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Online batch fault diagnosis with Least Squares Support Vector Machines ⋆

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Abstract: A new fault identification method for batch processes based on Least Squares Support Vector Machines (LS-SVMs; Suykens *et al.* [2002]) is proposed. Fault detection and fault diagnosis of batch processes is a difficult issue due to their dynamic nature. Principal Component Analysis (PCA)-based techniques have become popular for data-driven fault detection. While improvements have been made in handling dynamics and non-linearities, correct fault *diagnosis* of the process disturbance remains a difficult issue. In this work, a new data-driven diagnosis technique is developed using an LS-SVMs based statistical classifier. When a fault is detected, a small window of pretreated data is sent to the classifier to identify the fault. The proposed approach is validated on data generated with an expanded version of the `Pensim` simulator [Birol *et al.*, 2002]. The simulated data contains faults from six different classes. The obtained results provide a proof of concept of the proposed technique and demonstrate the importance of appropriate data pretreatment.

Keywords: batch control; fault detection; fault identification; data processing; statistical process control.

1. INTRODUCTION

In comparison to continuous processes, batch processes have a lower capital cost and a higher flexibility to produce multiple products or grades. Therefore, batch processes play an important role in the chemical and biochemical industries for the production of high added value products (e.g. pharmaceuticals, food products, polymers, semiconductors). A batch process can be prone to a number of process disturbances such as impurities in the raw materials, fouling of heat exchangers, sensor failures, plugged pipes, etc. The dynamic nature of batch processes presents a challenging problem for fault detection and diagnosis.

Today's process plants dispose of large historical databases containing the frequent measurements of online sensors on hundreds of variables. Statistical Process Monitoring (SPM) aims to exploit these existing databases for process monitoring, fault detection and fault diagnosis, and therefore has a tremendous potential for industrial applications.

Most recent research within the field of SPM has been devoted to fault detection and identification using techniques based on Principal Component Analysis (PCA). While progress has been made in improving fault detection performance by including process dynamics (e.g., *batch dynamic* PCA [Chen and Liu, 2002], *auto-regressive* PCA [Choi *et al.*, 2008]) or non-linear extensions of PCA (e.g., *kernel* PCA [Lee *et al.*, 2004]), correct diagnosis of the process disturbance remains a difficult issue.

Examining contribution plots, which chart the contribution of each variable to the out-of-control statistic, is by far the most popular approach to find the cause of an alarm signal [Westerhuis *et al.*, 2000]. The generation of contribution plots requires no prior knowledge about process disturbances. However, process knowledge is necessary for interpreting the contribution pattern and finding the actual cause.

Cho and Kim [2004] proposed a Fisher Discriminant Analysis (FDA)-based classifier which provides a more direct diagnosis. The classifier is trained on historical faulty data and assigns the cause of a detected fault to the class it most resembles. The drawback of this method is the need of a significant amount of historical faulty data as FDA requires a number of past fault batches greater than the dimensionality of the fault data. For example, Cho and Kim [2004] needed 700 faulty training batches per class in their case study. As process plants are monitored and controlled to achieve satisfactory product quality and prevent process faults, the number of faulty batches available is limited. Therefore, in most practical cases, pseudo-batches have to be generated to account for the data insufficiency [Cho and

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Kim, 2005]. The limited availability of faulty batches is an important consideration for the design of a data-driven fault diagnosis scheme. Cho [2007] extended the linear FDA approach to non-linear problems by employing *kernel* FDA and reduced the need for pseudo-batch generation.

Recently, Support Vector Machines (SVMs) were utilized as a learning algorithm for fault classification of continuous processes [Yélamos *et al.*, 2009]. SVMs are based on statistical learning theory developed by Vapnik [1998] and have shown to exhibit a large generalization performance, especially when the number of training samples is small [Abe, 2005]. This is an important advantage as the availability of faulty data is a common bottleneck in developing data-driven diagnosis techniques.

In this paper the application of Least Squares SVMs (LS-SVMs; [Suykens *et al.*, 2002]) to data-driven fault diagnosis of batch processes is explored. As a case study, data of an expanded version of the `Pensim` simulator developed by Birol *et al.* [2002] is used. First, the basics of PCA and its application to fault detection in batch processing are summarized in Section 2. Next, LS-SVMs are briefly introduced with a focus on multi-class problems in Section 3. The proposed LS-SVMs-based methodology for batch fault diagnosis is explained in Section 4. Section 5 describes the case study on which the fault diagnosis method is validated, followed by a discussion of the obtained results in Section 6. Finally, conclusions and future research directions are provided in Section 7.

