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Research article

Multivariate fault isolation of batch processes via variable selection in partial least squares discriminant analysis

Zhengbing Yan [a], Te-Hui Kuang [b], Yuan Yao [b,*]

[a] College of Physics and Electronic Information Engineering, Wenzhou University, Wenzhou 325035, China
[b] Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan

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ABSTRACT

In recent years, multivariate statistical monitoring of batch processes has become a popular research topic, wherein multivariate fault isolation is an important step aiming at the identification of the faulty variables contributing most to the detected process abnormality. Although contribution plots have been commonly used in statistical fault isolation, such methods suffer from the smearing effect between correlated variables. In particular, in batch process monitoring, the high autocorrelations and cross-correlations that exist in variable trajectories make the smearing effect unavoidable. To address such a problem, a variable selection-based fault isolation method is proposed in this research, which transforms the fault isolation problem into a variable selection problem in partial least squares discriminant analysis and solves it by calculating a sparse partial least squares model. As different from the traditional methods, the proposed method emphasizes the relative importance of each process variable. Such information may help process engineers in conducting root-cause diagnosis.

1. Introduction

In industrial manufacturing, batch processes have been widely used for producing low-volume and high-value-added products. For ensuring safe and efficient operation of such processes, various types of multivariate statistical process monitoring (MSPM) methods have been developed [1], among which multiway principal component analysis (MPCA) [2,3] is the most famous. Most of these methods focus on fault detection, while the issue of multivariate fault isolation has been discussed less frequently. Here, fault isolation is defined as identifying critical process variables contributing most to the detected process abnormality, which is the subsequent step of fault detection. In the literature, this step is also called fault diagnosis or fault identification. Since the latter two phrases have different meanings in different contexts, "fault isolation" is used in this paper.

Contribution plots are the most commonly used method of fault isolation, which can be applied to both continuous and batch processes [4]. Contribution plots calculate the contributions of different process variables to the monitoring statistic, and compare them with the corresponding control limits derived from the normal operation data. The interpretation of contribution plots is straightforward: the variables with contributions outside the control limits are regarded as faulty. However, the statistical basis of control limits calculation in contribution plots is debatable [5]. Although in normal operation the contributions of process variables follow a certain distribution, this does not necessarily mean that the contributions of non-faulty variables follow the same distribution when a fault occurs to the process, because of the correlations among variables. As a result, contribution plots often suffer from the smearing effect [6], i.e., the influence of faulty variables on the contributions of non-faulty variables, making the isolation results misleading. Such an effect may be more significant when contribution plots are applied to analyzing batch process data, due to the high autocorrelations and cross-correlations existing in variable trajectories within each batch. Other popular statistical isolation methods include reconstruction analysis [7,8] and its extension using branch-and-bound (B&B) search [9,10]. Usually, reconstruction analysis requires that the candidate fault directions are known or abundant historical fault data are available to estimate the fault directions. However, such requirements are unlikely to be fulfilled in real industrial applications. The utilization of B&B overcomes such problem with the price of heavy computations. In particular, the large number of expanded variables used in batch process monitoring may make the search more time-consuming.

In recent years, the utilization of the variable selection approaches, such as the least absolute shrinkage and selection operators (LASSO) [11] and elastic net (EN) [12], have been extended from regression modeling [13,14] to multivariate

* Corresponding author.
E-mail address: yyao@mx.nthu.edu.tw (Y. Yao).

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fault isolation [15,16]. In [17], the fault isolation problem is transformed into a variable selection problem in discriminant analysis, which can be solved efficiently using LASSO. Nevertheless, such a method is not applicable in dealing with batch process data. The reasons are of twofold. First, supposing that the dataset contains n observations and p variables, LASSO selects at most n predictors when $n < p$. In batch processes, it is common that there are more expanded variables than observations (i.e., batches). Therefore, LASSO may not provide correct results. Second, if there exist groups of highly correlated predictors, LASSO tends to select an arbitrary one from each group, which means that LASSO may not identify all faulty variables. Using EN instead of LASSO in variable selection may solve the problem partially [17]. However, a comparative study [18] has pointed out that sparse partial least squares (SPLS) [19] outperforms EN. In the case study in [18], EN selects a larger number of correlated variables.

In this research, a multivariate fault isolation method that is particularly useful for batch process data analysis is developed based on SPLS. Instead of giving a single suggestion on the set of faulty variables, the proposed method emphasizes the relative importance of each process variable by ranking the process variables based on their extent of influence on the fault. The organization of the rest of this paper is as follows. In Section 2, the link between fault isolation and SPLS-based discriminant analysis is revealed, based on which an SPLS-based fault isolation method is proposed. Then, in Section 3, the effectiveness of the proposed method is illustrated using an injection molding process, through the comparison with the traditional contribution plots and partial least squares discriminant analysis (PLS-DA). Finally, Section 4 concludes the paper with a summary.

2. Methodology

2.1. Link between fault isolation and SPLS-based discriminant analysis

The objective of multivariate fault isolation is to identify variables critical to the process abnormality already detected. Considering the normal operation data as from one class and the fault data as belonging to the other class, the variables to isolate are those discriminating these two classes. Hence, the task of fault isolation is equivalent to conducting variable selection in a two-class discriminant problem.

