Multivariate Statistical Process Control

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INTRODUCTION

Many quality characteristics of a manufactured product can be expressed in terms of a numerical measurement. A variable is a single measurable quality characteristic, such as length, diameter, or density. In general, for a manufactured product, there are requirements or goals set in the form of a minimum or a maximum limit for the variables (i.e, product characteristics of interest). That is, the observed values of these variables are supposed to lie within the limits with high probability. Variable or attribute control charts are used extensively to monitor these variables.

When monitoring a process variable, the focus is typically on both the mean value of the quality characteristic and its variability. The process mean can be monitored with a control chart for means, or the $\bar{x}$ chart. Control of the process variability is usually done with either a control chart for the standard deviation, called the S chart, or a control chart for the range, called an R chart. It is important to maintain control over both the process mean and process variability. We therefore, keep separate $\bar{x}$ and S (or R) charts for each variable of interest.

The purpose of this article is to examine the control limits in the control chart for process means of a multivariate procedure, to interpret the out-of-control signals, and to identify process conditions that can lead to nonrandom patterns in the control chart. In this article, the focus will be on monitoring the mean of the multivariate response vector.

UNIVARIATE CONTROL CHARTS

It is helpful to review single-variable or univariate control charts before discussing the multivariate control chart. One of the basic procedures used for monitoring the process mean of a variable is called the Shewhart control chart, a graphical display of a quality characteristic that has been measured or computed from a sample versus the sample number or time index. A horizontal line, called a center line, is placed at the average or aim value of the variable when the process is considered ``in control''. The chart also contains two other lines, the upper control limit (UCL) and the lower control limit (LCL), parallel to the center line. The UCL and LCL are chosen corresponding to the in-control state when we expect nearly all of the sample points will fall between these limits.

Suppose that an in-control quality characteristic is normally distributed with mean μ and standard deviation σ, where both μ and σ are known. A Shewhart control chart is a plot of the realized values of the variable of interest for each successive sample drawn with UCL, LCL and center line references included. Let x_1, x_2, ..., x_n be a sample of size n. The sample mean $\bar{x} = \dfrac{x_1 + x_2 + ... + x_n}{n}$ is the estimator of μ and is normally distributed with mean μ and standard deviation $\sigma_{\bar{x}} = \sigma / \sqrt{n}$ as long as the process is in

control. Thus, we would expect $100(1-\alpha)\%$ of the $\bar{x}$ values to fall between $\mu \pm Z_{\alpha/2}(\sigma/\sqrt{n})$. It is common to choose the constant $Z_{\alpha/2}$ to be 3, so that 99.7% of the in-control sample means will fall within the control limits. These are typically called "three-sigma" control limits. Therefore, the control limits for the standard Shewhart $\bar{x}$ chart when μ and σ are known are:

$$\text{UCL} = \mu + 3\,\frac{\sigma}{\sqrt{n}} \qquad \text{Centerline} = \mu \qquad \text{LCL} = \mu - 3\,\frac{\sigma}{\sqrt{n}}$$

Most often, the process μ and σ values are not known. Thus, a set of m preliminary samples must be collected in order to compute the estimates of μ and σ. The unbiased estimators of the unknown mean μ and standard deviation σ are, respectively,

$$\bar{\bar{x}} = \frac{\sum_{i=1}^{m}\bar{x}_i}{m} \quad \text{and} \quad \hat{\sigma} = \frac{\bar{s}}{c_4}, \quad \text{where} \quad \bar{s} = \frac{\sum_{i=1}^{m}s_i}{m}.$$

Values of c_4 for various sample sizes can be found in Montgomery (2005). Thus, the trial control limits for the $\bar{x}$ chart (assuming the samples were collected when the process is in control) are:

$$\text{UCL} = \bar{\bar{x}} + 3\,\frac{\hat{\sigma}}{\sqrt{n}} \qquad \text{Centerline} = \bar{\bar{x}} \qquad \text{LCL} = \bar{\bar{x}} - 3\,\frac{\hat{\sigma}}{\sqrt{n}}.$$

When a Shewhart $\bar{x}$ chart is used to monitor the process mean μ, an out-of-control signal occurs when a sample mean $\bar{x}$ is either below the LCL or above the UCL. Thus, it is possible to have a "false" out-of-control signal by chance when the process mean is actually on aim, or, to have a "true" out-of-control signal when the process mean has shifted from the aim.

