BATCH MONITORING THROUGH COMMON SUBSPACE MODELS

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Abstract: Multi-way statistical projection techniques have typically been applied in the development of monitoring models for single recipe or single grade production. As defined, implementation of these techniques in multi-product applications necessitates the development of a large number of process models. This issue can be overcome through the use of common sub-space models constructed by pooling the individual variance-covariance matrices. A second issue with multi-way approaches is the difficulty of interpreting multi-way contribution plots. An alternative approach is the U^2 statistic. In this paper an extension is proposed, the V^2 statistic, based on the cumulative contribution of variables at each sample point. The methodologies are demonstrated on two industrial applications.

Keywords:- Modelling; Statistical Analysis; Manufacturing Processes

1. INTRODUCTION

Over the last decade the emphasis in process manufacturing has changed. Quality and product consistency have become major consumer decision factors and are key elements in determining business success, growth and competitive advantage. Manufacturing products that meet their quality specifications first time result in higher productivity, reduced manufacturing costs through less re-work, give-away and waste. This all contributes to reducing the impact of the process on the environment by minimising raw materials and energy usage. The achievement of right first time production requires a reduction in process variability and thus the monitoring of process behaviour over time to ensure that the key process/product variables remain close to their desired (target) value is essential. This has led to a significant increase in the industrial application of statistical methods for interrogating the process to obtain an enhanced understanding of the process and the implementation of Statistical Process Control (SPC) for process monitoring and the early warning of the onset of changes in process behaviour.

An area of rapidly growing interest for the monitoring of processes is that of Multivariate Process Performance Monitoring (MPPM). MPPM schemes have typically been based on the statistical projection techniques of Principal Component Analysis (PCA) and Projection to Latent Structures (PLS) and their multi-way extensions for batch processes. Reported practical applications of MPPM have focused on the production of a single manufactured product i.e. one grade, one recipe, etc. with separate models being used to monitor different types of products (Kosanovich and Piovoso, 1995, Kourti *et al*, 1995, Rius *et al*, 1997, Martin *et al,* 1999). However, in recent years, process manufacturing has increasingly been driven by market forces and customer needs resulting in the necessity for flexible manufacturing to meet the requirements of changing markets and product diversification. Thus with many companies now producing a wide variety of products, there is a real need for process monitoring models which allow a range of products, grades or recipes to be monitored using a single process representation.

The elimination of between group variation is a prerequisite for statistical process monitoring, so that interest can focus on within process (product) variability. This normally requires constructing separate control charts for each type of product or grade to be monitored. In many process monitoring situations this may be impractical because of the large number of control charts required to monitor all the products being manufactured and the limited amount of data available from which to develop a process representation. An extension to multi-way PCA and multi-way PLS that allows the construction of a multiple group model is proposed based on combining the variance-covariance matrices of each of the individual groups. The loadings for the latent variables are then calculated from the pooled variance-covariance matrix of the individual groups. Previous work has been published on the multiple-group PCA algorithm, Lane *et al*, (2001) and thus the paper focuses on the multi-group PLS algorithm.

2. PROJECTION TO LATENT STRUCTURES

A brief overview of the PLS algorithm is presented. A more detail discussion of the methodology can be found in Garthwaite (1994). The objective of PLS is to determine a set of latent variable scores that "best" describe the variation in the process data set (**X**) data set that is most influential on the quality data set (**Y**) data set. Using these latent variables it is then possible to construct a set of latent variable scores for the process data i.e. $\mathbf{T} = \mathbf{XW}$, where **T** is the matrix of latent variable scores and **W** is the matrix containing the latent variable loadings. A number of different algorithms have been proposed to derive the loadings for the latent variables associated with PLS. One approach is based on the extensions to the NIPALS (Non-linear Iterative Partial Least Squares) method, which regresses the columns of **X** on **Y** directly. As a consequence, it is not feasible to combine a number of different data sets into a single model.