In discriminant analysis, PLS-DA is a promising method [20]. Compared with the traditional linear discriminant analysis method, such as Fisher discriminant analysis (FDA) [21], PLS-DA is better suited to the cases that the number of observations is smaller than the number of predictor variables, i.e., $n < p$, since it avoids the singular problem in matrix inversion by dimension reduction.

As is well known, PLS-DA is a variant of partial least squares (PLS) when the response is categorical. Consequently, the variable selection techniques developed for PLS can also be used in PLS-DA-based fault isolation. In the field of variable selection, recent developments, e.g., [11,12], are focusing increasingly on imposing sparsity in the midst of the regression model building step. In doing so, parameter estimation and variable selection are achieved simultaneously. SPLS [19] is one such method, which accomplishes variable selection at the same time of dimension reduction. Therefore, such a method is considered in this research.

2.2. Sparse partial least squares

PLS [22] is a well-known dimension reduction technique serving as an alternative to ordinary least squares (OLS) for solving ill-conditioned linear regression problems. The core of PLS is to transform the original predictors into a small number of orthogonal latent variables which maximize the covariance information between the inputs and the outputs. The latent structure of PLS is as follows:

$$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E}, \tag{1}$$

$$\mathbf{Y} = \mathbf{T}\mathbf{Q}^T + \mathbf{F}, \tag{2}$$

where $\mathbf{X} \in R^{n\times p}$ is the predictor matrix, $\mathbf{Y} \in R^{n\times q}$ is the response matrix, $\mathbf{T} \in R^{n\times K}$ is the score matrix representing K linear combinations of the original predictors, $\mathbf{P} \in R^{p\times K}$ and $\mathbf{Q} \in R^{q\times K}$ are the loading matrices containing coefficients, and $\mathbf{E} \in R^{n\times p}$ and $\mathbf{F} \in R^{n\times q}$ are the residual matrices composed of random errors. To specify the score matrix $\mathbf{T} = \mathbf{XW}$, PLS calculates the columns of the weighting matrix $\mathbf{W} = (\mathbf{w}_1, \mathbf{w}_2, \cdots, \mathbf{w}_K)$ projecting $\mathbf{X}$ to $\mathbf{T}$ by solving a number of successive optimization problems. The objective function for calculating the first weighting vector $\mathbf{w}_1$ is formulated as follows:

$$\max_{\mathbf{w}}\left(\mathbf{w}^T\mathbf{X}^T\mathbf{Y}\mathbf{Y}^T\mathbf{X}\mathbf{w}\right) \text{ subject to } \mathbf{w}^T\mathbf{w} = 1. \tag{3}$$

As seen in (3), the projection directions sought by PLS not only relate $\mathbf{X}$ to $\mathbf{Y}$, but also capture the most variation information in the $\mathbf{X}$ space. PLS has been widely applied in process monitoring [23–26] and soft sensor development [27–30], because of its good mathematical properties.

Although PLS is a popular way for dealing with ill-conditioned regression problems, it does not automatically lead to the selection of relevant predictors. Instead, the weighting vectors represent linear combinations of all original predictor variables. As shown in the literature [19], the asymptotic consistency of the PLS estimator does not hold with the very large p and small n paradigm. Therefore, it is necessary to impose sparsity in the optimization step for simultaneous regression modeling and variable selection. SPLS was proposed as a response to such a requirement [19].

In SPLS, the objective function for calculating the first weighting vector is modified as follows:

$$\min_{\mathbf{w},\mathbf{c}}\Big(-\kappa\mathbf{w}^T\mathbf{X}^T\mathbf{Y}\mathbf{Y}^T\mathbf{X}\mathbf{w} + (1-\kappa)(\mathbf{c}-\mathbf{w})^T\mathbf{X}^T\mathbf{Y}\mathbf{Y}^T\mathbf{X}(\mathbf{c}-\mathbf{w}) + \lambda|\mathbf{c}|_1 + \lambda^*|\mathbf{c}|_2^2\Big) \text{ subject to } \mathbf{w}^T\mathbf{w} = 1, \tag{4}$$

where $\mathbf{c}$ is an estimate of $\mathbf{w}$, the L_1 penalty introduces sparsity to $\mathbf{c}$, and the L_2 penalty addresses the potential singularity in $\mathbf{X}^T\mathbf{Y}\mathbf{Y}^T\mathbf{X}$ when solving for $\mathbf{c}$. After solving this optimization problem, $\mathbf{c}$ is rescaled to have norm 1 and then used as the estimated weighting vector instead of $\mathbf{w}$.

In (4), the value of λ controls the sparsity of $\mathbf{c}$. More specifically, a larger λ results in more zero entries in $\mathbf{c}$, and a smaller λ makes $\mathbf{c}$ less sparse and involves more variables in the regression model.

2.3. SPLS-based multivariate fault isolation

In [20], the utilization of PLS is extended from regression analysis to discriminant analysis by finding projection directions that focus on class separation. Such an application is called PLS-DA. Based on a similar idea, SPLS can also be implemented for classification. Moreover, owing to the variable selection property of SPLS, the most relevant variables for