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Research

Multivariate Statistical Process Control Charts: An Overview

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In this paper we discuss the basic procedures for the implementation of multivariate statistical process control via control charting. Furthermore, we review multivariate extensions for all kinds of univariate control charts, such as multivariate Shewhart-type control charts, multivariate CUSUM control charts and multivariate EWMA control charts. In addition, we review unique procedures for the construction of multivariate control charts, based on multivariate statistical techniques such as principal components analysis (PCA) and partial least squares (PLS). Finally, we describe the most significant methods for the interpretation of an out-of-control signal. Copyright © 2006 John Wiley & Sons, Ltd.

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1. INTRODUCTION

In a discussion paper, Woodall and Montgomery¹ stated that multivariate process control is one of the most rapidly developing areas of statistical process control. They also emphasized the need for review papers because such papers tend to spark new research ideas. Motivated by this, we present a review of the literature on multivariate process control chart techniques.

Nowadays, in industry, there are many situations in which the simultaneous monitoring or control of two or more related quality–process characteristics is necessary. Monitoring these quality characteristics independently can be very misleading. Process monitoring of problems in which several related variables are of interest are collectively known as *multivariate statistical process control*. The most useful tool of multivariate statistical process control is the quality control chart.

Multivariate process control techniques were established by Hotelling in his 1947 pioneering paper. Hotelling² applied multivariate process control methods to a bombsights problem. Jackson³ stated that any multivariate process control procedure should fulfill four conditions: (1) an answer to the question ‘Is the process in control?’ must be available; (2) an overall probability for the event ‘Procedure diagnoses an out-of-control state erroneously’ must be specified; (3) the relationships among the variables–attributes should be taken into account; and (4) an answer to the question ‘If the process is out of control, what is the problem?’ should be available.

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This paper is the result of an extended literature review of the most recent developments in the area of multivariate statistical process control, using control charting in particular. In Section 2 the basic theory of the multivariate Shewhart-type control charts is given. Section 3 describes the most significant multivariate cumulative sum (CUSUM)- and exponentially weighted moving average (EWMA)-type control charts. The use of principal components analysis (PCA) and partial least squares (PLS) in the field of multivariate statistical process control is presented in Section 4, while, in Section 5, developments with respect to the interpretation of an out-of-control signal are given. Finally, some concluding remarks are offered in Section 6.

2. MULTIVARIATE SHEWHART CONTROL CHARTS

In the literature, two distinct phases of control charting practice have been discussed (Woodall⁴).

- *Phase I: charts are used for retrospectively testing whether the process was in control when the first subgroups were being drawn.* In this phase, the charts are used as aids to the practitioner, in bringing a process into a state where it is statistically in control. Once this is accomplished, the control chart is used to define what is meant by a process being statistically in control. This is referred to as the retrospective use of control charts. In general, there is a great deal more going on in this phase than simply charting some data. During this phase the practitioner is studying the process very intensively. The data collected during this phase are then analyzed in an attempt to answer the question ‘Were these data collected from an in-control process?’. According to Duncan⁵, Phase I also includes the establishment of the process being statistically in control.
- *Phase II: control charts are used for testing whether the process remains in control when future subgroups are drawn.* In this phase, the charts are used as aids to the practitioner in monitoring the process for any change from an in-control state. At each sampling stage, the practitioner asks the question ‘Has the state of the process changed?’. In this phase, the practitioner is monitoring the process regardless of whether the parameters of the process, μ_0 and Σ_0 , were known or estimated. Note that in this phase the data are not taken to be from an in-control process, unless there is a clear indication of no change in the process.

Woodall⁴ states that much work, process understanding and process improvement are often required in the transition from Phase I to Phase II. Sparks⁶, Wierda⁷, Lowry and Montgomery⁸, Fuchs and Kenett⁹, Ryan¹⁰ and other statisticians and engineers agree with the above definition, which is also followed in this paper. Alt¹¹, gives a somewhat different definition for the two distinct phases of control charting. According to Alt¹¹, Phase I consists of using the charts for:

- (i) Stage 1 ‘Start-Up Stage’—retrospectively testing whether the process was in-control when the first subgroups were being drawn; and
- (ii) Stage 2 ‘Future Control Stage’—testing whether the process remains in control when future subgroups are drawn.

According to Alt¹¹, these are two separate and distinct stages of analysis. Phase II consists of using the control chart to detect any departure of the underlying process of standard values μ_0 and Σ_0 , when standard values μ_0 and Σ_0 are known, meaning that standard values are given by management or they have been estimated from a large set of past data and are assumed to be the true parameters.

Another crucial matter is the sample size n of each rational subgroup. If $n = 1$, then special care must be taken. As Lowry and Montgomery⁸ suggest, the appropriate use of a test statistic (χ^2 or T^2) can be divided into four categories:

- (1) Phase I and $n = 1$, working with individual observations;
- (2) Phase I and $n > 1$, working with rational subgroups;
- (3) Phase II and $n = 1$, working with individual observations;
- (4) Phase II and $n > 1$, working with rational subgroups.

At the time of writing we are not aware of any results in which sample sizes are taken to be unequal.

Mason and Young¹² give the basic steps for the implementation of multivariate statistical process control using the T^2 statistic, and they recently published a textbook on the practical development and application of multivariate control techniques using the T^2 statistic (Mason and Young¹³).

Control charts for the process mean ($n > 1$)

We first present multivariate control charts for controlling the process mean. Assume that the vector \mathbf{x} follows a p -dimensional normal distribution, denoted as $N_p(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$, and that there are m samples each of size $n > 1$ available from the process. Furthermore, assume that the vector observations \mathbf{x} are not time dependent. A control chart can be based on the sequence of the following statistic

$$D_i^2 = n(\bar{\mathbf{x}}_i - \boldsymbol{\mu}_0)^t \boldsymbol{\Sigma}_0^{-1} (\bar{\mathbf{x}}_i - \boldsymbol{\mu}_0) \quad \text{for } i = 1, 2, \dots, m$$

Here, $\bar{\mathbf{x}}_i$ is the vector of the sample means of the i th rational subgroup, where $\boldsymbol{\mu}_0$ and $\boldsymbol{\Sigma}_0$ are the known vector of means and the known variance–covariance matrix, respectively. The D_i^2 statistic represents the weighted distance (Mahalanobis distance) of any point from the target $\boldsymbol{\mu}_0$. Thus, if the value of the test statistic D_i^2 plots above the control limit (L_u), the chart signals a potential out-of-control process. In general, control charts have both upper (L_u) and lower control limits (L_l). However, in this case only an upper control limit is used, because extreme values of the D_i^2 statistic correspond to points far remote from the target $\boldsymbol{\mu}_0$, whereas small or zero values of the D_i^2 statistic correspond to points close to the target $\boldsymbol{\mu}_0$. The D_i^2 statistic follows a χ^2 -distribution with p degrees of freedom. Thus, a multivariate Shewhart control chart for the process mean, with known mean vector $\boldsymbol{\mu}_0$ and variance–covariance matrix $\boldsymbol{\Sigma}_0$, has an upper control limit of $L_u = \chi_{p,1-\alpha}^2$. This control chart is called a Phase II X^2 -chart or χ^2 control chart.

If $\boldsymbol{\mu}_0$ is replaced by $\bar{\bar{\mathbf{x}}}_0$, and $\boldsymbol{\Sigma}_0$ is replaced by $\bar{\bar{\mathbf{S}}}$, with $n > 1$ and $\bar{\mathbf{x}}_i$ the mean of the i th rational subgroup, then, according to Ryan¹⁰, the $D_i^2/c_0(p, m, n)$ statistic follows an F -distribution with p and $(mn - m - p + 1)$ degrees of freedom. Here $c_0(p, m, n) = [p(m - 1)(n - 1)](mn - m - p + 1)^{-1}$, $\bar{\bar{\mathbf{x}}}_0$ is the overall sample mean vector and $\bar{\bar{\mathbf{S}}}$ is the pooled sample variance–covariance matrix. Thus, a multivariate Shewhart control chart for the process mean, with unknown parameters, has the following control limit

$$L_u = \frac{[p(m - 1)(n - 1)]}{(mn - m - p + 1)} F_{1-\alpha, p, mn-m-p+1}$$

This control chart is called a Phase I T^2 -chart. We note that, for a Phase I T^2 -chart, the statement ‘if the process is in control the probability of at least one of the D_i^2 being outside the control limits is α ’ does not hold, because in this phase the D_i^2 are not independent (this is only valid for a given i). According to Woodall⁴ ‘To measure the statistical performance of a control chart in Phase I applications one considers the probability of any out-of-control signal with the chart. The false-alarm rate, for example, is the probability of at least one signal from the chart given that the process is in statistical control with some assumed probability distribution’. In practical problems, the T^2 -chart is typically recommended for the preliminary analysis of multivariate observations in process monitoring applications. Sullivan and Woodall¹⁴ discussed the problem of adapting control charts for the preliminary analysis of multivariate observations. They also recommend a method for preliminary analysis of multivariate observations that does not require simulation to determine the exact control limit, which is almost as effective as the multivariate CUSUM (MCUSUM) and multivariate EWMA (MEWMA) control charts in detecting a step shift. Nedumaran and Pignatiello¹⁵ considered the issue of constructing retrospective T^2 control chart limits to control the overall probability of a false alarm at a specified value. Furthermore, Mason *et al.*¹⁶ used the T^2 -chart for monitoring batch processes in both Phase I and Phase II operations. Recently, Kim *et al.*¹⁷ discussed the problem of Phase I analysis in the case where the quality of the process is characterized by a linear function. The authors recommend the use of a bivariate T^2 -chart in conjunction with a univariate Shewhart chart.

