Subspace identification for two-dimensional dynamic batch process statistical monitoring

Yuan Yao, Furong Gao*

Department of Chemical Engineering, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong SAR, People’s Republic of China

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Abstract

Dynamics are inherent characteristics of batch processes, which may be not only within a batch, but also from batch to batch. Two-dimensional dynamic principal component analysis (2-D-DPCA) method [Lu, N., Yao, Y., Gao, F., 2005. Two-dimensional dynamic PCA for batch process monitoring. AIChE Journal 51, 3300–3304] can model both kinds of batch dynamics, but may lead to the inclusion of large number of lagged variables and make the contribution plot difficult to read. To solve this problem, subspace identification technique is combined with 2-D-DPCA in this paper. The state space model of a 2-D batch process can be identified with canonical variate analysis (CVA) method based on the auto-determined support region (ROS). In 2-D-DPCA modeling, the utilization of state variables instead of lagged process variables reduces the number of variables and provides a clearer contribution plot for fault diagnosis.

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1. Introduction

Batch processes are widely applied in today’s industries to produce high-value-added products and meet the marking requirements which change frequently. To ensure the operation safety and product quality, multivariate statistical process modeling methods, such as principal component analysis (PCA) (Jackson, 1991), are extended from continuous process monitoring to batch process monitoring (Nomikos and MacGregor, 1994; Wold et al., 1996; Rännar et al., 1998; Lu et al., 2004). However, these methods are proposed based on the assumption of batch independency, which may not hold for many practical batch processes.

Dynamics are inherent characteristics of batch processes, which may exist not only within a batch but also from batch to batch. Many possible reasons may cause both types of batch dynamics, such as, the slow property changing of feed stocks, the drifting of process characteristics, process controllers designed in the manner of run-to-run adjustment, and the effects of slow response variables. Such batch process dynamics can be viewed as a kind of two-dimensional (2-D) dynamics including time-wise dimension and batch-wise dimension and can be described by a 2-D model structure. Based on such an idea, a 2-D dynamic principal component analysis (2-D-DPCA) method has been developed for batch process modeling and monitoring (Li et al., 2005), which integrates PCA into a 2-D model structure. After a proper determination of the support region (ROS), the 2-D dynamic information and cross-correlations among variables can be simultaneously extracted by performing PCA on an expanded data matrix which include both current variables and lagged variables in the ROS. The 2-D-DPCA method can provide efficient detection of on-line faults. Even small changes in correlation or process drifts can be detected effectively in both score and residual spaces of 2-D-DPCA (Lu et al., 2005; Yao and Gao, 2007). An automatic ROS determination algorithm has also been developed by the authors (Yao et al., 2007).

However, the 2-D-DPCA method incorporates a large number of lagged variables. In many industrial processes, there are dozens of process variables or even more. The inclusion of lagged variables can lead to a further significant increase of the number of variables. Although the similar problem has been analyzed and solved in dynamic continuous process monitoring and fault diagnosis (Treasure et al., 2004; Li et al., 2005), batch processes with 2-D dynamics have their own characteristics which are need to be considered.

In this paper, subspace identification (SI) technique is utilized to reduce the number of variables before 2-D-DPCA modeling. First, the ROS is determined by the auto-determination method. Then, the state space model of a 2-D batch process is identified with canonical variate analysis (CVA) method based on such ROS. The state variables are used instead of lagged process variables in 2-D-DPCA modeling of 2-D batch dynamics.
The paper is organized in the following way. In the next section, the preliminaries are introduced, including the review of 2-D-DPCA method, related subspace identification techniques and the existing combination method of PCA and subspace identification. Then, in Section 3, the subspace identification based 2-D-DPCA modeling method is proposed and described in details. In Section 4, simulations are given to show the benefit of the proposed method in fault diagnosis. Finally, conclusions are drawn.

2. Preliminaries

2.1. 2-D-DPCA

As mentioned in the first section, 2-D dynamics are common in many batch processes. To monitor the 2-D dynamic batch processes better, a parsimonious 2-D time series model structure is utilized together with PCA technique. This method is called 2-D-DPCA.

