ADVANCED MONITORING OF COMPLEX AUTOCORRELATED PROCESSES

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Abstract: In this work, the integration of ARMA filters into the multivariate statistical process control (MSPC) framework is presented to improve the monitoring of large-scale industrial processes. As demonstrated in the paper, such filters can remove auto-correlation from the monitored variables to avoid the production of false alarms. This is exemplified by application studies to a benchmark process from the literature.

Keywords: Statistical Process Control, ARMA Models, Auto Correlation, Large-Scale Systems, Process Models

1. INTRODUCTION

Modern industrial processes often present a large number of highly correlated process variables, which leads to huge amounts of process data to be analysed. MSPC methods are known to be effective in detecting and diagnosing abnormal behaviour in the above circumstances (MacGregor and Kourti, 1995; Wise and Gallagher, 1996). One of the most popular MSPC methods is principal component analysis (PCA), which aims to reveal linear relationships between the process variables by defining a reduced set of score variables. Using these variables, univariate statistics can be generated for on-line process monitoring.

The application of PCA, however, is based on the assumption that the process variables are stationary and normally distributed. In practice, this is rarely satisfied, as such processes are driven by random noise and disturbances. In addition, regulatory controller present feedback to the input variables, so that the impact of disturbances propagates through to both the input and output variables (MacGregor *et al.*, 1991; Kruger *et al.*, 2001). Thus, the process variables move around a steady state condition and exhibit some degree of auto-correlation.

For monitoring auto-correlated process variables, (Ku *et al.*, 1995) proposed the use of dynamic PCA (DPCA) for which time-series structures are incorporated into the PCA analysis. (Ku *et al.*, 1995) argued that: *Directly applying PCA on a data matrix actually constructs a linear static model. When the data contains dynamic information, applying PCA on the data will not reveal the exact relations between the variables, rather a linear static approximation.* It was stated further that: *The score variables will be auto-correlated and possibly cross-correlated* .

The contributions of this paper are as follows. Firstly, it is argued that if the process variables are highly correlated, the score variables can show a stronger degree of auto-correlation. Secondly, strongly auto-correlated score variables may lead to the production of false alarms that invalidate the on-line monitoring approach. Thirdly, the application of ARMA filters is proposed to remove auto-correlation from the score variables. The above findings are demonstrated using a benchmark example from the literature.

It should be noted that ARMA filters could also be applied directly to the recorded process variables. As industrial processes often present large variable sets, however, the application of ARMA filters to these variables may be practically difficult. Moreover, pre-filtering these variables may change the relationships between them, implying that PCA may be less successful in defining a much reduced set of score variables.

2. PROCESS MONITORING USING PCA

The application of PCA involves the construction of a reduced set of score variables that can describe significant variation of the process. The values of these variables can be obtained as follows:

$$\mathbf{t} = \mathbf{P}^T \mathbf{z}, \tag{1}$$

where $\mathbf{t} \in \mathbb{R}^n$ is a vector storing the values of the scores variables, $\mathbf{P} \in \mathbb{R}^{N \times n}$ is a transformation matrix, $\mathbf{z} \in \mathbb{R}^N$ is a vector in which the values of the process variables are stored and N, $n \in \mathbb{N}$ are the number of process variables and retained score variables, respectively. A more detailed analysis of PCA may be found in (Wold *et al.*, 1987).

2.1 Dynamic PCA

To accommodate auto-correlation of the process variables, (Ku *et al.*, 1995) showed that a linear time-series structure could be incorporated into the PCA analysis. This leads to an arrangement of the process variables to form an autoregressive with external input variables (ARX) model structure:

$$\mathbf{z}_k^{*^T} = \left(\mathbf{z}_k^T \ \cdots \ \mathbf{z}_{k-m}^T \right), \tag{2}$$

where $\mathbf{z}_k^{*^T}$ is an augmented set of variables, representing an ARX model structure of order m. Utilizing this "extended" set of process variables, a PCA analysis can then be carried out as described above. On the basis of the recommendations by (Zwick and Velicer, 1986), (Ku *et al.*, 1995) proposed the use of parallel analysis and a subsequent correlation analysis to determine the number of time-lagged values for the process variables and the number of retained PCs. This approach was also used here. Although more accurate relationships between the process variables can be extracted, the PCs are still to be auto-correlated, as can be seen from Equation (1).