If $\boldsymbol{\mu}_0$ is replaced by $\bar{\bar{\mathbf{x}}}_0$ and $\boldsymbol{\Sigma}_0$ is replaced by $\bar{\bar{\mathbf{S}}}$, with $n > 1$ and $\bar{\mathbf{x}}_f$ the mean of a future rational subgroup, then the $D_f^2/c_1(p, m, n)$ statistic follows an F -distribution with p and $(mn - m - p + 1)$ degrees of freedom, where $c_1(p, m, n) = [p(m + 1)(n - 1)](mn - m - p + 1)^{-1}$. Thus, a multivariate Shewhart control chart for

the process mean, with unknown parameters, has the following control limit

$$L_u = \frac{p(m+1)(n-1)}{mn-m-p+1} F_{1-\alpha, p, mn-m-p+1}$$

This control chart is called a Phase II T^2 -chart.

The average run length

The average run length (ARL) of the multivariate Shewhart chart when the process is in control and $\boldsymbol{\mu}_0$ and $\boldsymbol{\Sigma}_0$ are known can be calculated as $ARL_0 = 1/\alpha$, where α is the probability that D_i^2 exceeds L_u under the assumption that the process is in control. Furthermore, the out-of-control ARL (ARL_1) of the multivariate Shewhart chart depends on the mean vector and variance-covariance matrix only through the non-centrality parameter $\lambda^2(\boldsymbol{\mu}_1)$

$$\lambda^2(\boldsymbol{\mu}_1) = n(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^t \boldsymbol{\Sigma}_0^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) = n\boldsymbol{\delta}^t \boldsymbol{\Sigma}_0^{-1} \boldsymbol{\delta}$$

where $\boldsymbol{\mu}_1 = \boldsymbol{\mu}_0 + \boldsymbol{\delta}$ is a specific out-of-control mean vector, bearing in mind that the $\boldsymbol{\Sigma}_0$ is still in control. Hence, it is possible to consider the ARL_1 as a function of $\lambda(\boldsymbol{\mu}_1)$, the square root of $\lambda^2(\boldsymbol{\mu}_1)$, and to construct an ARL_1 curve by using the equation $ARL_1 = 1/(1 - \beta)$, where β is the probability of the event 'The procedure fails to diagnose an out-of-control situation'. In the literature (see, e.g., Pignatiello and Runger¹⁸), in cases in which it has been proven that the ARL depends only on the non-centrality parameter, the proofs were based on the assumptions that (i) $\boldsymbol{\Sigma}_0$ is the known variance-covariance matrix, and (ii) random sampling is carried out independently of a multivariate normal distribution.

The theory presented so far considers the case of a predefined and fixed n sample size. Jolayemi¹⁹ presented a power function model for determining sample sizes for the operation of a multivariate process control chart. Also, Aparisi²⁰ gave a procedure for the construction of a control chart with adaptive sample sizes.

Control charts for the process mean ($n = 1$)

For charts constructed using individual observations ($n = 1$), the test statistic for the i th individual observation has the form

$$D_i^2 = (\mathbf{x}_i - \boldsymbol{\mu}_0)^t \boldsymbol{\Sigma}_0^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_0)$$

where \mathbf{x}_i is the i th, $i = 1, 2, \dots, m$, observation following $N_p(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$, where $\boldsymbol{\mu}_0$ and $\boldsymbol{\Sigma}_0$ are the known vector of means and the known variance-covariance matrix, respectively. Moreover, we assume that the observations \mathbf{x}_i are not time dependent. The D_i^2 statistic follows a χ^2 -distribution with p degrees of freedom (Seber²¹). Thus, a multivariate Shewhart control chart for the process mean, with known mean vector $\boldsymbol{\mu}_0$ and known variance-covariance matrix $\boldsymbol{\Sigma}_0$, has a control limit $L_u = \chi_{p, 1-\alpha}^2$. This control chart is called a Phase II X^2 -chart.

If $\boldsymbol{\mu}_0$ is replaced by $\bar{\mathbf{x}}_0$, $\boldsymbol{\Sigma}_0$ is replaced by \mathbf{S}_0 and \mathbf{x}_i is the i th individual observation, which is not independent of the estimators $\bar{\mathbf{x}}_0$ and \mathbf{S}_0 , then the $D_i^2/d_0(m)$ statistic follows a β -distribution with $p/2$ and $(m - p - 1)$ degrees of freedom, where $d_0(m) = (m - 1)^2 m^{-1}$. Thus, a multivariate Shewhart control chart for the process mean, with unknown parameters, has the following upper control limit (Tracy *et al.*²²)

$$L_u = \frac{(m-1)^2}{m} B_{1-\alpha, p/2, (m-p-1)/2}$$

where $\bar{\mathbf{x}}_0$ is the overall sample mean and \mathbf{S}_0 is the overall sample variance-covariance matrix. This control chart is called a Phase I T^2 -chart. Tracy *et al.*²² also provided an analogous lower control limit. Alternative estimators of the variance-covariance matrix have been proposed by Sullivan and Woodall²³ and Chou *et al.*²⁴.

If $\boldsymbol{\mu}_0$ is replaced by $\bar{\mathbf{x}}_0$, $\boldsymbol{\Sigma}_0$ is replaced by \mathbf{S}_0 and \mathbf{x}_f is a future individual observation, which is independent of the estimators $\bar{\mathbf{x}}_0$ and \mathbf{S}_0 , then the $D_f^2/d_1(m, p)$ statistic follows an F -distribution with p and $(m - p)$ degrees

of freedom, where $d_1(m, p) = p(m + 1)(m - 1)[m(m - p)]^{-1}$. Thus, a multivariate Shewhart control chart for the process mean, with unknown parameters, has the following upper control limit (Tracy *et al.*²²)

$$L_u = \frac{p(m + 1)(m - 1)}{m(m - p)} F_{1-\alpha, p, m-p}$$

This control chart is called a Phase II T^2 -chart. Tracy *et al.*²² also provide an analogous lower control limit.

Control charts for the process dispersion

In the following, multivariate control charts for controlling process dispersion are presented. In the previous two sections, it was assumed that process dispersion remained constant and was equal to Σ . This assumption is generally not true and must be validated in practice. Process variability is summarized in the $p \times p$ variance-covariance matrix Σ , which contains $p \times (p + 1)/2$ parameters. There are two single-number quantities for measuring the overall variability of a set of multivariate data. These are: (1) the determinant of the variance-covariance matrix, $|\Sigma|$, which is called the generalized variance—the square root of this quantity is proportional to the area or volume generated by a set of data; (2) the trace of the variance-covariance matrix, $\text{tr}\Sigma$, which is the sum of the variances of the variables. In this section, two different control charts for the process dispersion are presented since different statistics can be used to describe variability.

Assume that the vector \mathbf{x} follows a $N_p(\mu_0, \Sigma_0)$ distribution, and that there are m samples of size $n > 1$ available. The first multivariate chart for the process dispersion, presented by Alt¹¹, can be based on the sequence of the following statistic

$$W_i = -pn + pn \ln n - n \ln[|\mathbf{A}_i| |\Sigma_0|^{-1}] + \text{tr}(\Sigma_0^{-1} \mathbf{A}_i)$$

for the i th, $i = 1, 2, \dots, m$, sample, where $\mathbf{A}_i = (n - 1)\mathbf{S}_i$ and \mathbf{S}_i is the sample variance-covariance matrix of the i th rational subgroup. The W_i statistic follows an asymptotic χ^2 -distribution with $p \times (p + 1)/2$ degrees of freedom. Thus, a multivariate Shewhart control chart for the process dispersion, with known mean vector μ_0 and known variance-covariance matrix Σ_0 , has an upper control limit of $L_u = \chi_{p(p+1)/2, 1-\alpha}^2$. Hence, if the value of the test statistic W_i plots above L_u , the chart signals a potential out-of-control process. This control chart is called a Phase II W -chart.

The second chart is based on the sample generalized variance $|\mathbf{S}|$, where \mathbf{S} is the $p \times p$ sample variance-covariance matrix. One approach in developing an $|\mathbf{S}|$ -chart is to utilize its distributional properties. Alt¹¹ and Alt and Smith²⁵ stated that if there are two quality characteristics, then

$$[2(n - 1)|\mathbf{S}|^{1/2}]|\Sigma_0|^{-1/2} \sim \chi_{2n-4}^2$$

Thus, the control limits for an $|\mathbf{S}|$ -chart are

$$L_u = [|\Sigma_0|(\chi_{2n-4, 1-\alpha/2}^2)^2][2(n - 1)]^{-2}$$

$$L_l = [|\Sigma_0|(\chi_{2n-4, \alpha/2}^2)^2][2(n - 1)]^{-2}$$

In a paper by Aparisi *et al.*²⁶, the distribution of the $|\mathbf{S}|$ -chart is studied and suitable control limits are obtained for the situation in which there are more than two variables. In addition, Alt¹¹ proposed a second approach in developing an $|\mathbf{S}|$ -chart by using only the first two moments of $|\mathbf{S}|$ and the property that most of the probability distribution of $|\mathbf{S}|$ is contained in the interval

$$E[|\mathbf{S}|] \pm 3\sqrt{V[|\mathbf{S}|]}$$

Also, Alt and Smith²⁵ proposed the $|\mathbf{S}|^{1/2}$ -chart. Furthermore, Alt¹¹ gave a proper unbiased estimator for $|\Sigma_0|$, in order to define a Phase I control chart for controlling process dispersion. Aparisi *et al.*²⁷ proposed the design of the $|\mathbf{S}|$ -chart with adaptive sample size to control process defined by two quality characteristics.