When 2-D dynamics exist, the current measurements are dependent not only on lagged measurements in the past time direction in the same batch, but also on lagged measurements in some past batches. Such lagged variables form a region which can reflect 2-D dynamic features of processes. This region is called the support region or the region of support (ROS). To build a good 2-D-DPCA model, an important step is to determine the ROS reasonably. A data-based ROS auto-determination method has been designed to achieve this objective. First, the lagged variables which have significant correlations with current sample are selected as components of a candidate region. This region is also called the initial ROS. The target proper ROS then can be obtained by eliminating unnecessary independent variables in the initial ROS. Iterative backward elimination procedures are designed to accomplish this task. In each run, a regression model is built to relate the candidate independent variables to current sample’s value. An index, which is a model evaluation criterion, is calculated for each regression model. Then, one independent variable which contributes least to the prediction is eliminated from the candidate region based on the model coefficients in each run. The above procedures are iterated. In the end, the best choice of the ROS is determined based on the comparison of the index values calculated during the iteration. Fig. 1 gives an illustration of initial ROS and proper ROS. For more details about ROS auto-determination, please refer to our previous work (Yao et al., 2007).

After the ROS is determined, an expanded data matrix is formed by including all the lagged measurements in ROS, together with current measurements. Then, PCA algorithm is performed on such matrix. Thus, the original data matrix is divided into two subspaces. Score space extracts systematic variation information, including both 2-D dynamics and cross-correlation information among variables. Measurement noises are retained in residual space. Therefore, SPE statistic and corresponding control limits can be calculated in order to perform process monitoring in residual space. The details of 2-D-DPCA modeling and SPE based monitoring are illustrated in Lu et al. (2005). The dynamics information retained in score space breaks the statistical basis of $T^2$ statistic based monitoring which requires time independence of the score variables. Therefore, 2-D multivariate score autoregressive (AR) filters are designed to remove most autocorrelations and cross-correlations in score space. Then, the $T^2$ statistic and its corresponding control limits can be calculated more reasonably based on the filtered scores (Yao and Gao, 2007). Thus, both residual and score space are monitored by 2-D-DPCA batch process model.

After a fault is detected by the $T^2$ or SPE control plot, fault diagnosis is necessary to find out the reason of the abnormal behavior. Contribution plots (Miller et al., 1998) are useful tools in fault diagnosis. When applied, the contribution of each PC or variable is often plotted on a bar plot which can make diagnosis visually. The calculations and effects of confidence limits for contribution plots are discussed by Conlin et al. (2000). Variable reconstruction (Dunia and Qin, 1998; Lieftucht et al., 2006) is another widely applied method in fault diagnosis. This method reconstructs each process variable in turn and compares the $T^2$ or SPE statistics before and after reconstruction to find out the faulty variables.

However, the proposed 2-D-DPCA method still has shortcomings. Recently, Treasure et al. (2004) discussed the shortcoming of dynamic PCA (DPCA) which makes use of a time series model structure. It is discussed that although the large number of lagged variables does not cause difficulty in establishing the univariate statistics, such as SPE, for abnormal behaviors monitoring, the fault diagnosis with contribution plot becomes more difficult. Similar to DPCA, 2-D-DPCA which utilizes a 2-D time series model structure also incorporates lagged variables into modeling. Since all lagged variables in ROS should be included in the expanded matrix for PCA decomposition, the number of lagged variables may be rather large, and make the contribution plots even much messier and much harder to read than in the 1-D cases. For the same reason, the computation burden of variable reconstruction is also increased largely. This problem will be solved in the later part of this paper.

![Fig. 1. Illustration of initial ROS and proper ROS.](image-url)
2.2. Related works on subspace identification

The basic idea of subspace model identification is to determine a set of state variables for process dynamics description. The state variables can be defined as "the minimum amount of information about the past history of a system which is required to predict the future motion" (Åström, 1970). The number of state variables produced is much smaller than the number of lagged variables used in time series model structure.