Lindgren *et a,l* (1993) presented a kernel algorithm for determining the latent variables that is based on the eigenvector decomposition of the variance-covariance matrix, $\mathbf{R} = \mathbf{X}^T\mathbf{Y}\mathbf{Y}^T\mathbf{X}$. By adapting the kernel algorithm, a multiple group model can be constructed by pooling the individual variance-covariance matrices ($\mathbf{R}_i$). In this way the formal statistical basis for the multiple group model, as given by Flury (1987), can be extended. The variance-covariance approach is based on the hypothesis that the first *a* eigenvectors of each of the individual variance-covariance matrices span the same common subspace. Although the model introduced by Flury (1987) related to common principal components, the hypothesis is also appropriate for PLS, since it is the variance-covariance matrices that are of interest. Krzanowski (1984) had previously shown that the common loadings for the latent variables could be extracted from a weighted sum of the individual variance-covariance matrices.

3. THE MULTIGROUP PLS ALGORITHM

The algorithm for constructing the multiple group model based on the kernel algorithm is as follows:

1. Calculate the kernel matrices for each individual group:

$$\mathbf{R}_i = \left(\frac{\mathbf{X}_{is}^T\mathbf{Y}_{is}}{n_i - 1}\right)\left(\frac{\mathbf{X}_{is}^T\mathbf{Y}_{is}}{n_i - 1}\right)^T \quad i = 1, \ldots, g \tag{1}$$

where $\mathbf{X}_{is}$ is the matrix of scaled process data for group i, $\mathbf{Y}_{is}$ is the matrix of scaled quality data for group i, n_i is the number of observations in group i, and g is the total number of groups.

2. Construct the pooled kernel matrix:

$$\mathbf{R}_p = \frac{\sum_{i=1}^{g}(n_i - 1)\mathbf{R}_i}{(N - g)} \qquad i = 1, \ldots, g \tag{2}$$

where $N = \sum_{i=1}^{g} n_i$

3. Calculate the loading vector ($\mathbf{w}_k$) for the process variables, where ($\mathbf{w}_k$) is the first eigenvector of the pooled kernel matrix ($\mathbf{R}_p$).

4. Once ($\boldsymbol{w}_k$) has been estimated, the latent variable scores for each group ($\boldsymbol{t}_{ik}$) can be calculated: -

$$\mathbf{t}_{ik} = \mathbf{X}_{is}\mathbf{w}_k \tag{3}$$

where $\mathbf{t}_{ik}$ is the matrix of principal component scores for group i and dimension k, $\mathbf{w}_k$ is the common latent variable loading for dimension k and $\mathbf{X}_{is}$ is the scaled data matrix for group i.

5. The loading vectors ($\mathbf{p}_i$) and ($\mathbf{q}_i$) are then calculated as:

$$\mathbf{p}_i = \frac{\mathbf{t}_{ik}^T\mathbf{X}_{is}}{\mathbf{t}_{ik}^T\mathbf{t}_{ik}} \qquad \mathbf{q}_i = \frac{\mathbf{t}_{ik}^T\mathbf{Y}_{is}}{\mathbf{t}_{ik}^T\mathbf{t}_{ik}} \tag{4}$$

where $\mathbf{Y}_{is}$ is the matrix of scaled quality data.

6. The process and quality data matrices are then deflated:

$$\mathbf{X}_{is\,new} = \mathbf{X}_{is} - \mathbf{t}_{ik}\mathbf{p}_i^T \tag{5}$$
$$\mathbf{Y}_{is\,new} = \mathbf{Y}_{is} - \mathbf{t}_{ik}\mathbf{q}_i^T$$

The next $(k + 1)^{\text{th}}$ latent variable is then calculated:

$$\mathbf{t}_{ik+1} = \mathbf{X}_{is\,new}\mathbf{w}_{k+1} \tag{6}$$

where $\mathbf{w}_{k+1}$ is the first eigenvector of the updated pooled kernel matrix:

$$\mathbf{R}_{p\,new} = \frac{\sum_{i=1}^{g}(n_i - 1)\mathbf{R}_{i\,new}}{N - g} \tag{7}$$

and

$$\mathbf{R}_i\ new = \left(\frac{\mathbf{X}_{is\,new}^T \mathbf{Y}_{is\,new}}{n_i - 1} \right) \left(\frac{\mathbf{X}_{is\,new}^T \mathbf{Y}_{is\,new}}{n_i - 1} \right)^T \quad (8)$$

The iteration process continues with new values for $\mathbf{p}_i$ and $\mathbf{q}_i$ being calculated. Finally the data matrices $\mathbf{X}_{isnew}$ and $\mathbf{Y}_{isnew}$ are deflated. The iteration process steps (1 to 6) are repeated until the required numbers of latent variables have been extracted.

