cumbersome.

Despite significant advantages of PCA in detecting the faults, most of the application of scores plane for fault identification and diagnosis have been confined to continuous processes (Kresta, MacGregor et al. 1991; Raich and Cinar 1997; Dunia and Qin 1998). For a batch process, in early work, the identification and diagnosis are limited to the utilization of the contribution plots (Kourti, Nomikos et al. 1995). Although the contribution plot can be used to identify which variable that contributes most to the out-of-control conditions, the actual cause is not directly diagnosed. Thus, the problem remains incompletely solved, in turns requires plant personnel to interrogate the variable further to diagnose the actual cause. In a typical continuous process, under a process upset, the scores are shifted to a new steady state which forming a new cluster. The classification of each fault cluster strongly relies on the assumption that the data is adequately represented by a normal distribution. However, as the batch/semi-batch process is continuously monitored, under a process upset, the scores do not form a new cluster instead they follow a certain trajectory. In this case, the normality assumption of the data distribution is clearly violated.

In this paper a fault detection and diagnosis for batch/semi-batch process based on the orthogonal nonlinear multi-way PCA is proposed. Rather than applying a nonlinear PCA directly onto unfolded data, a sequential application of a linear PCA and a nonlinear PCA is performed. The nonlinear PCA is applied only on selected principal components of the linear PCA. The main reason is since most of the nonlinearity has been removed, it is better to capture the remaining nonlinearity in more efficient manner. An improved nonlinear PCA called orthogonal nonlinear PCA is employed to improve the explained variance in the first few nonlinear principal components. For the fault diagnosis, a discriminant analysis based on the transient region is employed rather than out-of-boundary region. A single crossing point between the scores trajectory and boundary limit is used to classify the fault. It is expected that the proposed strategy is not only be able to maintain the diagnostic performance, but the foremost advantage is it provides a very fast diagnosis in view to a finite nature of the batch/semi-batch process.

The remaining of this paper is organized as follows. In the next section a brief overview on PCA and multi-way PCA is provided, followed by orthogonal NLPCA. Then, a complete framework for an orthogonal nonlinear multi-way PCA fault detection strategy is introduced. Finally, a discrimination analysis for fault diagnosis by using fault trajectory in the scores space is presented. An example is given to illustrate the performance of the proposed framework before concluding.

2. PRINCIPAL COMPONENTS ANALYSIS

2.1 Linear PCA.

Let X be a data matrix with n number of observations and m number of dimensions. The X matrix can be decomposed into two matrices as follows:

$$X = TP^T = \sum_{i=1}^{m} t_i p_i^T \qquad (1)$$

where T is called scores matrix and P is called loadings matrix. If the variables in X are collinear, the first f principal components can sufficiently explain the variability in data X. Thus, the data X can be written as follow in term of residual, E,

$$X = T_f P_f^{\ T} + E = \sum_{i=1}^{f} t_i p_i^T + E \qquad (2)$$

2.2 Multi-way PCA.

In typical batch processes, the process data is in the form of three-way matrix ($X(I\text{x}J\text{x}K)$). For a typical batch run, j = 1, 2, …, J variables are measured at k = 1, 2, …, K time intervals throughout the batch. There exists similar data on a number of batch run, i = 1, 2, …, I. In MPCA strategy, this matrix must be unfolded into a two-way matrix before PCA can be performed. There are several possible ways to unfold the matrix. In this case, the matrix is unfolded onto matrix $X(I\text{x}JK)$ as shown in figure 1. This allows us to obtain some variability analysis among the batches. In batch processes, some variables follow certain trajectories rather than maintain around specific steady state conditions. Thus, the mean trajectory of each variable can be removed by subtracting the mean of each column of the unfolded matrix. This will remove major portion of nonlinearity among batch variables. PCA then can be performed in conventional way once the unfold matrix has been auto-scaled.

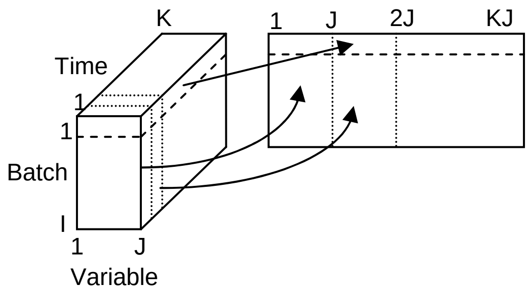

Fig. 1: Multi-way unfolding

One important performance of process monitoring is to detect the un-conformance condition as soon as possible by having on-line monitoring. However, the above unfolded matrix is not completed until the end of the batch. To handle the future missing data problem, a few suggestions have been proposed either by filling with zeros or using the current values, or using PCA projection (Nomikos and MacGregor 1995).