A state space model describing a one-dimensional dynamic process can be identified as

\[ \mathbf{x}(k+1) = A\mathbf{x}(k) + B\mathbf{u}(k) + \mathbf{e}(k), \]
\[ \mathbf{y}(k) = C\mathbf{x}(k) + D\mathbf{u}(k) + \mathbf{e}(k), \quad (1) \]

where \( \mathbf{y} \) is the vector of output variables, \( \mathbf{u} \) is the vector of input variables, \( \mathbf{x} \) is the vector of state variables, \( \mathbf{e} \) is the vector of state noise variables, \( \mathbf{e} \) is the vector of measurement errors and \( k \) is sampling index.

Most widely used techniques for subspace identification include CVA, partial least squares (PLS), numerical algorithms for state space subspace system identification (N4SID), balanced realization (BR) and so on. Some research works compared different subspace identification methods and CVA is found to outperform the other algorithms (Negiz and Cinar, 1997; Juricek et al., 1998, 2002), with better model stability and less number of state variables.

CVA is an application of canonical correlation analysis (CCA) (Hotelling, 1936) on process model identification. CCA models the correlation structure between two groups of multivariate data \( A \) and \( B \), and finds the sets of orthogonal canonical latent variables in both data spaces which are most correlated. Each pair of canonical latent variables is called a canonical pair. The mathematical expression of canonical correlation regression (CCR) is similar to PLS regression. But CCR does not care about the covariance information among the variables in input data space \( A \) while finding the direction that yield maximum correlation information, so it can achieve same prediction accuracy with PLS using fewer latent variables.

Larimore (1997) utilized CVA in subspace identification firstly. An important concept of the subspace identification with CVA is the past and future of a process. Suppose the output variables at time \( k \) is \( \mathbf{y}(k) \) and the input variables at time \( k \) is \( \mathbf{u}(k) \). At each time \( k \), the past vector \( \mathbf{p}(k) \) consists of the past outsputs and inputs with length \( d \) lags, and the future vector \( \mathbf{f}(k) \) consists of the outputs at time \( k \) or later.

\[ \mathbf{p}(k) = (\mathbf{y}(k-1)^T, \mathbf{y}(k-2)^T, ..., \mathbf{y}(k-d)^T, \mathbf{u}(k-1)^T, \mathbf{u}(k-2)^T, ..., \mathbf{u}(k-d)^T)^T, \quad (2) \]
\[ \mathbf{f}(k) = (\mathbf{y}(k+1)^T, ..., \mathbf{y}(k+1)^T)^T. \quad (3) \]

The state variables should summarize the information in \( \mathbf{p}(k) \) with lower (hopefully lowest) dimension space to predict \( \mathbf{f}(k) \). So CCA is performed on \( \mathbf{p}(k) \) and \( \mathbf{f}(k) \), and the first \( r \) canonical variables of \( \mathbf{p}(k) \) which extract most correlation information are chosen as state variables. Each state variable is a linear combination of the past process variables. There are several parameters need to be specified in CVA. Akaike (1976) proposed a method to choose the number \( d \) in Eq. (2). And the optimal state order \( r \) can be chosen based on Akaike information criterion (AIC) (Akaike, 1974).

2.3. DPCA using subspace identification

Treasure et al. (2004) combined subspace identification method with DPCA to solve the problem caused by large number of lagged variables which have been introduced in Section 2.1. Later, Li et al. (2005) improved the work. In their work, the N4SID algorithm is utilized to identify the process subspace model. Then PCA is performed on a matrix \( Z \) formulated as

\[ Z = [\mathbf{Y}, \mathbf{U}, \mathbf{X}], \quad (4) \]

where \( \mathbf{Y} \) is the matrix of output variables, \( \mathbf{U} \) is the matrix of input variables and \( \mathbf{X} \) is the matrix of state variables. Therefore, the state variables are included in the expanded matrix instead of lagged variables. Thus, the number of variables shown on contribution plots is reduced significantly.