Although $|\mathbf{S}|$ is a widely used measure of multivariate variability, it is a relative simplistic scalar representation of a complex multivariate structure. Therefore, its use can be misleading in some cases. Lowry and Montgomery⁸ presented three sample covariance matrices for bivariate data that all have the same generalized variance and yet have different correlations. Thus, it is often desirable to provide more than the single number $|\mathbf{S}|$ as a summary of \mathbf{S} . The use of univariate dispersion charts as supplementary to a control chart for $|\mathbf{S}|$ was proposed by Alt¹¹. In detecting changes in one or more of the variances (standard deviations), the $|\mathbf{S}|$ procedure would not perform as well as when using separate univariate dispersion charts. However, the question ‘How would one examine the data to see whether the signal may have occurred because of a change in one or more covariances/correlations between quality measurements?’ still remains. Mason *et al.*²⁸ examined the process conditions that lead to the occurrence of certain non-random patterns in a T^2 control chart while Low *et al.*²⁹ proposed a neural network procedure for detecting variations in the variances, with the assumption that the mean value of the multiple quality characteristics of a process is under control. Surtihadi *et al.*³⁰ considered several special cases of a process displacement affecting the covariance matrix and have developed control charts (both Shewhart-type and CUSUM) to detect these process changes.

Alternative charts

In this section, some alternative charts for controlling the mean or the dispersion of the process are pointed out. Hayter and Tsui³¹ proposed the use of independent control charts with exact simultaneous limits for monitoring the process mean. Guerrero³² has developed a control chart to determine the correlation structure of a multivariate process, by using the concept of ‘mutual information’. Also, Guerrero³³, proposed a ‘conditional entropy approach’ in which the correlation matrix is known or fixed. Two new overall variability measures have been defined based on the sample variances and ranges of the variables under consideration. Tang and Barnett³⁴ proposed the decomposition of the real variance–covariance matrix Σ_0 or the sample variance–covariance matrix $\bar{\mathbf{S}}$ into various statistically independent components each having a physical interpretation and known distribution. The problem with this method is that the ordering of the variables is not unique, so for a large p there are $p!$ possible permutations. Also, Tang and Barnett³⁵ compared their methods with various competing procedures. Moreover, Spiring and Cheng³⁶ demonstrated the use of an alternative control chart for controlling both the mean and the dispersion of a process. Sullivan and Woodall³⁷ introduced a preliminary control chart for detecting a shift in the mean vector, the covariance matrix or both, when multivariate individual observations are available, while Vargas³⁸ proposed a T^2 control chart based on robust estimators of location and dispersion, working with individual observations. Feltz and Shiau³⁹ proposed a control chart based on the empirical Bayesian approach. Wurl *et al.*⁴⁰ have developed a methodology to monitor a batch process during the start-up stage to reduce the length of this stage. Based on the problem of intrusion into an information system, Ye and Chen⁴¹, in order to overcome the scalability problem of Hotelling’s T^2 test when it is applied to large amounts of data, proposed an alternative to the T^2 control chart which is based on a χ^2 distance metric statistic, while Emran and Ye⁴² discussed the robustness of the χ^2 distance metric. Ye *et al.*⁴³ also compared the effectiveness of the scalable χ^2 procedure introduced by Ye and Chen⁴¹ with Hotelling’s T^2 control chart for monitoring processes with uncorrelated data variables. Chang and Bai⁴⁴ proposed a method for constructing multivariate T^2 control charts for skewed populations based on weighted standard deviations. Kim *et al.*¹⁷ proposed control chart methods for process monitoring when the quality of a process is characterized by a linear function.

Aparisi *et al.*⁴⁵ have recently investigated the performance of Hotelling’s X^2 -chart with supplementary runs rules. Specifically, in addition to the classical out-of-control criterion (one point above the L_u), they suggested using three additional rules based on two out of three scans and runs of length 7 and 8. As indicated, for moderate shifts, the combined use of all supplementary rules improves the ARL_1 value of the X^2 -chart by approximately 25% (when ARL_0 is kept fixed). Furthermore, Koutras *et al.*⁴⁶ combined the theory of success runs and Hotelling’s X^2 -chart, and have arrived at a procedure which improves the (weak) performance of Hotelling’s X^2 -chart in the case of relatively small mean vector shifts. The smooth performance of the suggested variation may be attributed, on the one hand, to the increased sensitivity of the runs statistic in detecting clustering of similar results and, on the other hand, to the substantial descriptive power of the X^2 -chart. He and Grigoryan⁴⁷

have proposed a multivariate extension of a double-sampling \bar{X} control chart with at least two sampling stages while Grigoryan and He⁴⁸ have introduced a multivariate double-sampling |S| control chart for controlling shifts in the variance–covariance matrix.

Multiaattributes control charts

In the literature, little work has been carried out that deals with multivariate attributes processes, which are very important in practical production processes. The first paper to deal with the methods of quality control, when the p -dimensional observations are coming from a multivariate binomial or multivariate Poisson population, was presented by Patel⁴⁹. Patel⁴⁹, assuming approximate normality, proposes an X^2 -chart. Lu *et al.*⁵⁰ gave a multivariate attribute control chart (MACC) which is a straightforward extension of the univariate np -chart and is called the MNP-chart. Also, Jolayemi⁵¹ gave a MACC that is based on an approximation for the convolution of independent binomial variables and on an extension of the univariate np -chart. Recently, Skinner *et al.*⁵² have developed a procedure for monitoring multiple discrete counts. This procedure is based on the likelihood ratio statistic for Poisson counts when input variables are measurable.

Autocorrelated multivariate processes

A process with serially correlated data may signal incorrectly and weaken the effectiveness of a control chart. On the other hand, detection and evaluation of the form of multivariate autocorrelation is quite difficult. A solution to this problem is to fit a time-series model to the multivariate data. Chan and Li⁵³ and Charnes⁵⁴ presented extensions of multivariate Shewhart charts that account for both autocorrelation within the process and correlation across the variables of a multivariate process.

A special type of autocorrelation that occurs in multivariate data is referred to as the multivariate step process. This occurs with decay processes such as continuous wear on equipment, with environmental contamination of equipment and with the depletion of certain components in a process. This type of autocorrelation, which is discussed by Mason *et al.*⁵⁵, may initially appear to be a location shift of the distribution, but on closer examination is a stage or step-change autocorrelation.

In many situations, the presence of measurement error arises when implementing process control. Fong and Lawless⁵⁶ and Lina *et al.*⁵⁷ presented models for correlated process variables with measurement error. Mastrangelo and Forrest⁵⁸ presented a program that can be used to generate multivariate data from a first-order vector autoregressive model with a shift in the mean vector of the noise series. The data can then be used to compare the shift detection properties of the multivariate control chart methods. Krogstad⁵⁹ also gave a method for simulating a multivariate Gaussian time series. Apley and Tsung⁶⁰ examined the use of Hotelling's T^2 -chart to monitor an autocorrelated process, while Dyer *et al.*⁶¹ provided a simulation study and evaluation of several multivariate approaches with regard to various autoregressive moving average ARMA(1,1) and autoregressive AR(1) processes, and a comparison with their univariate counterparts. Jiang⁶² gives a multivariate control chart for monitoring autocorrelated processes, which has an intrinsic relationship with the residuals-based generalized likelihood ratio test procedure discussed in the literature. Mahmoud and Woodall⁶³ studied the Phase I analysis of data when the quality of a process or product is characterized by a linear function. They assumed that simple linear regression data are available for a fixed number of samples collected over time, a situation common in calibration applications. Using a simulation study, they compared the performance of some of the recommended approaches used to assess the stability of the process. They also proposed a method based on using indicator variables in a multiple regression model. Woodall *et al.*⁶⁴ discussed the general issue involved in using control charts to monitor processes, which is better characterized by a relationship between a response variable and one or more explanatory variables. Also, Kalgonda and Kulkarni⁶⁵ proposed a multivariate quality control chart for autocorrelated processes in which observations can be modeled as a first-order autoregressive process.

Non-parametric schemes

Shewhart-type control charts require the assumption of multivariate normality. If the multivariate normal is not an appropriate model, there is very little literature available on alternative multivariate charting techniques.

An exception is the non-parametric control chart procedures put forward by Liu⁶⁶, who introduced several control charts using the concept of data depth. These charts are in the form of two-dimensional graphs for any p -dimensional observation. They can detect both shifts in the process mean and shifts of the process dispersion. According to Mason *et al.*⁶⁷, the methods introduced by Liu⁶⁶ assume that no standards are given, but the procedure may suffer some loss in the effectiveness of detecting a signal if the data follow a multivariate normal distribution.

Furthermore, the use of simulation to obtain accurate limits is an option in the absence of multivariate normality. Given a sufficiently large historical data set, one should be able to obtain reasonably accurate control limits by fitting a distribution to the variables. The use of simulation and bootstrap methods in process control has been discussed by Liu and Tang⁶⁸. A new robust Shewhart-type control chart for monitoring the location of a bivariate process using Hodges–Lehmann and Shamos–Bickel–Lehmann estimators has been introduced by Abu-Shawiesh and Abdullah⁶⁹.

Chou *et al.*⁷⁰ proposed a method to determine control limits, working with individual observations, in the case where the data come from a non-normal distribution. Sun and Tsung⁷¹ introduced a kernel-based multivariate control chart using support vector methods when the underlying distribution of the quality characteristics departs from normality. Also, Stoumbos and Sullivan⁷² investigated the effects of non-normality on the statistical performance of the MEWMA, and its special case, the X^2 -chart, while Qiu and Hawkins⁷³ propose a distribution-free CUSUM-type control chart. This chart is based on the ranks of the measurements, while Qiu and Hawkins⁷⁴ introduced a non-parametric CUSUM procedure which is based both on the order of information within the measurement components and on the order of information between the measurement components and their in-control means. Thissen *et al.*⁷⁵ used a combination of mixture modeling and multivariate statistical process control as a method for process monitoring in case of non-normality.

Chakraborti *et al.*⁷⁶ noted that, although multivariate process control problems are important, multivariate non-parametric statistical process techniques are not sufficiently well developed. From the above it is obvious that there is much more work to do in this area.

