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Statistical Performance Monitoring Using State Space Modelling and Wavelet Analysis

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Abstract

This paper describes the application of multiresolution analysis to the states and the model residuals calculated through the application of canonical variate analysis (CVA) for process performance monitoring. Applying Hotelling T^2 to the states and residuals and calculating the statistical limits will materialise in an excess of false alarms since the CVA model states and model residuals are observed to exhibit serial correlation. By applying wavelets to the states, the auto-correlation is removed and the standard monitoring metrics can then be applied. The performance and sensitivity of the proposed methodology was assessed for different monitoring indices using average run length (ARL) and false alarm rate as performance indicators. The basis of the study was a benchmark simulation of a continuous stirred tank reactor.

Keywords: Canonical variate analysis, Fault detection

1. Introduction

In the chemical process industries, the on-line monitoring and diagnosis of process operating performance is extremely important in terms of the contribution it can make towards plant safety and the maintenance of process yield and high quality production. Where process monitoring and control schemes are implemented on the basis of empirical techniques, not only is it essential to ensure that the process variables reflect process behaviour and that the data is fit-for-purpose, but it is essential that the appropriate techniques are applied that capture the underlying characteristics of the process (e.g. linear, non-linear or dynamic behaviour). By implementing the appropriate techniques, thereby developing a robust monitoring scheme, the operator is empowered to discriminate between normal and abnormal operation.

Under typical operating conditions, sensor measurements are highly correlated, consequently techniques such as principal component analysis (PCA), MacGregor and

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Kourti (1995), canonical variate analysis (CVA), Simoglou *et al*, (2002), have been applied to extract the information from the data. Although PCA has been widely applied, the most successful applications have theoretically been where the. methodology has been implemented for the analysis of steady state data that exhibits a linear relationship between the process variables. In industrial applications, the data generated does not necessarily satisfy such underlying assumptions, consequently where the process exhibits dynamic behaviour, techniques such as dynamic PCA (DPCA), Ku *et al,* (1996), and CVA, Simoglou *et al*, (2002), can be applied in the development of a monitoring scheme to capture the auto- and cross correlation present in the process data. Bakshi (1998) proposed multiscale PCA (MSPCA), which combines the ability of PCA to decorrelate the variables by extracting a linear relationship with the ability of wavelet analysis to extract the deterministic features and approximately decorrelate the autocorrelated measurements. An alternative approach proposed to capture the dynamics was proposed by Rosen and Lennox (2000) who combined adaptive PCA and multi-resolution analysis. More specifically, Simoglou *et al*, (2002) proposed a monitoring approach that utilizes a state space identification technique based on CVA to address the problem of process dynamics. This method takes the serial correlation into account during the dimension reduction step, as per DPCA, and then uses the state variables for computing the monitoring statistics. However, the states variables are autocorrelated, and thus neither Hotelling's T^2 or the Squared Prediction Error (SPE) follow a F or χ^2 distribution resulting in a higher than statistically desirable false alarm rate.

Within this paper a methodology is proposed that utilises CVA for the resolution of the multivariate problem and then multiscale analysis is applied for enhanced fault detection. That is, a CVA model is developed to address the challenges of variable autocorrelation and cross-correlation and dimensionality reduction. Multiscale analysis is then applied to the state variables and the residuals to approximately decorrelate the state variables and the residuals. The performance and sensitivity of the proposed methodology was assessed using Average Run Length (ARL) and false alarm rates of different monitoring metrics.