If the process variables are auto-correlated, the score variables, which are linear combinations of the original process variables, are auto-correlated too. In addition, if a time-series structure of auto-correlated process variables is considered, the auto-correlation of the score variables will accordingly be amplified. The application study in Section 4 illustrates that strongly auto-correlated score variables may lead to the production of false alarms. Consequently, the auto-correlation of the score variables must be removed in order to prevent such alarms to occur. The next section shows how the application of ARMA filters can remove auto-correlation from the score variables.

2.2 Univariate Statistics

A univariate statistic, denoted as T^2, can be established using the retained score variables:

$$T^2 = \mathbf{t}^T \mathbf{\Lambda}^{-1} \mathbf{t} \tag{3}$$

where $\mathbf{\Lambda}$ is a diagonal matrix storing the n largest eigenvalues of the covariance matrix $\mathbf{S}_{ZZ} = \frac{1}{K-1}\mathbf{Z}^T\mathbf{Z}$ with K being the number of mean centered and appropriately scaled observations stored successively as row vectors in $\mathbf{Z} \in \mathbb{R}^{K \times N}$. The time variation in T^2 can be plotted and its confidence limit obtained as discussed by (Jackson, 1980).

Note that a second univariate statistic, referred to as Q statistic and related to the residuals of the PCA model prediction, can also be defined. However, this statistic is not considered here, since these residuals are assumed to describe measurement uncertainty which is considered to be represented by identically and independently distributed (i.i.d.) variables that are superimposed on the "true" process variables. Hence, the auto-correlation of the process variables does not affect the Q statistic.

3. APPLICATION OF ARMA FILTERS

The application of ARMA filters is now proposed to remove auto-correlations from the score variables. The general form of an ARMA filter is given by (Box *et al.*, 1994) as:

$$\frac{\mu(B)}{h(B)} = \frac{\Theta(B)}{\Phi(B)}, \tag{4}$$

where μ and h are random variables, B is the backward shift operator, i.e. $B\mu_k = \mu_{k-1}$, and Θ and Φ are polynomials in B of dimension p and q, respectively. Moreover, the polynomial $\Theta(B) = 1+\theta_1 B+\cdots+\theta_p B^p$ is the moving average (MA) operator, whilst the polynomial $\Phi(B) = 1+\phi_1 B + \cdots + \phi_q B^q$ represents the autoregressive (AR) operator. The input sequence, $h(B)$, is assumed to be a normally distributed white noise sequence with zero mean and variance σ_h^2, i.e. $h \in \mathcal{N}\left(0, \sigma_h^2\right)$, and the sequence $\mu(B)$ represents the filtered sequence of $h(B)$ using the transfer function $R_{ARMA}(B) = \frac{\Theta(B)}{\Phi(B)}$.

Such ARMA(p, q) filters can be inverted so that $\mu(B)$ represents the input sequence and $h(B)$ represents the output sequence, i.e. $h(B) = R_{ARMA}^{-1}(B)\mu(B)$. This implies that the inverse filter can be employed to filter $\mu(B)$ so that a normally distributed white noise sequence can be produced. More precisely, the calculation of h using the filter $R_{ARMA}^{-1}(B)$ at the k^{th} time instance is given by:

$$h_k = \mu_k - \widehat{\mu}_k = \mu_k + \sum_{i=1}^{q} \phi_i \mu_{k-i} - \sum_{i=1}^{p} \theta_i h_{k-i}, \quad (5)$$

where $\widehat{\mu}_k$ represents the prediction of μ_k using the ARMA filter.