Economic models

Jolayemi and Berretoni⁷⁷ proposed an economic model that can be optimized to obtain the sample size, the intersample interval and the upper control limit, which minimizes the cost of operating a multivariate control chart. In addition, Jolayemi and Berretoni⁷⁸ presented another economic model for the optimal design of multivariate control charts in the presence of multiple assignable causes. Jolayemi⁷⁹ has developed a statistical model for the design of multivariate control charts with multiple control regions. The model produces the sample size and values of the control limits needed for the operation of a multivariate control chart with multiple control regions. Serel *et al.*⁸⁰ proposed the use of independent \bar{X} -charts, one for each of the p variables, with unequal probabilities, which the test statistic plots beyond the control limits under an in-control state, while Molnau *et al.*⁸¹ showed that the economic statistical design of a MEWMA gives better statistical properties without significantly increasing optimal total costs. Chou *et al.*⁸² have developed a procedure for the economic–statistical design of multivariate control charts by using a quality-loss function for monitoring the process mean vector and covariance matrix simultaneously. Noorossana *et al.*⁸³ summarized the assumptions as well as the consequences made regarding the out-of-control process shift in the economic design of multivariate control charts, while Love and Linderman⁸⁴ discussed the economic design of the MEWMA control chart. They concluded that the cost of the economic design of the MEWMA chart is not substantially affected by misspecification of the shape of the distribution of the process failure mechanism.

3. MCUSUM AND MEWMA CONTROL CHARTS

Multivariate Shewhart-type control charts use information only from the current sample and they are relatively insensitive to small and moderate shifts in the mean vector. MCUSUM and MEWMA control charts have been developed to overcome this problem.

CUSUM-type control charts

MCUSUM control charts are placed into two major categories. In the first, the direction of the shift (or shifts) is considered to be known (direction-specific schemes), whereas in the second the direction of the shift is considered to be unknown (directionally invariant schemes).

We first present CUSUM control charts, for which we assume that the direction of the shift (or shifts) is known. Woodall and Ncube⁸⁵ describe how a p -dimensional multivariate normal process can be monitored by using p univariate CUSUM charts for the p original variables or by using p univariate CUSUM charts for the p principal components. This multiple univariate CUSUM scheme is called the MCUSUM. The MCUSUM gives an out-of-control signal whenever any of the univariate CUSUM charts does likewise. ARL performance in a multivariate process is studied in relation to independent and dependent quality characteristics.

Healy⁸⁶ uses the fact that CUSUM charts can be viewed as a series of sequential probability ratio tests, in order to develop a MCUSUM chart. Let \mathbf{x}_i be the i th observation, which derives from $N_p(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ with an in-control $p \times 1$ mean vector $\boldsymbol{\mu}_0$ and a known $p \times p$ common variance–covariance matrix $\boldsymbol{\Sigma}_0$. Let $\boldsymbol{\mu}_1$ be the out-of-control $p \times 1$ vector of means. The CUSUM for detecting a shift in $\boldsymbol{\mu}_0$ towards $\boldsymbol{\mu}_1$ may be written as

$$S_i = \max[(S_{i-1} + \mathbf{a}^t(\mathbf{x}_i - \boldsymbol{\mu}_0) - 0.5\lambda(\boldsymbol{\mu}_1)), 0]$$

where $\lambda(\boldsymbol{\mu}_1)$ is the square root of the non-centrality parameter and $\mathbf{a}^t = [(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^t \boldsymbol{\Sigma}_0^{-1}] / \lambda(\boldsymbol{\mu}_1)$. This CUSUM scheme signals when $S_i \geq H$. As is clear, this CUSUM procedure reduces to a univariate procedure for detecting a shift in the mean of a normal variable. That is, all of the available theory for calculating ARL, H and S_0 for a univariate normal CUSUM can also be used for this multivariate normal CUSUM. A similar procedure is proposed by Healy⁸⁶ for controlling process dispersion. The CUSUM for detecting a change in the variance–covariance matrix, of the form $\boldsymbol{\Sigma}_1 = C\boldsymbol{\Sigma}_0$ (C is a real constant), may be written as

$$S_i = \max[(S_{i-1} + D_i^2 - K), 0]$$

where $K = p \log C / (C - 1)$ and $D_i^2 = (\mathbf{x}_i - \boldsymbol{\mu}_0)^t \boldsymbol{\Sigma}_0^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_0)$. This CUSUM scheme signals when $S_i \geq H$. We have been unable to find any proposal in the literature for an analogous charting procedure in the case where the mean vector and the variance–covariance matrix have to be estimated. Healy⁸⁶ has also proposed a lower-sided version of this CUSUM chart.

Hawkins⁸⁷ introduced CUSUMs for regression-adjusted variables based on the idea that the most common situation found in practice is departures from control having some known structure. In particular, it is assumed that the mean shifts with magnitude δ in only one variable.

Consider the multiple regression of X_j , the j th variable of \mathbf{x} , on all other variables of \mathbf{x} . Let Z_j be the residual corresponding to the linear regression of the j th variable on the rest of the variables, and suppose that Z_j has been rescaled to have unit variance. The Z_j may be used to determine whether there is a shift in the $\boldsymbol{\mu}_j$. The regression residual Z_j is given by $\mathbf{z} = [\text{diag}(\boldsymbol{\Sigma}^{-1})]^{-1/2} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_0)$, whose in-control distribution is $N(0, 1)$. Hawkins^{87,88} proposed to chart each Z_j using a CUSUM procedure because, in general, it is not known which of the p variables is out of control. For studying p individual charts simultaneously, Hawkins⁸⁷ proposed the following overall group diagnostics

$$MCZ = \max(L_{i,j}^+, -L_{i,j}^-) \quad \text{and} \quad ZNO = \sum_{j=1}^p (L_{i,j}^+ + L_{i,j}^-)^2$$

where $L_{i,j}^+ = \max(0, L_{i-1,j}^+ + Z_{i,j} - k)$, $L_{i,j}^- = \min(0, L_{i-1,j}^- + Z_{i,j} + k)$, $L_{0,j}^+ = L_{0,j}^-$, for $i = 1, 2, \dots, m$. MCZ is the MCUSUM statistic, introduced by Woodall and Ncube⁸⁵, applied to the CUSUM for \mathbf{z} . ZNO is the squared Euclidean norm of the resultant vectors of the CUSUM for upward and downward shifts in the mean. The CUSUMs L^+ , L^- test for shifts in location in the upward and downward directions, respectively. The plot of these CUSUMs on a common chart gives a better-performing CUSUM control chart for location. An out-of-control signal occurs when any of these four CUSUMs exceeds the decision interval h . The values of h and k are selected as in any univariate CUSUM chart because each is based on a single random variable that follows

the $N(0, 1)$ distribution. An out-of-control signal is indicated when MCZ and ZNO exceed a threshold value set to fix the in-control ARL. Hauck *et al.*⁸⁹ applied multivariate statistical process monitoring and diagnosis with grouped regression-adjusted variables.

Crosier⁹⁰ proposed two new multivariate CUSUM schemes. The first scheme is based on the square root of Hotelling's T^2 statistic, while the second can be derived by replacing the scalar quantities of a univariate CUSUM scheme with vectors. Moreover, Pignatiello and Runger¹⁸ introduced two new MCUSUM schemes. They refer to these MCUSUM charts as MCUSUM #1 and MCUSUM #2. Crosier⁹⁰ and Pignatiello and Runger¹⁸ have established MCUSUM schemes for cases where the direction of the shift is considered to be unknown.

The first CUSUM proposed by Crosier⁹⁰ is a CUSUM of the scalar D_i , the square root of the D_i^2 statistic, and is given by

$$S_i = \max[(S_{i-1} + D_i - K), 0], \quad i = 1, 2, 3, \dots$$

where $S_0 \geq 0$ and $K \geq 0$. This scheme signals when $S_i \geq H$, which is determined using the Markov chain approach. Crosier⁹⁰ noted that a search for the optimal K produces a sequence that closely resembles the square root of the number of variables.

A similar CUSUM was proposed by Pignatiello and Runger¹⁸, defined as

$$S_i = \max[0, S_{i-1} + D_i^2 - k], \quad i = 1, 2, 3, \dots$$

with $S_0 = 0$, and k chosen to be $0.5\lambda^2(\mu_1) + p$. The process is out of control if S_i exceeds an upper control limit H . Pignatiello and Runger¹⁸ used a Markov chain approach to determine the values of H .

Crosier⁹⁰ and Pignatiello and Runger¹⁸ found that ordinary one-sided univariate CUSUMs based on successive values of the D_i^2 or D_i statistic, respectively, do not have good ARL properties.

The second CUSUM proposed by Crosier⁹⁰ is a CUSUM of vectors. A vector-valued scheme can be derived by replacing the scalar quantities of a univariate CUSUM scheme with vectors and is given by

$$\gamma_i = [\mathbf{S}_i^t \boldsymbol{\Sigma}_0^{-1} \mathbf{S}_i]^{1/2}, \quad i = 1, 2, 3, \dots$$

where $\mathbf{S}_i = (\mathbf{S}_{i-1} + \mathbf{x}_i - \boldsymbol{\mu}_0)(1 - kC_i^{-1})$, if $C_i > k$ and $\mathbf{S}_i = \mathbf{0}$ otherwise and $C_i = [(\mathbf{S}_{i-1} + \mathbf{x}_i - \boldsymbol{\mu}_0)^t \boldsymbol{\Sigma}_0^{-1} (\mathbf{S}_{i-1} + \mathbf{x}_i - \boldsymbol{\mu}_0)]^{1/2}$. This scheme signals when $\gamma_i > h$, which is chosen to provide a predefined in-control ARL by simulation. Owing to the fact that ARL performance of this chart depends on the non-centrality parameter, Crosier⁹⁰ recommended that $k = \lambda(\mu_1)/2$ and $\mathbf{S}_0 = \mathbf{0}$. Both CUSUMs, as proposed by Crosier⁹⁰, allow the use of recent enhancements in CUSUM schemes. Among the CUSUM schemes proposed by Crosier⁹⁰, the vector-valued scheme has a better ARL performance than the scalar scheme.