2. Canonical Variate Analysis and Wavelets

2.1 Canonical Variate Analysis

CVA is a multivariate statistical technique that is receiving increasing attention for the development of models for linear systems. In CVA, the orthogonal basis is selected as those linear combinations of a data set (the past inputs and outputs, p) that are most predictive of the future outputs of the process, f):

$$\begin{aligned} p(t) = [&y_1(t-1)\ldots y_1(t-k_{y1})..y_n(t-1)..y_n(t-k_{yn}) \\ &u_1(t-1)\ldots u_1(t-k_{u1})..u_m(t-1)..u_m(t-k_{um})\ ]^T \end{aligned} \tag{1}$$

$$f(t) = [y_1(t)\ldots y_1(t+l-1)..y_n(t)..y_n(t+l-1)]^T \tag{2}$$

With the state space model identified using CVA taking the following form:

$$\mathbf{X}_{t+1} = \Phi\mathbf{X}_t + \mathbf{G}\mathbf{U}_t + \mathbf{W}_t \tag{3}$$

$$\mathbf{Y}_t = \mathbf{H}\mathbf{X}_t + \mathbf{A}\mathbf{U}_t + \mathbf{B}\mathbf{W}_t + \mathbf{V}_t \tag{4}$$

With knowledge of the canonical states and the plant data, the state space matrices Φ, **G**,**H**, **A** and **B** and the noise covariance matrix $\mathbf{Q} = \mathrm{E}(\mathbf{W}_t^k \mathbf{W}_t)$ and $\mathbf{R} = \mathrm{E}(\mathbf{V}_t^T \mathrm{V}_t)$ can be computed using least-squares regression. In this representation, $\mathbf{X}_t$ denotes the states, $\mathbf{Y}_t$, the outputs, and $\mathbf{U}_t$, the manipulated inputs. $\mathbf{W}_t$ describes the state or process noise, and $\mathbf{BW}_t + \mathbf{V}_t$ represents the measurement noise. Once the CVA model has been built, and the states identified, Simoglou *et al.* (2002) proposed the application of Hotelling's T^2 and SPE as the basis of the performance monitoring charts. The T^2 statistic is developed from the *k* CVA retained latent variables:

$$\mathrm{T}^2 = \mathbf{X}_{t,k}\mathbf{S}_k^{-1}\mathbf{X}_{t,k}^T \tag{5}$$

where $\mathbf{X}_{t,k}$ is the k^{th} retained state and $\mathbf{S}_k$ is the corresponding covariance matrix. The SPE is given by:

$$\mathrm{SPE}_w = \sum_{i=1}^{k} \mathbf{W}_i^2 \tag{6}$$

Simoglou *et al*, (2002) defined a number of metrics for monitoring the CVA states including the application of Hotelling's T^2 to the state space residuals, the excluded latent variables and the measurement residuals.

2.2 Wavelets and Multiscale PCA

The theory of wavelet transformations is based on multi-resolution analysis (Strang and Nguyen, 1996). The wavelet transformation can be applied to decompose a multivariate signal **X** into its approximate, $\mathbf{A}_1$ to $\mathbf{A}_L$, and detail, $\mathbf{D}_1$ to $\mathbf{D}_L$, coefficients for the first to L^{th} level respectively. The idea of using PCA and wavelets has previously been reported Bakshi, (1998) who developed a multi-scale PCA (MSPCA) process performance monitoring framework.

In this paper, the motivation for applying CVA and wavelets emanates from the fact that CVA deals with both the serial and cross correlation. However, the CVA states and residuals suffer from auto-correlation hence the metrics proposed by Simoglou *et al*, (2002) and Negiz and Cinar, (1997) for the monitoring of the CVA states and residuals will materialise in an excess of false alarms. This is due to the fact that the control limits for the T^2 metrics are calculated based on the assumption that the data is serially independent. To address this issue, Simoglou *et al*, (2002) proposed the use of control limits based on the empirical reference distribution (ERD) (Willemain & Runger, 1996). In this work, multi-scale PCA is applied to the CVA states and residuals. Wavelet analysis removes the autocorrelation within the states and the residuals and PCA is then applied to the wavelet coefficients to remove the correlation inherent within the states. The resulting scores and residuals are monitored using Hotelling's T^2 and SPE. Figure 1 presents a schematic diagram of the proposed fault detection and diagnosis scheme.

For on-line performance monitoring, a moving widow approach is adopted. A window of incoming states and residuals are analysed using the developed monitoring scheme.