In practice, however, many (if not most) process monitoring and control scenarios involve two or more related variables. Although creating a univariate control chart for each of the individual variables is a commonly-used approach to monitoring the means of the process variables, it can be very misleading.

MULTIVARIATE STATISTICAL QUALITY CONTROL

Suppose, there are p independent and normally distributed variables associated with a particular product. If an $\bar{x}$ chart with P{type I error} = α is maintained on each, then the true probability that all of the variables will simultaneously exceed their control limits when the process is really in control is α^p, which is considerably smaller than α. Then the true probability of a type I error for the joint simultaneous control procedure is $\alpha' = 1 - (1-\alpha)^p$, and the joint probability that all variables plot inside the control limits when they are in control is P{all p means plot in control} = $(1-\alpha)^p$. Clearly, the difference in the joint procedure compared to the p individual procedures can be severe, even for moderate values of p. Moreover, if the p quality characteristics are related to a

single product, they will most likely not be independent. In this case, there is no simple way to measure the true distortion between the joint and individual control procedures. On the other hand, it is possible that a point is inside the control limits on all the univariate $\bar{x}$ charts, yet when the variables are examined simultaneously, the unusual behavior of the point is fairly obvious.

The ellipse in Figure 1 represents an example of a bivariate control region, while the rectangular is formed by the separate control limits of the two variables. One way the corresponding multivariate control chart would produce a signal is when there is a data point falling outside the ellipse but inside the box. In other words, there is nothing apparently unusual about such a point when viewed individually, yet very different conclusion would quite likely be observed for this product based on the bivariate control region.
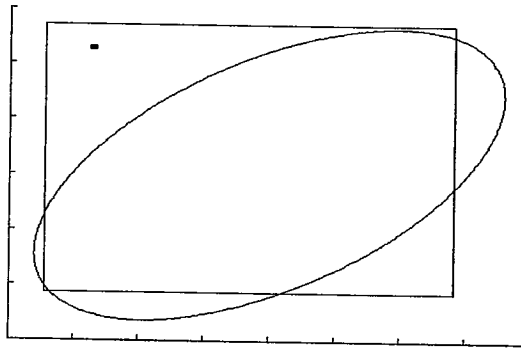

Figure 1: Individual Variable and Bivariate Control Regions

Besides the possibility that separate univariate control charts might fail to detect certain forms of lack of process control, the practitioner can not reliably guarantee that studying multiple charts can maintain process or product quality. Thus, monitoring the process with univariate SPC procedures on the same product is often less effective, and the use of multivariate control chart is recommended.

In multivariate statistical quality control applications, the p related quality characteristics are controlled jointly, and we generally use the multivariate normal distribution to describe the behavior of continuous quality characteristics of interest. The multivariate normal probability density function is

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} e^{-\frac{1}{2}(\mathbf{X}-\mu)'\Sigma^{-1}(\mathbf{X}-\mu)}$$

where $\mathbf{x}$ is a p×1 vector of the p variables. That is to say, $\mathbf{x}' = [x_1, x_2, ..., x_p]$. $\mu' = [\mu_1, \mu_2, ..., \mu_p]$ is the vector of the means of the x's, and the variances and covariance of the random variables in $\mathbf{x}$ are contained in a $p \times p$ covariance matrix Σ. The squared standardized distance from $\mathbf{x}$ to μ, therefore, is $(\mathbf{x}-\mu)'\Sigma^{-1}(\mathbf{x}-\mu)$.

Multivariate SQC based on Means

Sometimes we can group the multivariate data into rational subgroups in accordance with homogeneity within the subgroups created by the properties of the production process. Under these circumstances, μ, the in-control mean vector of the p quality characteristics, is occasionally known or is set as the standard based on the historical record. The same is true for the covariance Σ. In the unknown parameter case, the sample mean for each of the p quality characteristics from a sample of size n is computed, and the averages of each sample are contained in the $p \times 1$ vector

$$\overline{\mathbf{X}} = \begin{bmatrix} \overline{x}_1 \\ \overline{x}_2 \\ \cdot \\ \cdot \\ \cdot \\ \overline{x}_p \end{bmatrix}.$$