The second CUSUM proposed by Pignatiello and Runger¹⁸ can be constructed by defining MC_i as

$$MC_i = \max\{[\mathbf{D}_i^t \boldsymbol{\Sigma}_0^{-1} \mathbf{D}_i]^{1/2} - kn_i, 0\}, \quad i = 1, 2, 3, \dots$$

where $MC_0 = 0$, k is chosen to be $0.5\lambda(\mu_1)$, μ_1 is a specified out-of-control mean

$$\mathbf{D}_i = \sum_{l=i-n_i+1}^i (\mathbf{x}_l - \boldsymbol{\mu}_0)$$

and n_i is the number of subgroups since the most recent renewal (i.e. zero value) of the CUSUM chart, formally defined as

$$n_i = \begin{cases} n_{i-1} + 1 & \text{if } MC_{i-1} > 0 \\ 1 & \text{otherwise} \end{cases}$$

This chart operates by plotting MC_i on a control chart with an upper control limit of H (H is investigated by simulation). If MC_i exceeds H , then the process is out of control. Pignatiello and Runger¹⁸ proved that the ARL

performance of the MC_i -chart depends only on the square root of the non-centrality parameter and that it is better in relation to γ_i .

Ngai and Zhang⁹¹ gave a natural multivariate extension of the two-sided cumulative sum chart for controlling the process mean. Also, Chan and Zhang⁹² propose cumulative sum charts for controlling the covariance matrix.

Finally, as has already been mentioned, Qiu and Hawkins^{73,74} proposed non-parametric CUSUM-type control chart procedures.

Runger and Testik⁹³ provided a comparison of the advantages and disadvantages of MCUSUM schemes, as well as performance evaluations and a description of their interrelationships. A new derivation was also provided and extensive simulation results that include initial and steady-state conditions were presented. Geometric descriptions were used, and names were proposed based on these geometric characteristics.

MEWMA charts

MEWMA charts are the second category of charts examined. Let \mathbf{x}_i^t be the i th, p -dimensional observation. Also, assume that \mathbf{x}_i follows a $N_p(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ with a known variance–covariance matrix $\boldsymbol{\Sigma}$ and a known p -dimensional mean vector $\boldsymbol{\mu}_0$. A MEWMA control chart is proposed by Lowry *et al.*⁹⁴ as follows

$$\mathbf{z}_i = \mathbf{R}\mathbf{x}_i + (\mathbf{I} - \mathbf{R})\mathbf{z}_{i-1} = \sum_{j=1}^i \mathbf{R}(\mathbf{I} - \mathbf{R})^{i-j} \mathbf{x}_j, \quad i = 1, 2, 3, \dots$$

where $\mathbf{R} = \text{diag}(r_1, r_2, \dots, r_p)$ and $0 \leq r_k \leq 1$ for $k = 1, 2, 3, \dots, p$, and \mathbf{I} is the identity matrix. If there is no *a priori* reason to weight past observations differently for the p quality characteristics being monitored, then $r_1 = r_2 = \dots = r_p = r$. The initial value \mathbf{z}_0 is usually obtained as equal to the in-control mean vector of the process. It is obvious that if $\mathbf{R} = \mathbf{I}$, then the MEWMA control chart is equivalent to the T^2 -chart. The MEWMA chart gives an out-of-control signal if $\mathbf{z}_i^t \boldsymbol{\Sigma}_{\mathbf{z}_i}^{-1} \mathbf{z}_i > h$, where $\boldsymbol{\Sigma}_{\mathbf{z}_i}$ is the variance–covariance matrix of \mathbf{z}_i . The value h is calculated by simulation to achieve a specified in-control ARL. The ARL performance of the MEWMA control chart depends only on the non-centrality parameter, but in the case where unequal weighting constants are used, the ARL depends on the direction of the shift. This means that the MEWMA has the property of directional invariance. The variance–covariance matrix of \mathbf{z}_i is calculated via the following formula

$$\boldsymbol{\Sigma}_{\mathbf{z}_i} = \sum_{j=1}^i \text{Var}[\mathbf{R}(\mathbf{I} - \mathbf{R})^{i-j} \mathbf{x}_j] = \sum_{j=1}^i \mathbf{R}(\mathbf{I} - \mathbf{R})^{i-j} \boldsymbol{\Sigma} (\mathbf{I} - \mathbf{R})^{i-j} \mathbf{R}$$

or when $r_1 = r_2 = \dots = r_p = r$

$$\boldsymbol{\Sigma}_{\mathbf{z}_i} = (1 - (1 - r)^{2i})r/(2 - r)\boldsymbol{\Sigma}$$

An approximation of the variance–covariance matrix $\boldsymbol{\Sigma}_{\mathbf{z}_i}$ for i approaches $+\infty$ as follows

$$\boldsymbol{\Sigma}_{\mathbf{z}_i} = r/(2 - r)\boldsymbol{\Sigma}$$

However, the use of the exact variance–covariance matrix of the MEWMA leads to a natural fast initial response for the MEWMA chart. Inertia problems may occur with the MEWMA chart and the simultaneous use of a Shewhart-type chart is proposed.

Lowry *et al.*⁹⁴ studied the ARL of the MEWMA. The ARL performance of the MEWMA procedure depends only on $\boldsymbol{\mu}_0$ and $\boldsymbol{\Sigma}_0$ through the value of the non-centrality parameter. Since the MEWMA, the MCUSUM #1 and the vector CUSUM are all directionally invariant, these three charts can be compared with each other and with Hotelling's T^2 -chart. Such a comparison shows that the ARL performance of the MEWMA is at least as good as that of the vector-valued CUSUM and MCUSUM #1. Testik *et al.*⁹⁵ discussed the robustness properties of MEWMA control charts in the case where the data follow multivariate t and multivariate gamma distributions. Their study is an extension of the work by Borrór *et al.*⁹⁶ for the univariate EWMA control chart.

Rigdon^{97,98} gave an integral and a double-integral equation for the calculation of in-control and out-of-control ARLs, respectively. Moreover, Bodden and Rigdon⁹⁹ have developed a computer program for approximating the in-control ARL of the MEWMA chart. Runger and Prabhu¹⁰⁰ use a Markov chain approximation to determine the run-length performance of the MEWMA chart. In addition, Prabhu and Runger¹⁰¹ provide recommendations for the selection of parameters for a MEWMA chart. Molnau *et al.*¹⁰² presented a program that enables the calculation of the ARL for the MEWMA when the values of the shift in the mean vector, the control limit and the smoothing parameter are known.

Kramer and Schmid¹⁰³ proposed a generalization of the MEWMA control scheme of Lowry *et al.*⁹⁴ for multivariate time-dependent observations. Sullivan and Woodall¹⁴ recommended the use of a MEWMA for the preliminary analysis of multivariate observations. Fasso¹⁰⁴ has developed a one-sided MEWMA control chart based on the restricted maximum likelihood estimator.

Yumin¹⁰⁵ proposed the construction of a MEWMA using the principal components of the original variables. Choi *et al.*¹⁰⁶ proposed a general MEWMA chart in which the smoothing matrix is full instead of one having only diagonal. The performance of this chart appears to be better than that of the MEWMA proposed by Lowry *et al.*⁹⁴. Choi and colleagues have also provided a computer program for the estimation of control limits (Hawkins *et al.*¹⁰⁷). Yeh *et al.*¹⁰⁸ introduced a MEWMA which is designed to detect small changes in the variability of correlated multivariate quality characteristics, while Chen *et al.*¹⁰⁹ proposed a MEWMA control chart that is capable of monitoring simultaneously the process mean vector and process covariance matrix. Runger *et al.*¹¹⁰ showed how the shift detection capability of the MEWMA can be significantly improved by transforming the original process variables to a lower-dimensional subspace through the use of the U -transformation. The U -transformation is similar to principal components transformation. Tseng *et al.*¹¹¹ proposed a MEWMA controller under a linear multiple-input–multiple-output model, while Castillo and Rajagopal¹¹² gave a multiple-input–multiple-output extension to the univariate double EWMA, which was first used by Butler and Stefani¹¹³. In general, there are several different approaches to the design of MEWMA control charts: (i) statistical design; (ii) economic-statistical design; and (iii) robust design. A review and a comparison of these design strategies is provided by Testik and Borror¹¹⁴. Yeh *et al.*¹¹⁵ gave a likelihood-ratio-based EWMA control chart that effectively monitors small changes of variability of multivariate normal processes.

Margavio and Conerly¹¹⁶ have developed two alternatives to the MEWMA chart. The first of these is an arithmetic multivariate moving average; the second is a truncated version of the MEWMA. Sullivan and Jones¹¹⁷ proposed a self-starting control chart for individual observations. The use of this chart is advantageous when production is slow. Reynolds and Kim¹¹⁸ proposed MEWMA charts based on sequential sampling in which the total sample size taken at a sampling point depends on current and past data, while Kim and Reynolds¹¹⁹ discussed the use of the MEWMA control chart for monitoring the process mean when sample sizes are unequal.

4. MULTIVARIATE STATISTICAL PROJECTION METHODS

The use of traditional multivariate Shewhart charts or MCUSUM and MEWMA schemes may be impractical for high-dimensional systems with collinearities. A common procedure for reducing the dimensionality of the variable space is the use of projection methods such as PCA and PLS. These two methods are based on building a model from a historical data set, which is assumed to be in control. After the model has been built, the future observation is checked as to whether it fits well in the model. These multivariate methods have the advantage that they can handle process variables and product quality variables. The PCA approach for monitoring process variables ($\mathbf{X}_{n \times q}$) is used when product quality data ($\mathbf{Y}_{n \times p}$) are not available in the historical data set. The PLS approach for monitoring process variables has been developed from historical data sets, with measurements from both the process ($\mathbf{X}_{n \times q}$) and the quality variables ($\mathbf{Y}_{n \times p}$) obtained during in-control operation.