That is, multi-scale PCA is applied to the states and residuals and then Hotelling's T^2 and the SPE are calculated for each level of the wavelet decomposition. Once a fault is detected at a certain scale, fault identification is carried out to identify the source of the fault. Contribution plots for Hotelling T^2 of the states and the SPE of the measurement error in the time domain are derived based on the approach described in Westerhuis *et al*, (2000). This is in contrast to using contribution plots of the CVA states as proposed by Norvilas *et al* (2000) which are more difficult to interpret.

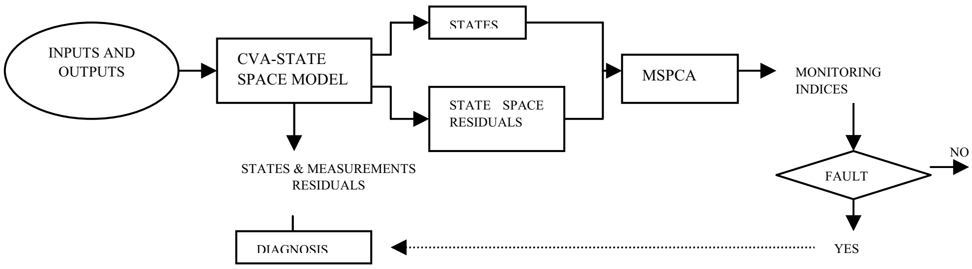

Figure 1. Framework for fault detection and diagnosis

3. Case Study: Monitoring of a Polymerization Reaction

The proposed detection and diagnosis method is now applied for detecting a subtle fault in the polymerization of vinyl acetate in a continuous stirred tank reactor. The polymerization process was modelled by Teymour (1989). In this study the same input and output variables as in Norvilas *et al* (2000) are considered with a CVA model comprising four states being developed. The four process variables considered were reactor temperature, conversion, reactor initiator concentration and polydispersity. The simulated fault is a gradual decrease of the overall heat transfer coefficient at time point 2000. The simulation was repeated 100 times to calculate the Average Run Length (ARL). The application of multi-scale PCA to the states and residuals for fault detection is compared with the theoretical control limits (TCL) and the ERD limits (Simoglou *et al*, 2002).

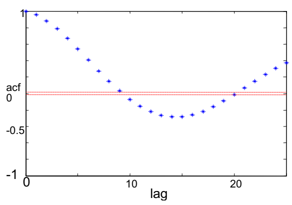

Figure 2a. ACF of the CVA states

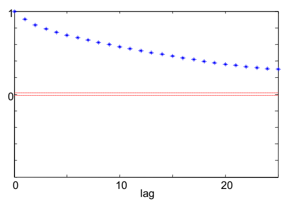

Figure 2b. ACF of Hotelling's T^2 of the CVA states

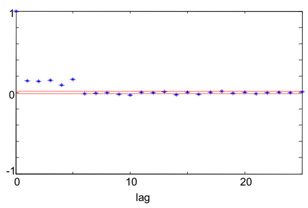

Figure 2c. ACF of the SPE of the CVA residuals

Figure 2 shows the autocorrelation function of Hotelling's T^2 based on the states and the SPE utilising the state-space residuals. As is observed from the autocorrelation function (ACF) (Figures 2b and c) of both Hotelling's T^2 and the SPE are not serially independent. Thus, the control limits calculated based on the assumption that the distribution of the data follows a F-distribution or a χ^2 distribution is incorrect, resulting in an excess of false alarms. However, to address this problem Simoglou *et al*, (2002), proposed using the ERD to derive the control limits. For the ERD, it is the in-control average run length (ARL) performance that determines the limits, however as a consequence of it not taking into account the serial correlation, wide limits result and hence the fault detection task is delayed. Consequently the issue of serial correlation is not addressed. This is illustrated in Figure 3. However, compared with the ERD limits, the theoretical control limits (TCL) have a higher false alarm rate.