4. MPCA AND MPLS FOR MONITORING BATCH DATA

Batch processes differ from continuous processes in that each variable, j, is measured at k time intervals for a total of I batches. The data set is thus three-dimensional (I x J x K). As a consequence interest is in both the "between" and "within" batch variability. The application of MPCA or MPLS to the three-dimension data array associated with batch manufacturing is equivalent to performing standard PCA or PLS on a large two-dimensional data matrix formed by unfolding the original three-dimensional array. The unfoding approach adopted in this paper is that proposed by Kourti *et* al, (1995) and demonstrated in Fig. 1. This approach allows the variability between batches to be analysed by summarising the variability in the data with respect to both variables and their time variation. The data contained in the two-dimensional matrix is mean centred and scaled prior to applying either MPCA or MPLS. By subtracting the mean of each column from the two-dimensional data matrix the non-linearities are effectively removed from the data.

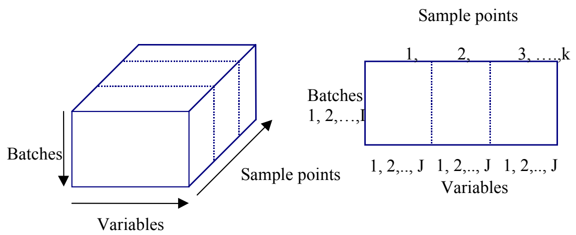

Fig. 1. Data unfolding

5. MULTIPLE GROUP MPCA AND MPLS

As described in Section 3, the pooled correlation (variance-covariance) approach is based on the existence of a common eigenvector subspace spanned by the first a eigenvectors of the individual correlation (variance-covariance) matrices. A formal statistical model was given by Flury (1987), who computed the common principal components using Maximum Likelihood Estimation (MLE). Krzanowski (1984) had previously demonstrated that the common principal components derived using the pooled correlation (variance-covariance) matrix were almost identical to those computed from MLE. In practice the pooled correlation (variance-covariance) approach proposed by Krzanowski (1984) is simpler to apply than the MLE approach, which requires the implementation of an iterative algorithm. The pooled correlation (variance-covariance) approach compares the subspaces defined by the eigenvectors associated with the largest eigenvalues. No conditions are placed on the MLE proposed by Flury (1987). This is a major consideration when determining the method to be used for calculating the latent variables for process monitoring. In process monitoring, it is convention to construct the process models using the eigenvectors corresponding to the largest eigenvalues. As a consequence determining the common latent variables from the pooled correlation (variance-covariance) matrix is more appropriate for industrial applications.

6. V^2 CONTRIBUTION PLOTS

The contribution plots introduced by Miller *et al*, (1998) are formulated from the weighted contribution of each variable to the principal component (latent variable) score at the sample points of interest. In the batch monitoring approach adopted in this paper there are a large number of variable contributions (variable x sample points) to analyse. In some situations this can make the contribution plots difficult to interpret. Furthermore the deviations usually impact on the manufacturing process over a number of sample points. As a consequence the development of a contribution plot that indicates the cumulative contribution of each variable to the principal component (latent variable) scores at each sampling point is desirable. The cumulative contribution of each variable is better related to the latent variable scores, whose deviation from the centre of the control region is usually caused by the cumulative affect of small deviations from the mean batch trajectory.