3. 2-D-DPCA combined with subspace identification

3.1. Basic idea and challenges

To alleviate the shortcoming of 2-D-DPCA discussed in Section 2.1, a combination method of 2-D-DPCA and subspace identification is proposed here. The basic idea is as following. First, the state variables are calculated with subspace identification method to extract 2-D dynamic information from history batch process data. Then, state variables are incorporated into an expanded data matrix instead of the 2-D lagged variables for 2-D-DPCA modeling. Then, the univariate statistics SPE and \( T^2 \) can be calculated for online process monitoring. The idea is similar to the one in the works of Treasure et al. (2004) and Li et al. (2005). However, this is not a simple application of their works. We need to know how to calculate state variables properly in the particular cases of 2-D batch process modeling. There are two requirements to meet. First, the state variables should reflect 2-D dynamic information correctly and sufficiently. Second, a minimal number of state variables is preferred.

A question may be asked is why not use subspace model directly in online monitoring without the 2-D-DPCA step. The answer is that subspace model only focuses on the model prediction ability without looking at the correlation structure among process variables. As mentioned in Shi and MacGregor's work (2000), "for process identification, SMI methods which ignore the covariance structure of the input space and focus only on the correlation with the outputs" yield better results with the smallest numbers of latent or state variables". "For process monitoring, latent variable methods (LVM) which also model the covariance structure of the past variables space are required". So the combination of 2-D-DPCA and subspace identification is needed.

3.2. State variables calculation for 2-D batch processes

In this work, CVA is chosen to identify the state variables for batch processes with 2-D dynamics. As mentioned before, it has several advantages over other algorithms, including that it is most possible to provide minimal number of state variables while extracting entire process dynamic information.

As indicated in Section 2.1, the 2-D dynamics of a batch process can be reflected by the correlations between current measurements and past measurements in the ROS. This gives an indication that, if such correlations can be extracted with a small number of latent variables, these latent variables are suitable to be chosen as the state variables. Performing CCA is a best choice, since it yields maximum correlation information between two data sets with a minimal number of canonical latent variables.

Suppose there is no process input. Here, we denote the process variables as \( y_j \), where \( j \) is the variable index. The proper ROS of a batch process consist of \( y_j(i, k-1), y_j(i, k), ..., y_j(i, k - q_j(i)), y_j(i-1, k + f_j(i-1)), y_j(i-1, k + f_j(i-1) - 1), ..., y_j(i-1, k), y_j(i-1, k - 1), ..., y_j(i-1, k - q_j(i-1)), y_j(i-1, k - q_j(i-1) - 1), ..., y_j(i-1, k - 1), ..., y_j(i-1, k), y_j(i-1, k), ..., y_j(i-p_j k), k), \) where \( i, j, k \) are the indices of batch, variable and time respectively, \( J = 1, 2, ..., J \) is the maximum number of lagged batch index in the proper ROS on variable \( j, q_j(v) \)
is the maximum number of lagged time index in the proper ROS in the $v$th batch on variable $j$, and $f_j(v)$ is the maximum number of future time index in the proper ROS on variable $j$. Then the past vector consists of all lagged variables in ROS, and the future vector consists of all current variables.

Therefore, the past matrix can be organized in the following way:

$$
\mathbf{Y}_p = \begin{bmatrix}
\mathbf{y}_{p+1,q+1}^T \\
\mathbf{y}_{p+1,K-f}^T \\
\vdots \\
\mathbf{y}_{l,k}^T \\
\vdots \\
\mathbf{y}_{l,K-f}^T
\end{bmatrix},
$$

(5)

where

$$
\mathbf{y}_{l,k}^T = [\mathbf{y}_j^T(i,k), \ldots, \mathbf{y}_j^T(i,k)],
$$

$$
\mathbf{y}_j^T(i,k) = [y_{j}(i,k-1), \ldots, y_{j}(i,k-q_j(i))],
$$

At the same time, the future matrix is written as

$$
\mathbf{Y}_f = \begin{bmatrix}
y_1(p+1,q+1) & y_2(p+1,q+1) & \cdots & y_j(p+1,q+1) \\
\vdots & \vdots & \ddots & \vdots \\
y_1(p+1,K-f) & y_2(p+1,K-f) & \cdots & y_j(p+1,K-f) \\
y_1(i,k) & y_2(i,k) & \cdots & y_j(i,k) \\
\vdots & \vdots & \ddots & \vdots \\
y_1(i,K-f) & y_2(i,K-f) & \cdots & y_j(i,K-f)
\end{bmatrix}.
$$