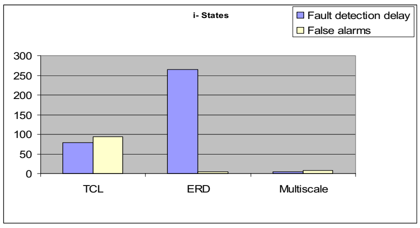

Figure 3a. Comparison of performance of different monitoring indices on the states for 100 runs.

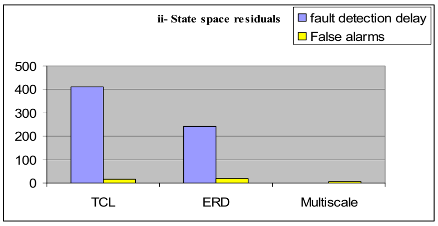

Figure 3b. Comparison of performance of different monitoring indices on the states space residuals for 100 runs.

As a consequence of these issues, wavelet analysis was performed on the states and residuals. More specifically Daubechies filter with 6 scales was applied. The number of scales was determined as described by Rosen and Lennox (2000). The number of scales being chosen in such a way that it allows sufficient separation between the stochastic (noise) and deterministic components of the variables.

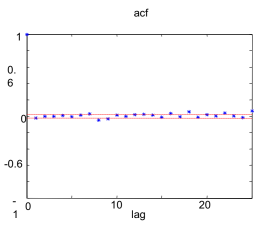

Figure 4a. ACF of scale 1 of the states

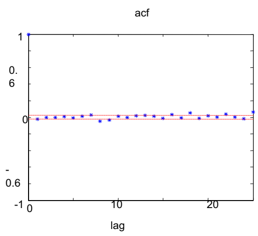

Figure 4b. ACF of Hotelling's T^2 of the states at scale 1

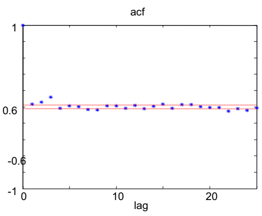

Figure 4c. ACF of Hotelling's T^2 of the state space residuals at scale 1

As can be seen from Figure 3 the application of multi-scale analysis to the states reduces the time to fault detection and the false alarm rate. By using wavelets, the observation of each state is decomposed into several scales, and the monitoring chart is defined at each scale. Thus, the state can be monitored according to the dynamic frequency thereby making it possible to detect a subtle fault in the monitoring chart for the small detail rapidly. Also, this approach suppressed false alarms because the individual decomposed signal does not exhibit auto-correlation as can be observed from the autocorrelation function for scale 1 (Figure 4). Once the fault has been identified, a contribution plot of the states and measurement residuals in the time domain is used to identify the variables that are indicative of the fault. Since fouling affects the difference in inlet and outlet jacket temperature of the reactor, it has a direct impact on the reactor temperature. This is confirmed by the Hotelling's T^2 contribution plots which show that temperature is primarily contributing to the fault.

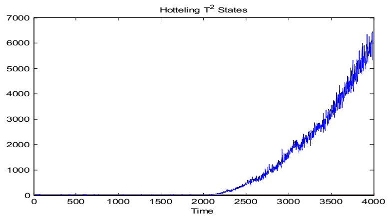

Fig. 4a. Hotelling's T^2 for the states

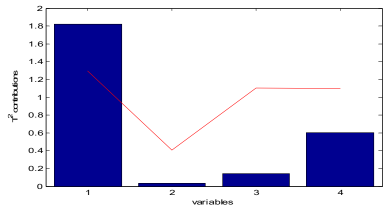

Fig. 4b. Contribution plot for Hotelling's T^2

4. Conclusions

This paper proposed a methodology for fault detection and diagnosis using the conjunction of CVA and wavelets. The performance and sensitivity of the proposed methodology was assessed using the Average Run Length (ARL) and the false alarm rate for different monitoring metrics. The results from the study demonstrated that the proposed methodology outperforms the conventional CVA monitoring metrics proposed by Simoglou *et al* (2002) for the detection of subtle faults. In addition the proposed methodology gave rise to fewer false alarms.

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