2.3 Nonlinear PCA.

For linearly correlated process data, linear PCA as mentioned above performs well to reduce the dimension of process data. For nonlinearly correlated process data Kramer has proposed a nonlinear PCA based on autoassociative neural network (Kramer 1991). The autoassociative neural network employs a feedforward structure with the bottleneck layer to represent the nonlinear principal components as shown in Figure 2. The overall structure consists of three hidden layers excluding input and output layers. A training procedure is conducted to perform identity mapping by reproducing the network input at the output layer. The trained network is split into two networks, mapping network which consists of input, 1st hidden and bottleneck (2nd hidden) layers, and de-mapping network which consists of 3rd hidden and output layers. NLPCA will be represented by the output of the mapping network. If the network training is properly conducted and the reasonable approximation has been achieved, the data input features must be well represented by the bottleneck layer.

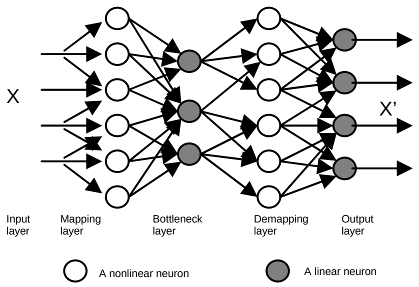

Fig. 2: Autoassociative NN Nonlinear PCA

2.4 Orthogonal Nonlinear PCA.

The NLPCA mentioned above shows one of the characteristics of linear PCA that it is capable of projecting the data to a lower dimension. Another important characteristic of linear PCA is that the first principal component always captures the highest variance of the input data followed by the second and so on. In NLPCA, the data information tends to be evenly distributed among the principal components (Chessari, Barton et al. 1995). In view of this drawback, a training algorithm using Gram-Schmidt process for NLPCA has been proposed in which the nonlinear scores produced are orthogonal at the end of training session(Chessari, Barton et al. 1995).

Although the Gram Schmidt scheme conceptually can provide some meaningful remedies for the orthogonality, in practice it suffers a constraint of trade-off between the main objective (overall convergence) and the secondary objective (orthogonal principal components). In the worst scenario, the orthogonal property may be severely affected as the main objective cannot be scarified at all. Otherwise, the network is not able to represent the data adequately. In view of orthogonal requirement and the drawbacks associated with the Gram-Schmidt approach, an alternative approach to orthogonal nonlinear principal component analysis is proposed. This approach utilizes the Hammerstein type model concept by incorporating a linear PCA model into the NLPCA strategy. In the proposed model formulation, the nonlinear and linear parts are separated into two blocks as shown in Figure 3.

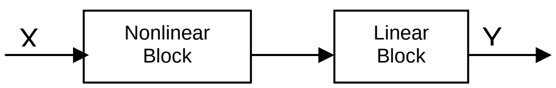

Fig. 3: Conceptual model architecture

In NLPCA, the bottleneck layer neurons are considered to be the principal components loadings, but they do not posses the orthogonal property. In order to build the orthogonal property on the model, a linear PCA module is incorporated as shown in Figure 4. In this case, the mapping network of NLPCA is the nonlinear block while the linear PCA is the linear block.

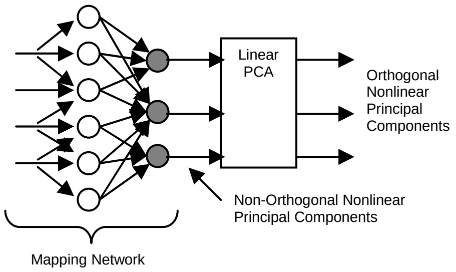

Fig. 4: Orthogonal Nonlinear PCA

In this proposal, the bottleneck layer nodes are called non-orthogonal nonlinear principal components and their outputs are called non-orthogonal scores. When linear PCA is applied on non-orthogonal score, it will produce orthogonal nonlinear principal components and orthogonal scores respectively. For the bottleneck layer in NLPCA, either a linear or nonlinear function can be used (Kramer 1991).

Let T be the non-orthogonal nonlinear scores matrix generated at the output of bottleneck layer. Thus, the non-orthogonal matrix T can be transformed into an orthogonal matrix U by

$$T = UP^T \qquad (3)$$

where P is the eigenvector matrix.