Then, the test statistic

$$\chi_0^2 = n\,(\overline{\mathbf{X}} - \mu)'\,\Sigma^{-1}(\overline{\mathbf{X}} - \mu) \tag{1}$$

is computed for each sample and plotted against the sample number in a chi-square (χ^2) control chart. Under the assumption that the samples are independent and the joint distribution of the p variables is multivariate normal, the upper and lower limits on the χ^2 control chart are

$$\text{UCL} = \chi_{\alpha,p}^2 \qquad \text{and} \qquad \text{LCL} = 0$$

The control limits can be derived from the theorem that that when $\Sigma^{-1}\Sigma = \mathbf{I}$ is idempotent, then $y'\Sigma^{-1}y$ is distributed as χ_p^2 if y is normally distributed. (Boik, 2005). The LCL based on chi-square distribution can be ignored in practice because any shift in the mean will lead to an increase in the statistic χ_0^2. Thus, the LCL can be set to zero instead. However, it should be noted that large values of χ_0^2 can be caused by the changes in the mean vector or by changes in the covariance matrix, which will be explained in detail later in the discussion of interpretations of out-of-control signals.

In practice, however, μ and Σ are frequently unknown and multivariate statistical quality monitoring has to be divided into two stages: Phase I and Phase II. Phase I is designed to estimate the process parameters from m preliminary samples of size n when the process is assumed to be in control. The usual estimate of μ is

$$\overline{\overline{\mathbf{X}}} = \frac{1}{mn}\sum_{i=1}^{n}\sum_{k=1}^{m}\mathbf{X}_{ik}\,.$$

The sample variance and covariance matrix for each sample is computed from

$$S_{jk}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_{ijk} - \overline{x}_{jk})^2 \quad \text{and}$$

$$S_{jhk}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_{ijk} - \overline{x}_{jk})(x_{ihk} - \overline{x}_{hk}) \quad (j,h = 1, 2, \ldots, p \quad \text{and} \quad j \neq h)$$

with S_{jk}^2 and S_{jhk}^h being the on-diagonal and off-diagonal entries of the matrix, respectively. The matrices for each subgroup are then averaged to get **S**, the estimate of the process covariance matrix. Next, we can get the test statistic

$$T^2 = n(\overline{\mathbf{x}} - \overline{\overline{\mathbf{x}}})' \mathbf{S}^{-1} (\overline{\mathbf{x}} - \overline{\overline{\mathbf{x}}}) \tag{2}$$

Alt (1985) pointed out that in multivariate quality control applications, one must be careful to select the control limits for Hotelling's T^2 statistic based on how the chart is being used. For phase I, the upper and lower control limits for the T^2 control chart are as follows:

$$\text{UCL} = \frac{p(m-1)(n-1)}{mn - m - p + 1} F_{\alpha, p, mn-m-p+1} \quad \text{and} \quad \text{LCL} = 0.$$

When establishing trial control limits, it is necessary for us to retrospectively test whether the process was in control when the m preliminary subgroups were drawn and the sample statistics $\overline{\overline{\mathbf{x}}}$ and S were computed. If assignable causes can be found for the out-of-control observations in the initial data, those outlying data points can be removed if it is approved by the experts of the production process. Observations with a T^2 value greater than the UCL are candidates for removal from the preliminary data set. The process of identifying outliers and removing special causes is repeated until a final data set is obtained that will represent an in-control process.

When the estimated in-control parameters can be trusted, they can be used to establish the control limits for Phase II, which is the monitoring of future production. In Phase II, the upper and lower control limits are given by

$$\text{UCL} = \frac{p(m+1)(n-1)}{mn - m - p + 1} F_{\alpha, p, mn-m-p+1} \quad \text{and} \quad \text{LCL} = 0.$$

Multivariate SQC based on Individual Measurements

In some industrial settings, the data are structured only as individual observations. That is, the rational subgroup size is naturally $n = 1$ because process characteristics do not necessarily produce homogeneous subgroups of large size. This can occur either when the production rate is too slow or when repeated measurements differ only because of laboratory or analysis error, as in many chemical processes. Under these circumstances, the test statistic for observation i is

$$T_i^2 = (\mathbf{X}_i - \overline{\mathbf{X}})'\mathbf{S}^{-1}(\mathbf{X}_i - \overline{\mathbf{X}}) \qquad (3)$$

Due to the high frequency of occurrence, the special case of control charting for individual observations draws more attention and extended studies. First, when the true parameters are known, we could use $\boldsymbol{\mu}$ and Σ in stead of $\overline{\mathbf{X}}$ and $\mathbf{S}$ in (3). Therefore, the test statistic is $T_i^2 = (\mathbf{X}_i - \boldsymbol{\mu})'\Sigma^{-1}(\mathbf{X}_i - \boldsymbol{\mu})$, and the distribution of this quadratic form follows a χ^2 distribution with p degrees of freedom.