An inverse ARMA filter can be utilised to remove the auto-correlation of the score variables. More precisely, an ARMA filter can be identified for each of the score variables and the residuals of each ARMA filter can then be employed instead of the original score variables. One could also consider removing the auto-correlation of the original process variables and then establishing a PCA model. However, this would be computationally more demanding, as there are usually considerably fewer score variables, i.e. $n < N$. Furthermore, the correlation structure between the process variables might then be changed, which implies that the variable reduction, performed by PCA, might not be as efficient.

3.1 Identification of ARMA Filters

A variety of approaches can be employed for identifying the parameters of the polynomials $\Theta(B)$ and $\Phi(B)$. For example, (Liu and Hudak, 1992) proposed a maximum likelihood estimation for minimizing the variance of $h(B)$, while (Box *et al.*, 1994) suggested a three-stage iterative procedure involving the identification, the estimation and diagnostic checking of the filter obtained.

To determine the orders of the polynomials $\Theta(B)$ and $\Phi(B)$, a number of approaches have been proposed. These can be divided into information based criteria, such as the Akaike information criterion (AIC) (Akaike, 1974), the BIC criterion (Schwarz, 1978) and the minimum description length (MDL) (Rissanen, 1978), and linear algebraic approaches, such as the determinant testing algorithm (Chow, 1972), SVD based methods (Cadzow, 1983; Zhang and Zhang, 1993) and the linear, dual, decoupled procedure (LD^2-ARMA) algorithm (Ribeiro and Moura, 1991).

(Broersen, 1998) highlighted that the residuals of an ARMA process provide an objective measure for assessing the quality of different filters. In the context of this paper, however, the purpose of the filter is to remove auto-correlation from the score variables. Hence, techniques that determine the "optimal filter order", i.e. the number of AR and MA terms, on the basis of residuals may not be suitable. In this work, the mismatch between the estimated auto-correlation function (ACF) and the "ideal ACF" within a window of length l is used. This mismatch can be calculated as follows:

$$J_\mu(p, q) = \frac{1}{l} \sum_{j=0}^{l} \left(r(j) - \widehat{r}_{\mu\mu}(p, q, j)\right)^2, \quad (6)$$

where $J_\mu(p, q)$ is a cost function, $r(j)$ is the "ideal ACF", i.e. $r(j) = \delta_{0j}$ with δ being the Kronecker delta and $\widehat{r}_{\mu\mu}(p, q, j)$ is the estimated ACF including p MA and q AR terms.

Since the BIC criterion provides a consistent estimation of the number of AR and MA terms (Pauler, 1998), it is adopted in conjunction with the above cost function:

$$BIC(p, q) = \log(J_\mu(p, q)) + 2\frac{(p + q)\log(K)}{K}. \quad (7)$$

The order of both polynomials, p and q, is then selected to minimise the BIC cost function.

3.2 Identifying an ARMA based PCA Model

The first step is to record reference data from the process. Note that reference data have to be selected with care, to ensure that abnormal process behaviour is not captured. Conversely, if the size of the reference data is too small, then normal variation within the process would not be adequately represented (Kruger *et al.*, 2001). A PCA model then needs to be established. After defining the order of dynamics m using parallel analysis, (Wold *et al.*, 1987) showed that the transformation matrix $\mathbf{P}$ is constructed by the dominant eigenvectors of $\mathbf{S}_{ZZ}$, which are stored as column vectors. The number of retained score variables can also be determined by parallel analysis, including a subsequent correlation analysis to avoid that the score variables which capture process variation are not discarded. The score variables can now be determined as shown in Equation (1), and the "optimum" number of AR and MA terms then found to remove auto-correlation from these variables.

3.3 Application of ARMA based PCA Models

After the identification of an ARMA model for each score variable, on-line process monitoring can be established as follows. Given that a new observation becomes available:

(1) Obtain the values of the score variables by applying Equation (1).

(2) Apply the identified ARMA filters to each of the score variables –Equation (5).
(3) Determine the T^2 statistic –Equation (3).
(4) Update the monitoring chart.

4. APPLICATION STUDIES

This section presents an application study to a benchmark example from the literature to illustrate the influence of auto-correlated process variables on the T^2 statistic. This example involves two process input variables and two process output variables. From this process, a data set was generated which represents an ARMA process and dynamic PCA was subsequently applied.