An additional advantage of this approach compared to conventional NLPCA is that the specified number of bottleneck layer neurons can be relaxed as long as the number is reasonably selected. In a conventional NLPCA, it is necessary to optimize the number of neurons in bottleneck layer to the optimal minimum value.

3. FAULT DETECTION

In our proposed strategy, the monitoring is performed by sequentially performing the linear PCA followed by the nonlinear PCA. Only the first few linear principal components are utilised to develop the nonlinear PCA. The orthogonal nonlinear PCA is utilised to improve the distinct characteristics among the nonlinear principal components. The strategy is depicted in Figure 5.

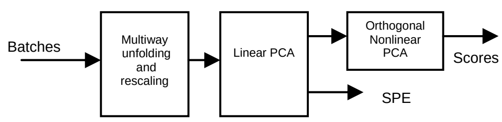

Fig. 5: Nonlinear Multi-way PCA Strategy

Using all retained principal components to develop nonlinear PCA model will not add any additional improvement. In spite it may over-shadow the remaining nonlinearity characteristics. There is no definite criterion on how few the number of principal components to be chosen. In this study, firstly we apply Jollife's approach (0.7 of average eigenvalues) to decide how many principal components to be retained for scores and squared prediction error (SPE) analysis (Jolliffe 1986). This is simply to screen unnecessary principal components since total principal components number is very large (equal to input dimension). Based on the retained principal components, the number of PC that explain 50~70% of data variability will be used to develop the nonlinear PCA model. Alternatively, a cross-validation approach can be used to decide the number of principal components used for nonlinear PCA modelling. With this approach, a ratio between the numbers of batches to variables (input dimension) will be tremendously improved for nonlinear PCA model development. For a SPE analysis (Q-Statistics) a similar approach and procedure in conventional MPCA approach is utilised. However, the significance of applying nonlinear PCA on the selected PC depends on the data variability distribution. If 50% explained variance constitutes a very small PC number, it clearly indicates that the nonlinearity is very minimal and the nonlinear PCA should not be applied.

Once appropriate model has been developed, the fault can be detected by testing the future data based on the Hotelling's T^2 statistics. Assuming that the multivariate normal distribution adequately represents the scores distribution, the confidence limits for T^2 can be calculated using *F*-distribution (Tracy, Young et al. 1992). For a SPE analysis (*Q*-Statistics) a similar approach and procedure in conventional MPCA approach is utilised. The critical value for *Q*-Statistic can be calculated by approximating the distribution as the quadratic form of a normal distribution (Jackson and Mudholkar 1979).

4. FAULT DIAGNOSIS

The orthogonal nonlinear multi-way PCA model developed in the previous section provides a good platform for fault diagnosis in the scores subspace. It provides low-dimensional principal components which are sensitive enough to faults.

The envelope of normal operating region (NOR) described by three principal components scores is illustrated in Figure 6. All points encapsulated by the sphere are considered statistically in-control with respect to scores space. For a continuous process, under a process upset, the scores are shifted to a new steady state which forming a new cluster as marked by the triangle (fault 1). Then the statistical analysis is performed on the new cluster to classify each different fault. The fault diagnosis can be performed by discriminating the test cluster mean against the known clusters mean.

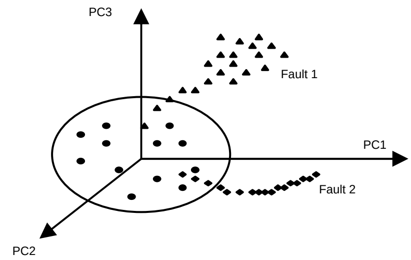

Fig. 6: Normal Operating Envelope

However, in on-line batch/semi-batch process monitoring, the fault is represented by a trajectory as marked by the diamond (fault 2). There is no new steady state cluster is attained in which it violates the vital assumption of the normality of the data distribution. As a result the cluster population mean approach will not work properly. The discriminant analysis must be performed on the trajectory rather than the cluster for batch/semi-batch processes. In this study, the crossing point between the trajectory of faulty batch and the boundary limits is proposed to perform the discriminant analysis. This representation is considerably acceptable because the same faults produce the same effects. Eventually, they will be characterized by the same trajectories in the scores subspace. Since the batch/semi-batch process is a finite process in nature, it is very essential to diagnose the problem as soon as the fault is detected. Thus examining the transient region will give much advantage rather than conducting an analysis on abnormal region. The process model and its boundary limit must be defined by using the reference data of past successful batches. The reference data must represent normal operating conditions and should be free from any fault or abnormality. Then each fault will be classified by the crossing point between its score trajectory and the boundary limit.