More often, the multivariate process control for individual observations contains two stages because the true parameters are unknown. In that case, m preliminary observations are measured to get the estimates. Traditionally, the in-control process mean and variance/covariance matrix are estimated, respectively, by

$$\overline{\mathbf{X}} = \frac{1}{m}\sum_{j=1}^{m}\mathbf{X}_j \quad \text{and} \quad \mathbf{S} = \frac{1}{m-1}\sum_{j=1}^{m}(\mathbf{X}_j - \overline{\mathbf{X}}) \times (\mathbf{X}_j - \overline{\mathbf{X}})' \ .$$

for the in-control process. Four other methods have been suggested for estimating the variance and covariance matrix. A comparison of these methods will be made later in this writing project.

Assuming that $\mathbf{S}$ is used as the estimator of the parameter, Tracy, Young, and Mason (1992) mention that the distribution of the statistic in Phase I is proportional to a beta distribution. That is, we employ a control chart with upper and lower limits

$$\text{UCL} = \frac{(m-1)^2}{m}\beta_{\alpha,p/2,(m-p-1)/2} \quad \text{and} \quad \text{LCL} = 0$$

to test whether the process was in control when the m preliminary observations were drawn.

In Phase II, when the true parameters are unknown and x_i's are future individual observations, the test statistic, based on the quadratic form in ▓▓▓▓, is claimed to have a Hotelling's T^2 distribution that is proportional to an F distribution. Thus, the upper and lower control limits for the control chart of individual multivariate observations are

$$\text{UCL} = \frac{p(m+1)(n-1)}{m^2 - mp}F_{\alpha,p,m-p} \quad \text{and} \quad \text{LCL} = 0$$

Mason, Tracy and Young (1992) derived the upper control limit based on the theorem that if $\mathbf{y} \sim N_d(\mathbf{0}, \Sigma)$, $\mathbf{W} \sim W_d(\mathbf{m}, \Sigma)$, where $\mathbf{y}$ and $\mathbf{W}$ are statistically independent, then, for $T^2 = m\mathbf{y}'\mathbf{W}^{-1}\mathbf{y}$, we have $\dfrac{m-d+1}{d}\dfrac{T^2}{m} \sim F(d, m-d+1)$.

From the preliminary m individual observations, we can estimate the in-control process mean as $\overline{X} \sim N_p(\mu, \Sigma/m)$ and the covariance as $(m\text{-}1)S \sim W_p(m-1, \Sigma)$. Also, X_f, the future observations in phase II, are independent from $\overline{X}$ and S. Thus,

$$\sqrt{\frac{m}{m+1}}(X_f - \overline{X}) \sim N(0, \Sigma).$$

If one defines a statistic $Y = (\frac{m}{m+1})(X_f - \overline{X})'S^{-1}(X_f - \overline{X})$, then,

$$\frac{(m-p)}{p}\frac{Y}{(m-1)} \sim F(p, m-1-p+1),$$

which leads to

$$\frac{m-p}{p(m-1)}\frac{m}{(m+1)}(X_f - \overline{X})'S^{-1}(X_f - \overline{X}) \sim F(p, m-p)$$

and

$$(X_f - \overline{X})'S^{-1}(X_f - \overline{X}) \sim \frac{p(m-1)(m+1)}{m(m-p)}F(p, m-p)$$

INTERPRETATION OF OUT-OF-CONTROL SIGNALS

One of the major problems encountered with a multivariate quality control plan is the interpretation of an out-of-control signal. This is primarily caused by attempting to reduce a p-dimensional data vector into a uni-dimensional statistic. In multivariate SPC, a signal can be produced in several ways, including (i) by the unusual behavior of one of the p variables, (ii) by a relationship between two or more of the variables contradicting the structure established by the historical data, and (iii) resulting from combinations of the first two cases with some variable being out of control while others having counter-relationships.

When the measurement of an observation is located outside the univariate control limits in the univariate Shewhart $\overline{x}$ charts for one or more of the variables, we do not need to take the trouble of decomposing the corresponding T^2 values. In that case, a T^2 signal is generated by individual variables that are out of control. To solve that type of problem, our initial step is to examine the variables marked out-of-control by univariate control charts, and try to bring them into control.