4.1 Process Description

The process under study had the following description (Ku *et al.*, 1995):

$$\begin{pmatrix} x_k^{(1)} \\ x_k^{(2)} \end{pmatrix} = \begin{bmatrix} 0.118 & -0.191 \\ 0.847 & 0.264 \end{bmatrix} \begin{pmatrix} x_{k-1}^{(1)} \\ x_{k-1}^{(2)} \end{pmatrix} + \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix} \begin{pmatrix} v_{k-1}^{(1)} \\ v_{k-1}^{(2)} \end{pmatrix} \tag{8}$$

$$\begin{pmatrix} y_k^{(1)} \\ y_k^{(2)} \end{pmatrix} = \begin{pmatrix} x_k^{(1)} \\ x_k^{(2)} \end{pmatrix} + \begin{pmatrix} f_k^{(1)} \\ f_k^{(2)} \end{pmatrix},$$

where $\mathbf{v}_k^T = \begin{pmatrix} v_k^{(1)} & v_k^{(2)} \end{pmatrix}$ and $\mathbf{x}_k^T = \begin{pmatrix} x_k^{(1)} & x_k^{(2)} \end{pmatrix}$ represented the process input and output variables at the k^{th} time instance, respectively, and $\mathbf{f}_k^T = \begin{pmatrix} f_k^{(1)} & f_k^{(2)} \end{pmatrix}$ represented measurement noise superimposed to the "true" values of the output variables to form the measured output variables $\mathbf{y}_k^T = \begin{pmatrix} y_k^{(1)} & y_k^{(2)} \end{pmatrix}$. The input variables of the above process were defined as follows:

$$\begin{pmatrix} v_k^{(1)} \\ v_k^{(2)} \end{pmatrix} = \begin{bmatrix} 0.811 & -0.226 \\ 0.477 & 0.415 \end{bmatrix} \begin{pmatrix} v_{k-1}^{(1)} \\ v_{k-1}^{(2)} \end{pmatrix} + \begin{bmatrix} 0.193 & 0.689 \\ -0.320 & -0.749 \end{bmatrix} \begin{pmatrix} w_{k-1}^{(1)} \\ w_{k-1}^{(2)} \end{pmatrix} \tag{9}$$

$$\begin{pmatrix} u_k^{(1)} \\ u_k^{(2)} \end{pmatrix} = \begin{pmatrix} v_k^{(1)} \\ v_k^{(2)} \end{pmatrix} + \begin{pmatrix} g_k^{(1)} \\ g_k^{(2)} \end{pmatrix},$$

here $\mathbf{w}_k^T = \begin{pmatrix} w_k^{(1)} & w_k^{(2)} \end{pmatrix}$ represented sequences of normally distributed values with zero mean and unit variance, i.e. $w_k^{(1)}$ and $w_k^{(2)} \in \mathcal{N}\{0, 1\}$. In contrast to the simulation model by (Ku *et al.*, 1995), measurement noise was also superimposed on the "true" values of the input variables, i.e. $\mathbf{g}_k^T = \begin{pmatrix} g_k^{(1)} & g_k^{(2)} \end{pmatrix}$, to form the measured input variables $\mathbf{u}_k^T = \begin{pmatrix} u_k^{(1)} & u_k^{(2)} \end{pmatrix}$. The measurement noises were sequences of normally distributed variables with zero means and variances chosen to be 5% of the variance of each individual process variable, i.e.: $f_k^{(i)} \in \mathcal{N}\{0, 0.05 \cdot E\{x_k^{(i)^2}\}\}$ and $g_k^{(i)} \in \mathcal{N}\{0, 0.05 \cdot E\{v_k^{(i)^2}\}\}$.

The output variables were then recorded as shown in Equation (8) prior to the introduction of measurement noise to the input and output variables. Since auto-correlated process behaviour is achieved by describing the input and output variables by ARMA sequences, this process is further referred to as the ARMA process and the corresponding data set is denoted as the ARMA data set.