The crossing point can be determined when the calculated T^2 at time *i* is equal to the T^2-statistical threshold as calculated in the fault detection scheme. Then the future fault is diagnosed by discriminating its crossing point to the crossing points of known faults. The discriminant statement is minimizing the Euclidean distance between the two points of scaled scores as follows:

$$\min_j \left\| a - b_j \right\|_2 \qquad (4)$$

where *a* is the crossing test point and *b* is the reference crossing points of known fault *j*.

Since the boundary limits are utilised to represent the trajectory, the proposed discriminant approach inherits the good statistical properties itself. The fault diagnosis can be performed at different level of confidence limits. The lower limit gives a faster diagnosis with less confidence while the higher limit validates the lower limit observations. Although a boundary limit less than 90% confidence is rarely used, but it is quite useful as a guideline to perform a routine preventive checking to ensure the process is adequately controlled and operated.

5. CASE STUDY

In order to demonstrate the proposed process monitoring strategy, a well developed mechanistic model of styrene/MMA emulsion copolymerisation semi-batch process is utilised (Alhamad, Romagnoli et al. 2005). There are 8 variables being measured and sampling is performed for every 30 sec (150 time intervals) of 4500 sec batch run. The process is seeded for 1500 sec before the continuous feeds are introduced. Autocorrelations are added to all system feeds and temperature. 30 good batches are simulated to create a reference batches to build the orthogonal nonlinear MPCA model. Variations are introduced in each good batch by random variations in initial charges within acceptable limits.

The main objective of this process is to produce a polymer product with a specific bi-modal particle size distribution (PSD). Any significant changes in monomers, surfactant and initiator conditions will distort the required bi-modal PSD. Two abnormal batches are created. For the first batch, the surfactant initial charge is set at 20% below the base recipe. As the process is under surfactant starvation, there are not enough micelles being produced for new nucleation. Thus most of the monomers favour in the particle growth rate in which it shifts the distribution to a higher particle size range. This eventually distorts the required bi-modal distribution. For the second batch, a 50% step drop in surfactant feed flow rate is simulated at the middle of the batch run.

In general, the overall monitoring is usually performed by using an adequate number of principal components regardless the strategies used. However, the significant advantage of the proposed strategy is in low-dimensional monitoring. If each principal component is individually sensitive enough to detect the fault, this advantage could be exploited to extract more information regarding the fault. One of important exploitations is in a fault diagnosis. Thus, the performance of proposed nonlinear strategy is evaluated by performing an on-line monitoring on a single principal component. For future data substitutions, the simplest approach (zero deviation) is utilised. The nonlinear MPCA strategy performance is compared with the conventional MPCA strategy for a comparison purpose. Solid line and dotted line in Figure 7 and 8 represent nonlinear and linear strategy respectively. All scores are scaled to zero means and unit variance. A simple 99% limit is calculated based on assumption the scaled scores follow the normal distribution.

Figure 7 shows a T^2 plot for the first fault batch. In this case, the linear strategy fails to detect the fault since it does not cross the limit. Whereas the proposed orthogonal nonlinear MPCA strategy depicts its superiority by crossing the 99% limit at the middle of batch run.

The T^2 plot for the second fault batch is illustrated in Figure 8. As the surfactant feed is reduced at the middle of the batch run, the nonlinear strategy responses faster than linear strategy and predicts that the product is off-specification by crossing the 99% limit before the batch run ends. Whereas the linear strategy response is much slower, resulting the off-specification in product cannot be highlighted.

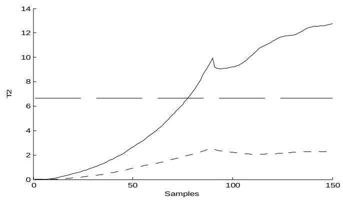

Fig. 6: T^2 plot for the first fault

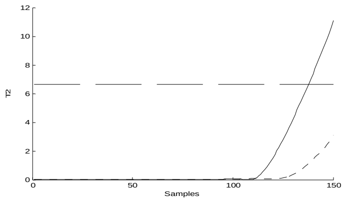

Fig. 7: T^2 plot for the second fault

To test the performance of the proposed framework of fault diagnosis for batch/semi-batch processes, the additional 25 abnormal batches are simulated. There are five fault classes (FA, FB, FC, FD and FE) and in each class contains five batches which have been numbered from 1 to 5. FA, FB and FC belong to initial condition problems while FD and FE belong to faults that occur in the middle of semi-batch run. Each batch is assigned with different common variation and fault magnitude which is randomly assigned. For fault FD and FE, the timing of fault occurrence is also randomly assigned. This setting is very important due to the fact that the faults in the same class occur at different magnitude and time. In general, each fault is considered unique although they belong to same category. The first batch of each fault class is considered as the fault reference set while the remaining four batches are considered as the test sets. Three principal components are utilised to build the discriminant model. Three different boundary levels (70%, 90% and 99%) are utilised to calculate the cross-point.