(6)

CCA is performed to extract the correlations between $\mathbf{Y}_p$ and $\mathbf{Y}_f$. The canonical latent variables of $\mathbf{Y}_p$ are calculated. The number $A$ of retained canonical variables can be determined by AIC criterion as stated before. Then the retained canonical variables are chosen to be state variables of this 2-D batch process. The state variables at each sampling interval are calculated in the following way:

$$
x_l^T(i,k) = \tilde{Y}_{l,k}^T C = [x_1(i,k), x_2(i,k), \ldots, x_A(i,k)],
$$

(7)

where $x_j$ is the $j$th state, $C$ contains canonical correlation vectors for $\mathbf{Y}_p$ as columns and tells how the past process variables combined into state variables.

### 3.3. 2-D-DPCA modeling with state variables

After the states are calculated, the state variables are utilized in 2-D-DPCA modeling instead of lagged variables in ROS. PCA algorithm is performed on an expanded data matrix $Z$, where

$$
Z = [Y,X].
$$

(8)

In Eq. (8), $Y$ is the matrix of process data and $X$ is the matrix of states:

$$
Y = [y_1, y_2, \ldots, y_j],
$$

(9)

where $y_j$ is the data vector of the $j$th process variable.

$$
X = [x_1, x_2, \ldots, x_A],
$$

(10)

where $x_j$ is the vector of the $j$th state variable.
After performing PCA, the 2-D dynamics and variable cross-correlation information are extracted by the score space and noises are retained in the residual space. The control limits of $T^2$ based on filtered scores and SPE can be calculated for online process monitoring.

After an abnormal behavior is detected by the $T^2$ or SPE control plot, the contribution plots or variable reconstruction method can be used to find out the reason causing the fault. Since this 2-D-DPCA model only includes $J + A$ number of variables, the contribution plot is much easier to read than the one including all lagged variables in the ROS. The computation burden of variable reconstruction can also be reduced.

3.4. Procedures of 2-D-DPCA modeling and monitoring using state variables

The procedures of 2-D-DPCA modeling using state variables are illustrated in Fig. 2(a). With the normal history data, the ROS determination can be carried on. Then CVA algorithm is used for subspace identification based on the determined ROS. The expanded data matrix is formed by including process variables and state variables. PCA is then performed on it to extract the dynamics and correlation information in score space and leave noise in residual space. The scores are filtered before calculation of the $T^2$ and corresponding control limits. The values of SPE together with its control limits are calculated also for online monitoring.

Fig. 2(b) shows the steps of online monitoring. After new online data coming, the states are calculated. Then the filtered scores and residuals can be got based on 2-D-DPCA model using state variables. The $T^2$ and SPE are calculated to be compared with corresponding control limits. If one of them is out of control, an abnormal behavior is detected. Then contribution plots are called for fault diagnosis to find out the reason.

Although we suppose there is no input process variable in Sections 3.2 and 3.3, the proposed method can be extended to a 2-D batch process with input process variables. The procedures of modeling and online monitoring are same.

4. Simulation results

4.1. Modeling of a 2-D batch process

In this section, simulations are performed to show the benefits of the proposed 2-D-DPCA method using state variables comparing to the 2-D-DPCA method using lagged variables. A batch process with 2-D dynamics (Lu et al., 2005) is simulated as the description
By the lagged variables of \( y \) are 200 samples in each batch. The data matrix is expanded in the way of \( y \) consists of six variables totally. Two of six score variables are chosen to be the first two canonical variates. The AIC criterion indicates to retain two canonical variate pairs. The correlation structure change based on 2-D-DPCA using state variables.