A data set containing a total number of 2000 samples was generated as described above. The first 500 samples were selected as the reference data and the remaining 1500 samples served as testing data to evaluate the performance of the established monitoring scheme. Given the construction of the process variables, the PCA analysis was based on the following dynamic data matrix:

$$\mathbf{Z} = \begin{bmatrix} y_2^{(1)} & y_2^{(2)} & y_1^{(1)} & y_1^{(2)} & u_1^{(1)} & u_1^{(2)} \\ y_3^{(1)} & y_3^{(2)} & y_2^{(1)} & y_2^{(2)} & u_2^{(1)} & u_2^{(2)} \\ & \vdots & & & \vdots & \\ y_{2000}^{(1)} & y_{2000}^{(2)} & y_{1999}^{(1)} & y_{1999}^{(2)} & u_{1999}^{(1)} & u_{1999}^{(2)} \end{bmatrix}. \tag{10}$$

Since the "true" values of the output variables were linear combinations of previous "true" values of the input and output variables, a total number of 4 PCs needed to be retained. The measurement noise was represented by the 2 discarded PCs. The confidence limits for the T^2 statistic was determined with a confidence of 99%.

4.2 Monitoring of the ARMA Processes

After establishing a PCA model using the first 500 samples, the auto-correlation function of the 4 retained PCs was determined. Figure (1) shows that particularly the first two score variables were strongly auto-correlated. Figure (2) shows the T^2 statistic. The number of violations of the 99% confidence limit was excessive after about 1500 samples into the data set. Furthermore, some of these violations occur in sections, i.e. more than one consecutive T^2 value violates the confidence limit. More precisely, almost 3.5% of the last 500 T^2 values violate the 99% confidence limit. This highlights the fact that the process was out-of-statistical-control.

In summary, the application of an MSPC based monitoring approach to a stationary process with auto-correlated variables may lead to false alarms

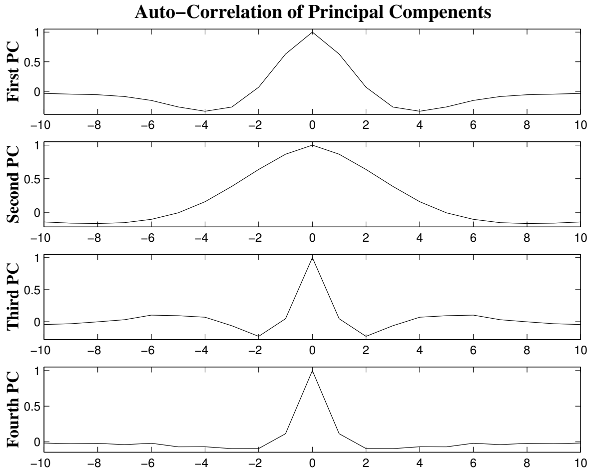

Fig. 1. Auto-correlation functions of retained PCs (original PCs)

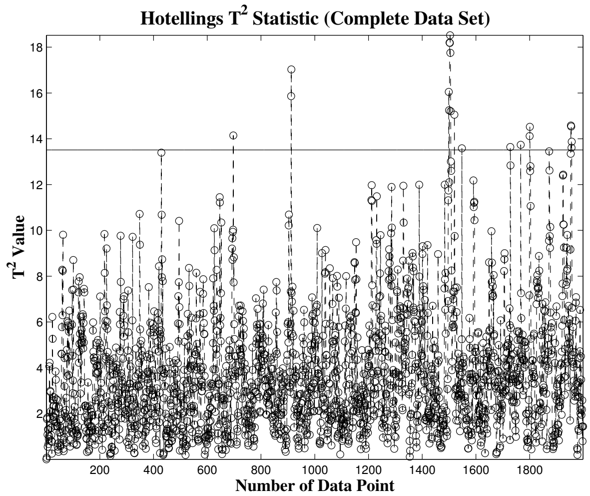

Fig. 2. Hotelling's T^2 statistic based on original score variables)

being produced although the process itself behaves normally. To circumvent such violations, the auto-correlation must be removed or filtered out as discussed in the next subsection.