Using PCA

The principal components method is a common multivariate procedure for reducing the dimensionality of the quality variable space (Jackson³). This method is based on a key result from matrix algebra: a $p \times p$ symmetric,

non-singular matrix, such as the sample variance–covariance matrix \mathbf{S} , may be reduced to a diagonal matrix \mathbf{L} by premultiplying and postmultiplying it by a particular orthonormal matrix \mathbf{U} such that $\mathbf{U}^t\mathbf{S}\mathbf{U} = \mathbf{L}$. The diagonal elements of L , $l_1 \geq l_2 \geq \dots \geq l_p$ are the characteristic roots, or eigenvalues, of S . The columns of \mathbf{U} are the characteristic vectors, or eigenvectors, of \mathbf{S} .

Furthermore, let \mathbf{x} and $\bar{\mathbf{x}}$ be $p \times 1$ vectors of observations of the original variables and their means, respectively. The transformed variables are the principal components of \mathbf{x} . The i th principal component is

$$Z_i = \mathbf{u}_i^t[\mathbf{x} - \bar{\mathbf{x}}]$$

and has mean zero and variance l_i under the assumption that the eigenvectors \mathbf{u}_i are normalized, that is $\mathbf{u}_i^t\mathbf{u}_i = 1$ for $i = 1, 2, \dots, p$. The quantity $l_i \times (l_1 + l_2 + \dots + l_p)^{-1}$ is the proportion of variability in the original data explained by the i th principal component, owing to the valid relationship $\text{tr}S = \text{tr}L = l_1 + l_2 + \dots + l_p$. The great advantage of this method is the reduction of the dimensionality. Since the first k ($k < p$) principal components explain the majority of the process variance they can be used for inferential purposes. In addition, the residual term $Q = (\mathbf{x} - \hat{\mathbf{x}})^t(\mathbf{x} - \hat{\mathbf{x}})$ exists because of the use of only the first k significant principal components, where $\hat{\mathbf{x}}$ is the estimated value of \mathbf{x} using the PCA model. Thus, the value k must be decided. A number of different methods for choosing k exist. In addition, Runger and Alt¹²⁰ presented a method for choosing k specifically for process control problems.

The method of principal components is very useful in multivariate quality control. Jackson³ presented three types of principal components control charts: (1) a T^2 control chart obtained from principal components scores; (2) a control chart for principal components residuals; and (3) a control chart for each independent principal component's scores. Thus, having established a PCA model based on historical data collected only when a common cause of variation was present, future multivariate observations can be projected onto the plane defined by the principal components loading vectors (U), to obtain their scores and the residuals.

In this section we are assuming that \mathbf{x}_i derives from a $N_p(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ distribution.

Control chart of principal components scores—working with individual observations ($n = 1$)

Principal components charts based on Hotelling's D_i^2 can be plotted for either all of the p principal components or the first k principal components. Using PCA, the original form of D_i^2 statistic, as can be easily derived from Jackson³, is transformed to

$$D_i^2 = \sum_{i=1}^k Z_i^2 l_i^{-1} + \sum_{i=k+1}^p Z_i^2 l_i^{-1}$$

If all p principal components are used, the critical value for D_i^2 , as given by Jackson³, is

$$L_u = p(m + 1)(m - 1)[m(m - p)]^{-1} F_{1-\alpha, p, m-p}$$

where the total number of independent individual observations is m . On the other hand, if the first k principal components are used, the critical value for D_i^2 is given by the same formula replacing p with k . Thus, if a D_i^2 value is greater than L_u , then the process is said to be out of control.

Control chart of PCs scores—working with rational subgroups ($n > 1$)

In the case where a number, m , of rational subgroups, each of size $n > 1$, are taken in a homogeneous time interval, the D_i^2 statistic for use with principal components has the following form

$$D_i^2 = n \left(\sum_{i=1}^k \bar{Z}_i^2 l_i^{-1} + \sum_{i=k+1}^p \bar{Z}_i^2 l_i^{-1} \right)$$

where \bar{Z}_i is the average of each of the p z -scores over the n observations in the subgroup. Thus, the critical value as given by Jackson³ is

$$L_u = p(m - 1)(n - 1)(mn - m - p + 1)^{-1} F_{1-\alpha, p, mn-m-p+1}$$

In the case where the first k principal components are used, the critical value is given by the same formula, replacing p with k . Consequently, if a D_i^2 value is greater than L_u then the process is said to be out of control.

Control chart of principal components residuals

The residual term Q can be tested by means of the sum of squares of the residuals (Jackson³)

$$Q = (\mathbf{x} - \widehat{\mathbf{x}})^t(\mathbf{x} - \widehat{\mathbf{x}}) = \sum_{i=k+1}^p l_i y_i^2 = \sum_{i=k+1}^p z_i^2$$

where $\widehat{\mathbf{x}} = \bar{\mathbf{x}} + \mathbf{Uz}$, \mathbf{U} is $p \times k$ and \mathbf{z} is $k \times 1$. The critical value for Q is

$$Q_\alpha = \vartheta_1 [c_\alpha (2\vartheta_2 h_0^2)^{1/2} \vartheta_1^{-1} + \vartheta_2 h_0 (h_0 - 1) \vartheta_1^{-2} + 1]^{1/h_0}$$

where $\vartheta_T = \sum_{i=k+1}^p l_i^T$, $h_0 = 1 - 2\vartheta_1 \vartheta_3 / \vartheta_2^2$ and c_α is the normal deviate cutting off an area of α under the upper tail of the distribution if h_0 is positive and under the lower tail if h_0 is negative. This distribution holds whether or not all of the significant components are used, even when some non-significant components are employed. The quantity c is approximately normally distributed with zero mean and unit variance, and is given by the formula

$$c = \vartheta_1 \times [(Q\vartheta_1^{-1})^h - (\vartheta_2 h_0 (h_0 - 1) \vartheta_1^{-2}) - 1] (2\vartheta_2 h_0^2)^{-1/2}$$

Another test statistic for the residuals has been proposed by Hawkins⁸⁷ using the unweighted sums of squares of the unretained principal components $D_i^2 = y_{k+1}^2 + \dots + y_p^2$, which is distributed as $k(m-1)(n-1)(mn - m - k + 1)^{-1} F_{1-\alpha, p-k, n-p+k}$.

In the case of m rational subgroups, each of size $n > 1$, the residual term can be tested by means of the sum of squares of the residuals $Q_M = n(\bar{\mathbf{x}} - \widehat{\bar{\mathbf{x}}})^t(\bar{\mathbf{x}} - \widehat{\bar{\mathbf{x}}})$, where $\widehat{\bar{\mathbf{x}}}$ is the predicted average vector. The Q_M statistic has the same distribution with the same degrees of freedom as for Q itself.

Univariate control charts of principal components scores

In the case where $n = 1$, the independent Z_i principal components can be charted for controlling the process in single univariate charts for each i . The control limits are $\pm Z_{1-\alpha/2} \sqrt{l_i}$ with $L_c = 0$ (center line), where $Z_{1-\alpha/2}$ is the corresponding $1 - \alpha/2$ percentile of the standard normal distribution. Moreover, in the case of rational subgroups, the independent Z_i principal components can be charted for controlling the process in single univariate charts for each i and the control limits are $L = \pm Z_{1-\alpha/2} \sqrt{l_i/n}$ with $L_c = 0$ (Jackson³).

PCA and autocorrelated data

The PCA method is also widely used in cases where data are autocorrelated. Ku *et al.*¹²¹ extended the use of PCA models in process monitoring to account for autocorrelation. Likewise, Runger¹²² proposed a model which allows autocorrelation and crosscorrelation in the data. Mastrangelo *et al.*¹²³ explored the use of PCA in autocorrelated processes. Wilkstrom *et al.*¹²⁴ applied ARMA models in principal components.

Alternative control charts using PCA

Several control charts using PCA have been proposed in the literature. The first is the U^2 -chart (U transformation is similar to PCA transformation) proposed by Runger¹²⁵.

Chen *et al.*¹²⁶ proposed a robust PCA approach via hybrid projections pursuit. Nijhuis *et al.*¹²⁷ demonstrated the use of PCA by applying process control in chromatography, while Nijhuis *et al.*¹²⁸ proposed a new control chart based on PCA that is called the $(TC)^2$ -chart; it is used for applying process control in gas chromatography. Furthermore, Wilkstrom *et al.*¹²⁹ applied multivariate statistical process control to an electrolysis process. A mixed control chart is presented which permits the simultaneous monitoring of principal component scores and principal component residuals; it is called the SMART-chart (Simultaneous Monitoring And Residuals Tracking). Wilkstrom *et al.*¹²⁴ apply multivariate statistical process control to an electrolysis process, incorporating PCA, PLS and ARMA techniques into the analysis.

Tsung¹³⁰ presented a method focused on process control schemes that are based on a combination of the process outputs and automatic control actions using adaptive PCA. Chiang *et al.*¹³¹ discussed the use of discriminant analysis, PCA and PLS for fault diagnosis in chemical processes. Norvilas *et al.*¹³² have developed an intelligent process-monitoring and fault-diagnosis environment by interfacing multivariate statistical process control monitoring techniques and knowledge-based systems for monitoring multivariate process operation. Lane *et al.*¹³³ proposed an extension to PCA which enables the simultaneous monitoring of a number of product grades or recipes. Schippers¹³⁴ proposed an integrated process control model using statistical process control, total productivity management and automated process control. Kano *et al.*¹³⁵ proposed a novel statistical monitoring method which is based on PCA, called moving PCA, in order to improve process-monitoring performance. The aim of this method is to identify changes in the correlation structure. Chen and Liu¹³⁶ proposed on-line batch process monitoring using dynamic PCA and dynamic PLS models. Finally, Arteaga and Ferrer¹³⁷ dealt with the missing-data problem in the estimation of latent variables scores from an existing PCA model. Badock *et al.*¹³⁸ proposed two alternative projection techniques that focus on the temporal structure of multivariate data. Ramaker *et al.*¹³⁹, using simulation, studied the effect of the size of the training set and number of principal components on the false-alarm rate in statistical process monitoring.