4.2. Comparisons of monitoring and fault diagnosis results

To demonstrate the benefits of the proposed 2-D-DPCA method using state variables on fault diagnosis, two different types of faults are generated. The first fault is caused by changing the variable correlation structure. From batch 61, process variable \( y_2 \) is formulated as

\[
y_2(i, k) = 0.3 \cdot y_2(i - 1, k) + 0.85 \cdot y_2(i, k - 1) - 0.05 \cdot y_2(i - 1, k - 1) + \epsilon_2.
\]  

As shown in Fig. 4, the changes in variable’s value are not obvious in batch 61, although the autocorrelation is changed quite significantly. This makes the fault detection not so easy. The other fault is a kind of small process drift on variable \( y_2 \) from batch 61 by adding a signal that increases slowly with time and batch.

Fig. 5(a) shows the online monitoring result of correlation structure change diagnosis based on 2-D-DPCA using state variables. Fig. 6 shows the diagnoses based on the 2-D-DPCA using state variable. It is clear that process variable \( y_2 \) is significantly outside the control limits, while process variables \( y_3 \) and \( y_4 \), which correlate to \( y_2 \), are also out of

\[
y_1(i, k) = 0.8 \cdot y_1(i - 1, k) + 0.5 \cdot y_1(i, k - 1) - 0.33 \cdot y_1(i - 1, k - 1) + \epsilon_1,
\]

\[
y_2(i, k) = 0.44 \cdot y_2(i - 1, k) + 0.67 \cdot y_2(i, k - 1) - 0.11 \cdot y_2(i - 1, k - 1) + \epsilon_2,
\]

\[
y_3(i, k) = 0.65 \cdot y_1(i, k) + 0.35 \cdot y_2(i, k) + \epsilon_3,
\]

\[
y_4(i, k) = -1.26 \cdot y_1(i, k) + 0.33 \cdot y_2(i, k) + \epsilon_4.
\]
Fig. 7. SPE contribution plot for correlation structure change diagnosis based on 2-D-DPCA using lagged variables.

Fig. 8. Monitoring result of process drift with 2-D-DPCA using state variables and with 2-D-DPCA using lagged variables (dash curve: 95% control limit; solid curve: 99% control limit).

control. State variable $x_1$ is contributed most by the lagged value of $y_2$, so it is also outside the control limits significantly. These indicate process variable $y_2$ is most possible to be the reason of the fault. Fig. 7 shows the diagnosis based on the 2-D-DPCA using lagged variables. There are totally 16 variables plotted on the contribution plot, which is much more than the variables plotted in Fig. 6. This makes the contribution plots messy and need more time to analyze before drawing a reasonable conclusion. Variable reconstruction gives similar diagnosis results. 2-D-DPCA using state variable can also reduce the computation burden of variable reconstruction since the number of variables to be reconstructed is reduced significantly.

The monitoring results of process drift are shown in Fig. 8. Again, two 2-D-DPCA models show similar fault detection efficiencies. And from Figs. 9 and 10, we can find that the 2-D-DPCA model using state variables again give a tidier contribution plot which is easier to read. When variable reconstruction based fault diagnosis is performed, 2-D-DPCA using state variable again reduces the computation burden.

In the above examples, only SPE control plots and contribution plots are used. Actually, the statistic $T^2$ can also be calculated for monitoring. As introduced in Section 2.1, the details of filtered scores
based monitoring can be found in our previous work (Yao and Gao, 2007).

5. Conclusion

As a lagged variable method, 2-D-DPCA method proposed previously (Lu et al., 2005) includes a large number of lagged variables into the batch process model. This does not affect the online monitoring ability, but does make the contribution plots hard to read. To solve this problem, the subspace identification technique is utilized to reduce the number of variables included into the 2-D-DPCA model. Based on the auto-determined process ROS, CVA method is used to identify the state variables. Then, state variables are used in 2-D-DPCA modeling instead of lagged process variables. Therefore, the number of variables is reduced and the contribution plots are clearer, which makes fault diagnosis easier. Simulation examples have shown the benefits of the 2-D-DPCA method using state variables.

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References