Table 1 shows the result of the diagnostic decision. In general the overall performance is satisfactory with an overall diagnosis success rate (DSR) is 82%. The diagnostic performances for 90% and 99% boundary limit are equal at 85% DSR. However as a lower boundary limit is being utilised (70%) the diagnostic performance is slightly degraded to 75% DSR. Despite this degradation, the performance is still considerably good. Therefore, the lower boundary limit can be utilised as a guideline to conduct a routine preventive check list. Fault C has the best performance with 100% DSR, while fault D and E have the lowest performances. Since the magnitude and the timing of fault D and E are randomly assigned, this increases the complexity of the diagnosis.

Table 1: Diagnostic performance of trajectory-boundary-limit cross point approach

	Test Set												DSR			
	1			2			3			4						
Fault class	70%	90%	99%	70%	90%	99%	70%	90%	99%	70%	90%	99%	70%	90%	99%	Overall
FA	FE	FE	FE	✓	✓	✓	✓	✓	✓	✓	✓	✓	0.75	0.75	0.75	0.75
FB	✓	✓	FC	✓	✓	✓	✓	✓	✓	✓	✓	✓	1	1	0.75	0.92
FC	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	1	1	1	1
FD	FE	✓	✓	✓	✓	✓	FA	✓	✓	FB	FB	FB	0.25	0.75	0.75	0.58
FE	✓	✓	✓	✓	✓	✓	✓	✓	✓	FA	FE	✓	0.75	0.75	1	0.67
DSR	0.6	0.8	0.6	1	1	1	0.8	1	1	0.6	0.6	0.8	0.75	0.85	0.85	0.82

As the incorporation of O-NLPCA improves the fault detection sensitivity as has been illustrated in the above, the trajectory-boundary-limit cross point strategy improves the diagnostic effectiveness. To illustrate this advantage, a comparison study to the conventional PCA fault diagnosis approach is carried out. With the multi-way unfolding and orthogonal nonlinear PCA approaches are preserved, the diagnostic analysis is performed by discriminating between the populations means. Only the scores that exceeding the boundary limits are used to calculate the population mean. Each fault population mean is derived from the same model rather than being derived on its individual model. The single-model PCA can significantly outperform the multi-model PCA for diagnosing faults because it utilizes information from all fault classes and projects the data onto the same dimensions for each class (Chiang, Braatz et al. 2001). In this comparison, 90% boundary limit is utilised and the diagnostic is performed only after a complete run. Table 2 shows the diagnostic decision for the conventional PCA approach.

Table 2: Diagnostic performance of population means approach

Fault class	Test Set				DSR
	1	2	3	4	
FA	✓	✓	✓	✓	1
FB	FE	FE	✓	FE	0.25
FC	✓	✓	✓	✓	1
FD	✓	✓	FA	FB	0.5
FE	✓	✓	✓	✓	1
DSR	0.8	0.8	0.8	0.6	**0.75**

Comparing Table 2 content to Table 1 content (for 90% limit), the overall performance of proposed trajectory-boundary limit cross points is better with 85% overall DSR compared to conventional PCA with 75% overall DSR. For the proposed method, the diagnostic performance is considerably consistent through out the fault classes. For the conventional method, it has a bias superior performance towards particular faults where three fault classes (FA, FC and FE) have 100% DSR. However, the most significant advantage of the proposed discriminant approach is the faults are diagnosed as soon as they are being detected. Therefore, the operator will have an ample time to take a proper corrective action.

6. CONCLUSION

In this paper the framework of fault detection and diagnosis for batch/semi-batch processes has been presented. The strategy utilises a sequential application of PCA and orthogonal nonlinear PCA which captures the nonlinearity characteristic in an efficient manner. In addition, the sequential approach reduces the complexity of nonlinear PCA development and compact the information to a very low dimension. The trajectory-boundary limit crossing point discriminant analysis has been proposed to improve the diagnostic performance and foremost the fault is diagnosed as it is being detected.

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