Sometimes, a signal is produced while all the variables are in-control according to the individual $\bar{x}$ charts. This indicates something is astray with the relationship between the various variables. Due to the complexity, we need extra effort to interpret the signals.

One method for interpreting such signals is to decompose the T^2 statistic into components that reflect the contribution of each individual variable. A new statistic indicating the relative contribution of the ith variable to the overall statistic is obtained by

$$d_i = T^2 - T^2_{(i)} \qquad (4)$$

where T^2 is the current value of the statistic, and $T^2_{(i)}$ is the value of the statistic associated with all process variables except for the ith one. With an out-of-control signal occurring when all variables are in-control individually, the distinct d_i's are computed. We recommend focusing attention on the variable with relatively large d_i. Usually, the relationship between this variable and the others changes relative to the historical structure.

Other analysis of the out-of-control signals have been documented and used. For instance, Alt (1985) discussed the use of an elliptical control region. However, this process has the disadvantage that it can be applied only in the special case of two quality characteristics. The MYT decomposition suggested by Mason, Tracy, and Young (1997) decomposes a T^2 value into two types of orthogonal components that are themselves generalized distance measures. The first type, referred to as an *unconditional component*, is used to check whether an individual variable is out-of-control. The second type, called a *conditional component*, is used to determine if an observation vector generating a signal satisfyies the linear relationships among the variables. Advocates of discrimination analysis, e.g., Murphy(1987) and Chua and Montgomery (1992), developed procedures which are variations on the statistical procedure designed for classifying and grouping observations. Jackson (1991) proposed that when the variables are transformed to be uncorrelated principal components, they might provide some insight into the nature of the out-of-control condition, and then lead to the examination of particular original observations. However, these procedures require more extensive computations and more elaborate decompositions, especially when the number of potential variables increases.

IMPROVEMENT OF THE SENSITIVITY OF THE CONTROL CHART

From Phase I, the value of the mean vector of the in-control process is taken as the estimate and is used to set up the limits in the control chart to monitor the production process in the future. Suppose there are on m preliminary individual observations. Then the traditional covariance matrix estimator is

$$\mathbf{S}_1 = \frac{1}{m-1} \sum_{j=1}^{m} (\mathbf{X}_j - \overline{\mathbf{X}}) \times (\mathbf{X}_j - \overline{\mathbf{X}})'$$

There are, however, several alternative covariance estimators that can be used when constructing the T^2 statistics in equation (3) for individual observations.

The second estimator, denoted $\mathbf{S}_2$, is formed by classifying the observations into groups of size $p+1$. In order to use all observations, it is acceptable that not all groups be of equal size. $\mathbf{S}_2$ is then calculated by averaging the sample covariance matrix for each group, when the weight (subject to the degrees of freedom) is taken into consideration if the size of the groups are different.

The third estimator, denoted $\mathbf{S}_3$, uses overlapping groups, which make the sample covariance matrices for the groups not statistically independent as they are for $\mathbf{S}_2$. The data are divided into k groups, and each contains r observations numbered k, $k+1$, ..., $k + r - 1$, with r being the group size. The sample covariance matrix is then computed for each group, and the results are averaged to give $\mathbf{S}_3$.

The forth estimator, denoted $\mathbf{S}_4$, is based on the moving range approach. It is calculated by partitioning the data into two independent, non-overlapping groups. The last observation can be discarded if necessary so the two groups are the same size. Let the difference between nonoverlapping successive pairs of observations in each group be

$$y_i = x_{2i} - x_{2i-1}, \quad i = 1, ..., m/2,$$

where $\lfloor \ \rfloor$ stands for the greatest integer function and y_i's are independent for this scenario. Then, estimator four is calculated by

$$S_4 = \frac{1}{2} \frac{Y'Y}{\lfloor m/2 \rfloor},$$

where the matrix $\mathbf{Y}$ contains $\lfloor m/2 \rfloor$ row vectors of the differences.