2. PCA-BASED FAULT DETECTION

2.1 PCA for batch data

Industrial data is typically heavily correlated as the measured variables are connected through physical laws, mass balances, redundancy of sensors, etc. PCA reduces the number of measured variables to a smaller number of uncorrelated variables or *scores* by exploiting these correlations [Jollife, 1986].

While PCA is applicable to two-dimensional matrices only, a batch data set is inherently three-dimensional as it contains I batches of which J variables are measured at K different time points. Nomikos and MacGregor [1994] solved this issue by first unfolding the $I \times J \times K$ batch data array to a two-dimensional matrix. In this paper, the data is normalized around the mean trajectory to zero mean and unit variance and subsequently unfolded using the variable-wise unfolding method proposed by Wold *et al.* [1998]. The $K \times J$ measurements of each batch are placed under each other to obtain an $IK \times J$ data matrix $\mathbf{X}$. After unfolding, each column of the variable-wise unfolded data matrix $\mathbf{X}$ is normalized before applying PCA.

The PCA model approximates $\mathbf{X}$ with a lower dimensional matrix $\mathbf{T}$ containing R scores ($R \leq J$) for each row of $\mathbf{X}$. The scores matrix is found by projecting $\mathbf{X}$ on a loading matrix $\mathbf{P}$:

$$\mathbf{X} = \mathbf{T}\mathbf{P}^{\mathrm{T}}(+\mathbf{E_X}). \tag{1}$$

where $\mathbf{E_X}$ represents the residuals. The sizes of the matrices $\mathbf{T}$, $\mathbf{P}$, and $\mathbf{E_X}$ in Eq. 1 are $IK \times R$, $J \times R$ and $IK \times J$ respectively. The R columns of $\mathbf{P}$ correspond to the principal components. The first principal component is the direction of maximum variance in the data; subsequent components explain gradually less variance. When applying PCA to process data, large variance are assumed to be important dynamics, while smaller variances represent noise. The number of principal components R to include has to be decided by the user.

2.2 Fault detection statistics

In Statistical Process Monitoring, abnormal behavior is detected by comparing measured process data against a reference dataset obtained under Normal Operating Conditions (NOC). Each new $1 \times J$ measurement vector $\mathbf{x}_k$ is projected on $\mathbf{P}$ to obtain its $1 \times R$ score vector $\mathbf{t}_k$ and $1 \times J$ residual vector $\mathbf{e}_k$. The current score vector and residuals are compared to the NOC data by computing two scalar fault detection statistics. The Hotelling's T^2 statistic monitors the scores and checks if a new observation projects onto the model plane defined by the loading matrix $\mathbf{P}$ within the limits determined by the NOC data. The Squared Prediction Error (SPE) statistic monitors the residuals to detect the occurrence of any abnormal events that cause new observations to move away from the model plane. Upper control limits are established for both statistics based on the reference data set [Nomikos and MacGregor, 1994].

2.3 Fault detection versus fault identification

Fault detection statistics only indicate if process behavior is normal in comparison to the NOC reference data. When a fault is detected, they provide no information about the cause of the out-of-control signal. In this work, an LS-SVM classifier is trained on historical data of past faulty batches to provide online fault *diagnosis*.

3. INTRODUCTION TO LS-SVMs

The concept of LS-SVMs and their extension to multi-class problems is discussed in Section 3.1 and 3.2 respectively. For more information on LS-SVMs, the interested reader is referred to the book of Suykens *et al.* [2002] for a detailed treatment.

3.1 LS-SVM basics

Consider a dataset consisting of N samples of M-dimensional input data $\mathbf{x}_i$ ($i = 1 \dots N$) belonging to two classes (Fig. 1). Each sample can be labeled with a scalar $y_i \in \{-1, +1\}$ for the positive and the negative class respectively. In their simplest form, LS-SVMs train a linear decision function or hyperplane

$$y = \mathbf{w}^{\mathrm{T}}\mathbf{x} + b \tag{2}$$

to separate the input data, where $\mathbf{w}$ is an M-dimensional vector and b a scalar bias term. For a new data point $\mathbf{x}_k$, Eq. 2 is evaluated and $\mathbf{x}_k$ is labeled as the sign of y_k. An infinite number of separating hyperplanes exist. LS-SVMs seek the hyperplane that maximizes the margin between the two classes (Fig. 1b). This maximum margin principle leads to a higher generalization performance, i.e. an increased correct classification rate of unseen data points. The four samples lying on the margin in Fig. 1b are called support vectors.