Multi-way PCA

Multi-way PCA is used to analyze a historical set of batch trajectory data. In a typical batch run, p variables are measured at k time intervals through the batch. Similar data will exist on m similar process batch runs. The vast amount of data involved can be organized into a three-way array $\underline{\mathbf{X}}_{m \times p \times k}$. In general, multi-way PCA is equivalent to unfolding the three-dimensional array $\underline{\mathbf{X}}_{m \times p \times k}$ slice by slice, rearranging the slices into a large two-dimensional matrix \mathbf{X} , and then performing a regular PCA. Four multidimensional statistical methods (Tucker model, PARAFAC (parallel factor) model, canonical decomposition, three mode factor analysis) have been proposed for decomposing such data arrays into the sum of a few products of vectors and matrices and for summarizing the variation of the data in the reduced dimensions of the spaces. A presentation of the Tucker model and the PARAFAC model and a comparison of these methods with the method multi-way PCA were given by Louwerse and Smilde¹⁴⁰. Nomikos and MacGregor^{141,142} gave a detailed presentation of multi-way PCA. Wise *et al.*¹⁴³ presented an application of PARAFAC2 to fault detection and diagnosis in semiconductors. Cho and Kim¹⁴⁴ proposed a new method for predicting future observations in the monitoring of the batch that is currently being operated. This method makes extensive use of past batch trajectories.

Using PLS

In general, PLS is a method, or rather a class of methods, which accomplishes dimension reduction by working on the sample variance-covariance matrix $(\mathbf{X}^t\mathbf{Y})(\mathbf{Y}^t\mathbf{X})$, where $\mathbf{X}_{n \times q}$ is the matrix of process characteristics and $\mathbf{Y}_{n \times p}$ is the matrix of quality variables. The use of PLS as a regression technique has been promoted primarily within the area of chemometrics, although PLS would be equally useful in any application that has multiple predictors. MacGregor *et al.*¹⁴⁵, Nomikos and MacGregor¹⁴⁶, MacGregor and Kourti¹⁴⁷ and Kourti and MacGregor¹⁴⁸ presented the use of PLS in multivariate statistical process control, while Wang *et al.*¹⁴⁹ presented the use of the recursive PLS modeling technique in the multivariate statistical process control framework. The multivariate control chart is, again, a T^2 -chart on the first k latent variables.

Multi-way PLS

Nomikos and MacGregor¹⁴⁶ gave a detailed presentation of multi-way PLS, which is an extension of PLS for handling data in three-dimensional arrays. The relation between multi-way PLS and PLS is that multi-way PLS is equivalent to performing PLS on a large two-dimensional matrix $\mathbf{X}_{m \times pk}$ formed by unfolding $\underline{\mathbf{X}}_{m \times p \times k}$.

Multi-block PLS

In the multi-block PLS approach, sets of process variables \mathbf{X} are broken into meaningful blocks $\mathbf{X}_1, \mathbf{X}_2, \dots$; each block usually corresponds to a process unit or a section of a unit. These blocks are then related simultaneously to \mathbf{Y} . Multi-block PLS is not equivalent to performing PLS on each block separately;

all of the blocks are considered together. MacGregor *et al.*¹⁴⁵ and Kourti *et al.*¹⁵⁰ discussed applications of multi-block PLS to process monitoring and diagnosis. In addition, they presented an algorithm for performing multi-block PLS. Martin *et al.*¹⁵¹ used an industrial ethylene propylene rubber compounding process in order to illustrate some of the issues that arise in the monitoring of the manufacturing performance of a process comprised of both batch and continuous unit operations.

Applications of PCA and PLS

Several applications of PCA and multi-way PCA, or modifications thereof, in real or in simulated processes, have been discussed by numerous authors including Zullo¹⁵², Gallagher *et al.*¹⁵³, Runger *et al.*¹⁵⁴, Stover and Brill¹⁵⁵, Tates *et al.*¹⁵⁶, Howarth *et al.*¹⁵⁷, Chen and Liu¹⁵⁸, Marengo *et al.*¹⁵⁹, Wang *et al.*¹⁶⁰, Yoon and MacGregor¹⁶¹, Albazzaz and Wang¹⁶², Skoglund *et al.*¹⁶³ and Garcia-Munoz *et al.*¹⁶⁴. Applications of PLS, multi-way PLS, PCA and multi-way PCA, or their modifications in real or in simulated processes, have also been discussed by numerous authors. Among these are Kourti *et al.*^{150,165}, Wise and Gallagher¹⁶⁶, Martin *et al.*^{167,168}, Martin and Morris¹⁶⁹ and Simoglou *et al.*¹⁷⁰. Kourti¹⁷¹ also provided a discussion on multi-block, multi-way PCA/PLS. Some of the methods that have appeared in the literature are examined as to their assumptions, their advantages and disadvantages and their range of applicability. Kourti¹⁷² gave an overview of the latest developments of multivariate monitoring based on latent variable methods for fault detection and isolation in industrial processes.

Neural networks and non-linear models

Neural networks are well suited for solving the same types of problem as those confronting human brains, such as recognition and classification (see Bose and Liang¹⁷³). Dayal *et al.*¹⁷⁴ used feedforward neural networks and PLS for modeling the 'kappa number' in a continuous Kamyr digester. In their study, inferential models for the kappa number were developed using PLS and neural networks. The advantages and limitations of each method were evaluated followed by a comparison with other modeling approaches. A novel nonlinear PCA method based on the input-training neural network was proposed by Jia *et al.*¹⁷⁵, together with non-parametric control charts. Another nonlinear PCA algorithm was proposed by Shao *et al.*¹⁷⁶ for process performance monitoring based on an input-training neural network. Prior to assessing the capabilities of the monitoring scheme in relation to the use of an industrial dryer, the data were first pre-processed to remove noise and spikes through wavelet de-noising. The wavelet coefficients obtained were used as the inputs for the nonlinear PCA algorithm. Performance monitoring charts with non-parametric control limits were then applied to identify the occurrence of non-conforming operation. Ganesan *et al.*¹⁷⁷ presented a literature review of wavelet-based, multiscale statistical process monitoring. In their paper, over 150 published and unpublished papers are cited for this important subject, and some extensions of the current research are discussed.

5. INTERPRETATION OF AN OUT-OF-CONTROL SIGNAL

In the previous sections, multivariate Shewhart, MCUSUM and MEWMA control charts, as well as PCA and PLS, procedures were reviewed in relation to monitoring the process mean and the process variability. These control charts are able to recognize an out-of-control process. If a univariate control chart gives an out-of-control signal, then someone can easily detect the problem and find a solution since a univariate chart is associated with a single variable. This is not valid for a multivariate control chart, as a number of variables are involved and, also, correlations exist among them. The identification of an out-of-control variable or variables after a multivariate control chart signals has been an interesting topic for many researchers over the last few years. In this section, methods for detecting which of the p different variables are out-of-control are presented.

Using univariate control charts with standard or Bonferroni control limits

An obvious idea is to consult the corresponding univariate control charts. The use of p univariate control charts gives the first evidence for which of the p variables are responsible for an out-of-control signal.

However, as already stated, the use of p independent univariate control charts can be very misleading if they have not been properly designed. The use of the Bonferroni inequality was proposed by Alt¹¹. Thus, p individual control charts would be constructed, each with a probability that the test statistic plots beyond the control limits under an in-control state equal to α/p and not α .

Hayter and Tsui³¹ extended the idea of Bonferroni-type control limits by giving a procedure for exact simultaneous control intervals for each of the variable means, using simulation. Hence, for a known variance–covariance matrix Σ and a chosen probability that the test statistic plots beyond the control limits under an in-control state, equal to α , the experimenter first evaluates the critical point $C_{R,\alpha}$. The choice of $C_{R,\alpha}$ depends on the correlation matrix R . The authors give guidance and various tables for choosing the critical point $C_{R,\alpha}$. Then, following any observation \mathbf{x}^t , the experimenter constructs intervals for the statistic $(X_i - \sigma_i C_{R,\alpha}, X_i + \sigma_i C_{R,\alpha})$, where σ_i is the standard deviation of the i th variable, for each of the p variables. This procedure ensures that an overall probability α is achieved. The new procedure can be thought of as triggering an alarm when $M = \max[|X_i - \mu_{0i}|/\sigma_i] > C_{R,\alpha}, i = 1, 2, \dots, p$. A graphical control display can be created by charting the M statistic for each multivariate observation.

The next method that is discussed is the use of an elliptical control region. This method is discussed by Alt¹¹ and Jackson³ and can be applied only in the special case of two quality characteristics distributed as a bivariate normal. In this specific case, an elliptical control region can be constructed. This elliptical region is centered at $\boldsymbol{\mu}_0^t = (\mu_1, \mu_2)$ and can be used in place of the Phase II X^2 -chart. All points lying on the ellipse have the same value of X^2 . The X^2 -chart gives a signal every time the process is out of control, while the elliptical region is useful for indicating which of the variables led to an out-of-control signal. An extension of the elliptical control region as a solution to the interpretation problem was given by Chua and Montgomery¹⁷⁸. They use a MEWMA control chart for identifying out-of-control observations and the hyperplane method for identifying the variable or variables that caused the problem. Mader *et al.*¹⁷⁹ presented the use of the elliptical control region for power supply calibration as a process-monitoring technique.

Another control chart that gives evidence about which variable caused the out-of-control signal is that presented by Sepulveda and Nachlas¹⁸⁰. This chart, called the simulated minimax control chart, monitors the maximum and minimum standardized sample mean of samples taken from a multivariate process. It is assumed that the data are normally distributed and that the variance–covariance matrix is known and constant over time. Hence, by monitoring the maximum and minimum standardized sample mean, an out-of-control signal is directly connected with the corresponding out-of-control variable. Sepulveda and Nachlas¹⁸⁰ also discussed the statistical properties and the ARL performance of the minimax control chart.