The V^2 statistic is an extension of the U^2 statistic of Runger (1996) and Runger and Alt (1996) and is proposed as a technique for examining the cumulative contribution of each variable individually or as a group of variables, at each sample point. The V^2 statistic is calculated as the difference between two T^2 statistics. The first includes the entire variable set and the second excludes the variable or groups of variables whose contribution is of interest. To examine the cumulative contribution to the batch scores, a V^2 statistic is calculated at each sample point this requiring the calculation of:

$$V_1^2 = T^2 - T_1^2 \quad (9)$$

where T_1^2 excludes the variable or variables of interest at the first sample point. At the second sample point (V_2^2) is calculated from:

$$V_2^2 = T^2 - T_2^2 \quad (10)$$

where T_2^2 excludes the variable(s) of interest at both the first and second sample points. The calculation is repeated at each sample point to obtain V_3^2, V_4^2, etc. until the end of the batch run. Each individual V^2 statistic can then be plotted as a bar graph, which shows the cumulative contribution of each variable or group of variables at each sample point.

7. PROCESS PERFORMANCE MONITORING

7.1 Case Study 1

To demonstrate the application of multiple group multi-way PCA, three sets of data from a metal etcher process were considered (Wise *et al,* 1999). Data was supplied from an A1-stack etching process that was being performed using a Lam 9600 plasma-etching tool. The objective of the process is to etch the NiN/A1-0.5% Cu/TiN/oxide stack with an inductively coupled BCI_3/CI_2 plasma. The standard manufacturing process consists of a series of six steps. The first two are for the achievement of gas flow and stabilisation. Steps 3 and 4 are the brief plasma ignition step and the main etch of the A1 layer terminating at the A1 endpoint respectively. The next step acts as an over etching for the underlying TiN and oxide layers whilst the final step is associated with the venting of the chamber.

Etching of an individual wafer is analogous to a single batch in a chemical process. Changes in the process mean are a result of a residue building up on the inside of the chamber following the cleaning cycle, differences in the incoming materials resulting from changes in the upstream process and drift in the process monitoring sensors themselves. As a result of the changes in the process mean there are three distinct operating levels identified in the data set. When the data is combined into a single data set, the scores of principal component 1 and principal component 2 identify the discrete operating levels as seen in Fig. 2.

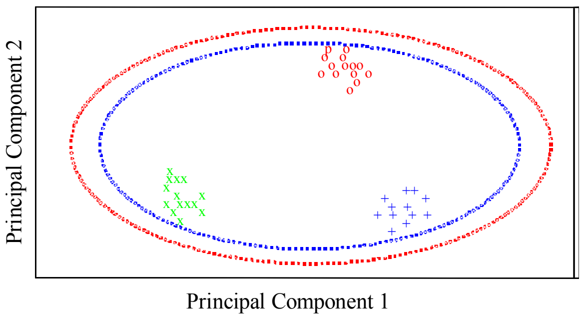

Fig. 2. Bivariate scores plot (Mixed covariance model)

In this case the major source of variation explained by the individual principal components is the variation of each variable from the overall mean of the data set and thus identifies the different operating conditions of each variable. This between group variation present in the data set causes the principal component scores to cluster according to which operating region, or grade of product, they represent. When such clustering occurs there are two issues that impact on process monitoring: (i) the control limits may be conservative and assignable cause process events may not be detected and (ii) an assignable cause reflected in the movement of a principal component score into another cluster when the operating conditions have not been changed may result in the real process event not being detected. As a consequence of the clustering observed and due to the changing mean levels, the process data was divided into three subsets one for each of the operating levels. The composition of each of these data sets is presented in Table 1.

Table 1. The Metal Etcher Data Sets

Operating level	Observations	Variables	Batches
1	90	17	17
2	90	17	16
3	90	17	18

A reference model for the multiple group application was then constructed using the three data sets. By analysing each of the data sets, it was inferred that the different operating levels share common characteristics that determine the process behaviour and as a consequence the use of the multiple group modelling approach was validated. Ten principal components were selected from cross-validation explaining 68%. A bivariate scores plot for principal components 1 and 2, Fig. 3, shows that the scores are independent and identically distributed. As a result it was inferred that the multiple group monitoring model provided a good representation of the overall etch process.