4.3 Monitoring of the ARMA Process Using Box-Jenkins Filters

It is now shown that ARMA filters can remove auto-correlation from the PCs. The filters were identified using the same data set as in the previous subsection. The number of AR and MA terms, p and q, was determined by applying Equations (6) and (7). From analysing the ACF of each PC (Figure 1), the window length l was chosen as 10. Table (1) shows the selected number of AR and MA terms. The resultant ACF of each filtered PCs is shown in Figure (3) from which it can be seen that only very marginal auto-correlation remains. By comparing Figures (2) and (4), it can be seen that:

Table 1. Number of AR and MA terms for Retained PCs –ARMA Process

#PC	#AR Terms (p)	#MA Terms (q)
1	7	0
2	6	1
3	8	3
4	3	1

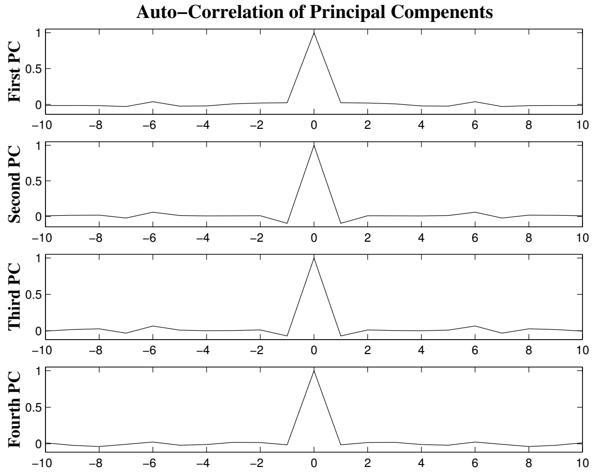

Fig. 3. Auto-correlation functions of retained PCs (filtered PCs)

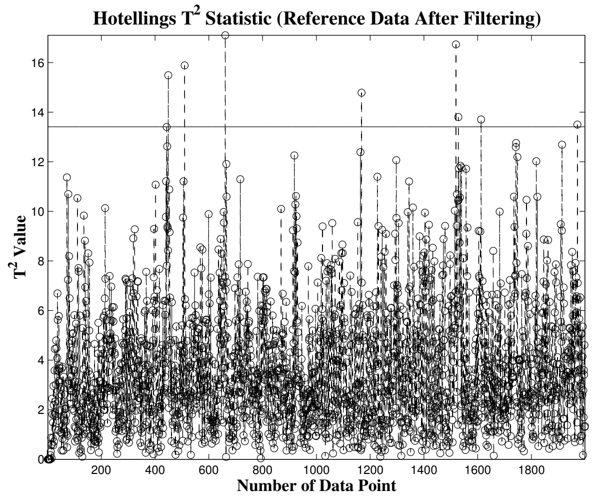

Fig. 4. Hotelling's T^2 statistic based on filtered score variables

(i) the number of violations is less than 1%; and
(ii) violations of consecutive samples, as seen in Figure (2) at around 1500 data points into the data set, were removed.

The process was therefore in-statistical-control, whereas without filtering, the T^2 statistic and the scatter diagrams suggested incorrectly that the process was out-of-statistical-control. Applying ARMA filtering of the PCs has thus prevented false alarms being produced.

5. CONCLUSIONS

This paper has studied the incorporation of ARMA filters into the MSPC framework, motivated by the fact that monitoring processes with strongly auto-correlated variables may lead to the production of false alarms. This was demonstrated using a benchmark simulation from the literature.

It was shown that the application of ARMA filters removes auto-correlation from the reduced set of PCs, thus circumventing the production of false alarms. A more robust monitoring scheme was hence established for the application study used in this work.

The benefits of filtering the PCs instead of the physical process variables are that (i) the number of ARMA filters to be established is much smaller then the number of physical process variables, (ii) the reduced variable set is then statistically independent in contrast to the large number of highly correlated process variables and (iii) auto-correlation of the PCs can be removed.

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