Using T^2 decomposition

Many authors have suggested using decomposition techniques for identifying particular subsets that cause an out-of-control signal.

The most promising method is T^2 decomposition, proposed by Mason *et al.*¹⁸¹. The main idea behind this method is to decompose the T^2 statistic into independent parts, each of which reflects the contribution of an individual variable. The main drawback of this method is that the decomposition of the T^2 statistic into p independent T^2 components is not unique as $p!$ different non-independent partitions are possible. An appropriate computing scheme that can greatly reduce the computational effort required was given by Mason *et al.*¹⁸². This method was developed to deal with individual observations, but it can easily be generalized to handle rational subgroups. Mason *et al.*⁵⁵ presented an alternative control procedure for monitoring a step process, which is based on a double decomposition of Hotelling's T^2 statistic. Mason and Young¹⁸³ showed (using T^2 decomposition) that by improving model specification at the time that the historical data set is constructed, it may be possible to increase the sensitivity of the T^2 statistic to signal detection.

Murphy¹⁸⁴ proposed a method that stems from the idea of discriminant analysis and uses the overall T^2 value, comparing it with a $T_{p_1}^2$ value based on a subset of p_1 variables, which are suspect as regards the out-of-control signal. Then, T_p^2 is the full squared distance and $T_{p_1}^2$ is the reduced distance corresponding to the subset of the p_1 variables which are suspected of being associated with the out-of-control signal.

Finally, the difference $D = T_p^2 - T_{p_1}^2$ is calculated, following a χ^2 -distribution with p_1 degrees of freedom, under the null hypothesis that the subvector $\bar{\mathbf{x}}_{p_1}$ follows a p_1 -dimensional distribution with mean μ_{01} and variance-covariance matrix Σ_{01} .

The main idea of the method proposed by Doganaksoy *et al.*¹⁸⁵ is the univariate t ranking procedure using the test statistic

$$t = (\bar{X}_f - \bar{X})[s(n_f^{-1} + n^{-1})]^{-1/2}$$

where f stands for the observation that gave the out-of-control signal, n is the sample size and \bar{X} , s are the mean and the standard deviation of the reference data set, respectively. This method is based on use of p unconditional T^2 terms. The diagnostic approach is triggered by an out-of-control signal from a T^2 -chart.

Wierda⁷ recommended a step-down procedure, assuming that there is an *a priori* ordering (which variable is the most sensitive to shifts) among the means of the p variables and sequentially tested subsets using this ordering to determine the sequence. The test statistic has the form

$$F_j = (T_j^2 - T_{j-1}^2)\{1 + [T_{j-1}^2/(n-1)]\}^{-1}$$

where the T_j^2 represents the unconditional T^2 for the first j variables in the chosen group. In the setting of a multivariate control chart, F_j would be the charting statistic which, under the null hypothesis, follows an $(n_f - 1)j(n_f - j)^{-1}F_{p_j, n_f - j}$ distribution. This procedure can be considered as an alternative to using the regular T^2 -chart and not only as a supplement because the numerator of F_j is a conditional T^2 value.

Timm¹⁸⁶ proposed the use of finite intersection tests (FITs). He assumes that there is an *a priori* ordering among the means of the p variables. Although T^2 is optimal for finding a general shift in the mean vector, it is not optimal for shifts that occur for certain subsets of variables. Timm¹⁸⁶ states that when this occurs the optimal procedure is to utilize a FIT. In the same paper, Timm¹⁸⁶ described a stepdown FIT procedure for the situation where the variance-covariance matrix Σ is unknown. Runger *et al.*¹⁸⁷ simplified previous recommendations given by Wierda⁷ and Timm¹⁸⁶, considering all subsets of variables.

Cause-selecting control chart and regression adjusted variables

Wade and Woodall¹⁸⁸ considered a two-step process in which the steps are not independent. In particular, when the incoming variable X_1 (the first step of the process) is charted in its own right, the outgoing quality X_2 (the second step of the process) is monitored after adjusting for the incoming quality X_1 . A chart for X_1 and $Z = X_2 - \hat{X}_2$ respectively, where \hat{X}_2 is the predicted value for X_2 based on the regression line, connecting X_1 and X_2 , is used. Thus, the Z_i are independent normal. If controllable, assignable causes are present, the distribution of Z_i shifts from the normal distribution for some values of i .

Another chart that uses the concept of regression adjustment is that of Hawkins. Hawkins^{87,88}, as already mentioned, defined a set of regression-adjusted variables in which he regressed each variable on all of the others. Hawkins^{87,88} proposed charting each Z_j using a CUSUM procedure because, in general, it is not known which of the p variables is out of control. His test statistic involves p -adjusted values, which can be shown to be related to the statistics presented in Mason *et al.*¹⁸¹ decompositions. Kalagonda and Kulkarni¹⁸⁹ recently proposed a diagnostic procedure using the dummy variable regression technique. This technique enables the identification of the causative factors, such as the mean and/or relationship shift, responsible for out-of-control signalling. The technique also indicates the direction of the shift, i.e. whether the mean is increased or decreased.

Using principal components

Principal components can be used to investigate which of the p variables are responsible for the creation of an out-of-control signal. Writers have proposed various methods for using principal components to interpret an out-of-control signal.

The most common practice is to use the first k most significant principal components, in these cases where T^2 control charts show an out-of-control signal. The principal components control charts that were analyzed in

the corresponding section can be used. The basic idea is that the first k principal components can be physically interpreted and named. Therefore, if the T^2 -chart shows an out-of-control signal and, for example, the chart for the second principal component also gives an out-of-control signal, then from the interpretation of this component, a direction can be taken as regards which variables are out-of-control suspects. This transforms the variables into a set of attributes. The discovery of the assignable cause that led to the problem, using this method, demands further knowledge of the process itself on the part of the practitioner. The basic problem is that the principal components do not always lead themselves to physical interpretation.

According to Jackson³, the procedure for monitoring a multivariate process using PCA can be summarized as follows. For each observation vector, obtain the z -scores of the principal components and from these compute T^2 . If this is in control, continue processing. If it is out of control, examine the z -scores. As the principal components are uncorrelated, they may provide some insight into the nature of the out-of-control condition, which may then lead to the examination of certain original observations.

Kourti and MacGregor¹⁴⁸ provided a different approach based on PCA. T^2 is expressed in terms of normalized principal components scores of the multinormal variables. When an out-of-control signal is received, the normalized score with high values is detected, and contribution plots are used for finding the variables responsible for the signal. A contribution plot indicates how each variable involved in the calculation of that score contributes to it. This approach is particularly applicable to large, ill-conditioned data sets owing to the use of principal components. Contribution plots were also explored by Wasterhuis *et al.*¹⁹⁰.

Maravelakis *et al.*¹⁹¹ have proposed a new method based on PCA. Theoretical control limits were derived and a detailed investigation of the properties and limitations of the new method was given. Furthermore, a graphical technique which can be applied in these limiting situations was also provided. Choi *et al.*¹⁹² have developed a fault-detection method based on a maximum likelihood-PCA mixture.

Graphical techniques

Fuchs and Benjamini¹⁹³ presented a method for simultaneously controlling a process and interpreting out-of-control signals. The new chart (graphical display) used emphasizes the need for fast interpretation of an out-of-control signal. The multivariate profile (MP) chart is a symbolic scatterplot. Summaries of data for individual variables are displayed via a symbol, and global information about the group is displayed by means of the location of the symbol on the scatterplot. A symbol is constructed for each group of observations, the symbol used representing the adoption of a profile plot that encodes visually the size and sign of each variable from its reference value. Fuchs and Kenett⁹ have developed a Minitab macro for creating MP charts.

Sparks *et al.*¹⁹⁴ presented a method for monitoring multivariate process data based on the Gabriel biplot. In contrast with existing methods that are based on some form of dimension reduction, Sparks and colleagues used reduction to two dimensions for displaying the state of statistical control. This approach allows them to detect changes in location, variation and correlation structure accurately but still display concisely a large amount of information. They illustrated the use of the biplot using an example involving industrial data. Nottingham *et al.*¹⁹⁵ have developed radial plots as an SAS-based data visualization tool that can enhance the ability of the process controller to monitor, analyze and control a process.

6. CONCLUSIONS

Today, multivariate Shewhart are the most commonly used control charts in industry. Owing to this, the need for further research on these kinds of chart is considered to be of great importance. In this paper, we have extended the review carried out by Mason *et al.*⁶⁷. The most crucial points of interest in this area are robust design of the T^2 -chart and non-parametric control charts. Autocorrelation and measurement error is an area that must be further investigated. The construction of a T^2 -chart with supplementary run rules may be a promising research area, and research into MACCs also shows promise. In general, MEWMA control charts perform better than classical Shewhart charts. Likewise, MCUSUM charts perform better than Shewhart charts, while having a performance similar to that of the MEWMA. An extensive comparison covering all possible scenarios between

MCUSUM, MEWMA and multivariate Shewhart control charts may be useful. The extension of MCUSUM techniques to autocorrelated observations is also an important area of research. Furthermore, economic models for MCUSUM should be investigated. Finally, a challenging area for research is the development of non-parametric MEWMA and MCUSUM control charts. Techniques such as PCAs and PLS are used primarily in the area of chemometrics, but they seem to be very promising in relation to any kind of multivariate process. Of the interpretation methods that have been reviewed, the most promising is the T^2 decomposition. The problem of interpreting an out-of-control signal is an open one which needs further investigation. In general, there are many examples of methods to be found in the literature that involve the graphical display of multivariate data by the use of symbols. Graphical methods such as polyplots, starplots, Andrews' curves, Chernoff faces and others can be used in the field of process control and their performance can be evaluated.

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