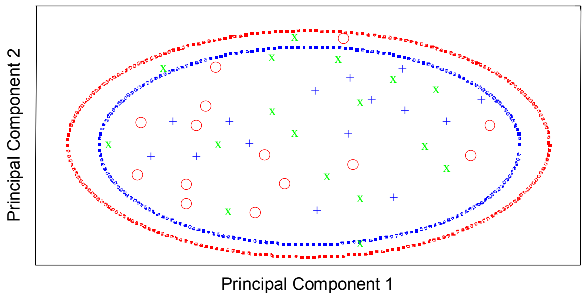

Fig. 3. Bivariate scores plot (Pooled covariance model)

To evaluate the detection and diagnostic capabilities of the multiple group model, a data set containing an increase in the TCP power was projected onto the reference model. This was done in a manner so as to simulate an on-line monitoring situation. Each observation that is projected onto the monitoring chart represents the status of an 'on-line batch' at successive sampling points during the etch process. The bivariate scores plot of principal components 1 and 2 (Fig. 4) detects the change in the operating conditions as a slow drift away from the centre of the control region.

At the beginning of the etch run, the principal component scores lie in the centre of the control region. After the first few sample points the scores gradually drift away from the centre towards the control limits. An out-of-statistical-control signal is flagged as the scores cross the action limits. In this particular example no remedial action was taken and the scores continue to drift away from the control region until the conclusion of the process run.

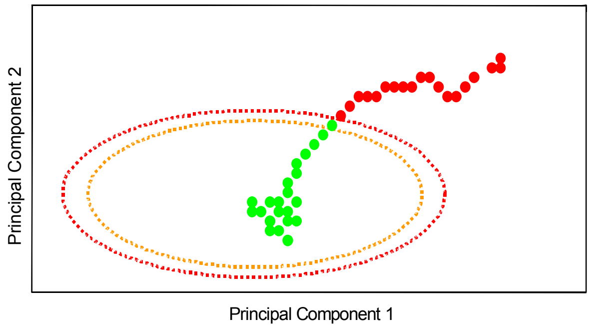

Fig. 4. Bivariate scores plot

The V^2 contribution plot, Fig. 5, identifies the variable indicative of the out-of-statistical-control signal. For clarity only the contribution from a single variable is plotted and it can be seen that the contribution from the variable follows a similar profile to the principal component scores shown in Fig. 4. These results demonstrate the power of the multi-group modelling approach and confirm the findings of Wise *et al*, (1999).

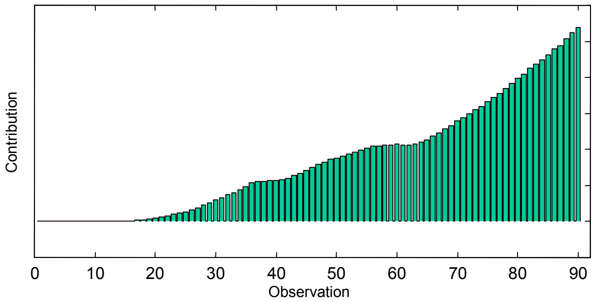

Fig. 5. V^2 Contribution Plot

7.2 Case Study 2

The industrial process used to demonstrate the on-line application of the multiple group multi-way PLS model is a polymer film manufacturing process. The manufacture of polymer film can be considered as a series of unit operations that are applied to convert polymer pellets to a rolled film product (e.g. Weighell *et al*, 2001). A number of different film types are manufactured using the same process equipment through changes in the operating conditions being made and the types of polymer pellets used. Following the production of each roll of film, a number of quality attributes are measured at the end of the roll. As a consequence each roll of film can be considered as a separate batch of product. In this example, 105 process variables and 3 quality variables are included in the model. These provide a description of the "well being" of the process and its manufacturing performance, although at present the process operators only monitor a few "key" process variables.

Separate performance monitoring charts were constructed for each unit within the manufacturing process. In this example the unit of interest is the sheet forming process. Two grades of film manufactured using two different production lines were used to construct the multiple group model. In this particular plant there are a number of different lines manufacturing polymer film and as a consequence there is both between line variation in the data as well as the between polymer grade variation. The composition of each data set is shown in Table 2. Again as in the previous Case study, initially all the data was combined into a single data matrix. For comparative purposes, standard single group MPLS was carried-out on the combined data matrix.

Table 2. The Films Production Line Data

Data Set	Line	Grade	Obs.	Proc Vars	Qual Vars	Btch's
1	1	1	100	19	3	23
2	1	2	100	19	3	23
3	2	1	100	19	3	19
4	2	2	100	19	3	19

Inspection of the bivariate scores plot of latent variables 1 and 2 showed, as expected, the scores to be clustered into four distinct regions (not shown). Combining the data into a single matrix and applying standard multi-way PLS does not result in a satisfactory model for on-line process monitoring (Lane *et al*, 2001). Inspection of the bivariate scores plot of latent variables 1 and 2 for the multiple group model showed the latent variable scores to be independent and normally distributed (not shown), implying that the multiple group model was appropriate for monitoring the polymer film manufacturing process.

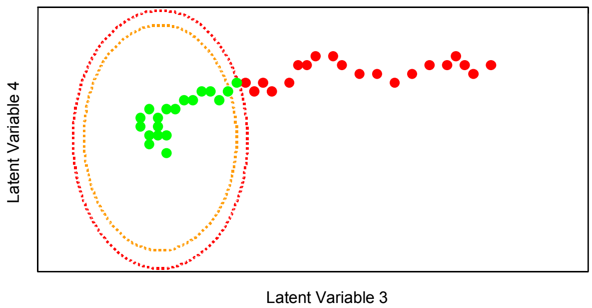

Fig. 6. Bivariate scores plot of latent variable 3 versus latent variable 4

A data set containing a process fault, a reduction in the pressure, was projected onto the reference model. Fig. 6, represents the on-line status of the batch at successive sample points during the manufacturing process. The bivariate scores plot of latent variables 3 and 4, Fig. 6, detects a process disturbance. As with the multiple group multi-way PCA Case Study, the scores are seen to drift away from the centre of the control region. Again in this particular application no remedial action could be taken when the abnormal situation was detected.

Once the out-of-statistical-control operation was signalled, a V^2 contribution plot was used to determine the variables indicative of the out-of-statistical-control signal. In this case a change in pressure impacted on two of the process variables. Fig. 7 shows the V^2 statistic for the joint contribution of these two variables. In this case the V^2 statistic is calculated by omitting both variables from the T_i^2 statistic (Equations 9 and 10) at each sample point.

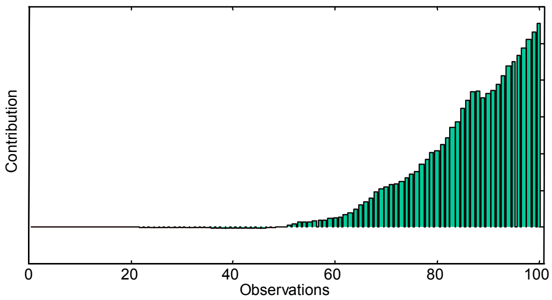

Fig. 7. V^2 contribution plot

8. CONCLUSIONS AND DISCUSSION

The applications presented in the paper are from manufacturing processes where the amount of data from each distinct set of operating conditions or product grade was limited. Prior analysis of the individual data sets suggested that the data available was not sufficient to give a true reflection of the underlying process variability. By applying the pooled correlation (variance-covariance) approach, all the products being manufactured could be monitored using a small number of monitoring charts. In this way the cost and time required to update the models can be significantly reduced allowing the faster on-line implementation of process performance monitoring schemes. The multiple group process monitoring techniques were also demonstrated to have good fault detection and diagnostic capabilities.

An alternative contribution plot for batch processes has also been proposed. The objective of the multi-group modelling methodologies proposed is to monitor the deviation of each variable from its mean trajectory. As a consequence, most out-of-statistical-control signals are the result of a variable, or group of variables deviating from their mean trajectories over a number of sample points. By examining the cumulative contribution of each variable, or group of variables, at each sample point a clear indication of their influence on the out-of-statistical-control signal can be obtained.

9. ACKNOWLEDGEMENTS

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