The fifth estimator, denoted $\mathbf{S}_5$, is similar to $\mathbf{S}_4$, except the differences between $m-1$ overlapping successive pairs of observation are used. The vectors consisting of the differences between successive observations are calculated as

$$v_i = x_{i+1} - x_i, \quad i = 1, ..., m-1.$$

In this case, the v_i's are not independent. The estimator of Σ is one-half of the sample covariance matrix of these differences. That is,

$$S_5 = \frac{1}{2} \frac{V'V}{(m-1)}.$$

Some common models for out-of-control data have been studied, and more powerful procedures based on these alternative estimators of Σ are recommended to optimize the effectiveness of a T^2 statistical control chart. In most cases, step change, trend, and outliers are the most common problems occurring in a production process.

Mean Vector Step Changes

With a *step change* in the mean vector, one pair of adjacent observations will have different mean vector. Suppose a shift occurs after k observations. Then, this can be modeled as

$$\mu_i = \mu_0 + \delta, \quad i = k+1, ..., m$$

where μ_0 is the in-control mean vector and δ is some nonzero vector. Subject to this special cause, the separation of the observations from the center is $\delta'\Sigma^{-1}\delta$.

Due to independent groups being used in estimators S_2 and S_4, shifts coincident with a group boundary do not affect the "within" estimate of Σ. Thus, S_2 and S_4 might miss the shift in a single location. However, S_3 and S_5, the two estimators based on overlapping groups, provide greater statistical power than the corresponding estimators using independent groups of data. According to a simulation study with 1200 sets of data (Sullivan and Woodall 1996), using the true value of the covariance matrix is the most sensitive for detecting shift locations, and is followed by S_5, S_3, S_2 and S_4. The commonly-used chart based on S_1 has the least statistical power.

Mean Vector Trend

W now consider a ramp in the mean vector, also called a *drift* or *trend*. The mean vector changing by the same amount for each observation can be modeled as

$$\mu_i = \mu_0 + \frac{i-1}{m-1}\delta, \quad i = 1, ..., m$$

where μ_0 is the in-control mean vector, and δ is the vector difference between the mean vectors of the first and last observations.

From the study by Sullivan and Woodall (1996), S_1 fails to show an increase in detecting the trend as the severity of the shift δ increases. Again, estimators based on overlapping groups, produce a more powerful control chart than the corresponding estimators using independent groups. When there is a large shift, S_2, S_3 and S_5 can be as powerful as knowing the true value of the covariance matrix.

Outlier Vectors

Outlier vectors are more likely to generate a signal on the chart using S_1 because it is more sensitive to extreme values. Next, S_2 and S_3, the estimators based on averaging of sample covariance matrix of subgroups, produces better results than S_4 and S_5, the difference-based estimators.

If the serial nature of the observations is somehow known, one of the alternative methods to estimate the covariance matrix can be used to generate a more powerful analysis.

NON-RANDOM PATTERNS OF THE CONTROL CHART

When the statistic is not contained in the control limits, the control chart generates an out-of-control signal. In addition to signals, out-of-control conditions can also be indicated by a nonrandom pattern in the plotted statistic.

In practice, some non-stationary processes may contain inherent variation due to ramp change, step change and even a weak level of autocorrelation, which occurs often in the chemical processing industry. Given this situation, it is necessary to identify process conditions that can lead to nonrandom patterns in a chart. Thus, in Phase I, certain nonrandom patterns that occur in the chart of a preliminary data can be used as a diagnostic data tool.

Because individual observations are frequently seen in the chemical process industry, the estimates of parameters of the process are

$$\overline{\mathbf{X}} = \frac{1}{m}\sum_{j=1}^{m}\mathbf{X}_j \quad \text{and} \quad \mathbf{S} = \frac{1}{m-1}\sum_{j=1}^{m}(\mathbf{X}_j - \overline{\mathbf{X}}) \times (\mathbf{X}_j - \overline{\mathbf{X}})',$$

and non-random patterns occurring in T^2 control chart based on these estimates are illustrated in this paper.

Ideally, under in-control conditions, (i) many T^2 values are expected to be close to zero in a T^2 control chart, (ii) larger T^2 values should be randomly dispersed throughout all the values instead of occurring in clusters, (iii) no T^2 value will exceed the UCL, and (iv) no systematic pattern is observed. Sometimes, however, certain types of patterns will be observed.

Cyclic Patterns

Cyclic patterns associated with serially correlated data may result from many causes, such as the difference between night and day temperature, equipment change, operator fatigue, or change of operators. Thus, the statistic $(x_i - \overline{\mathbf{X}})/\mathbf{S}$ will indicate a

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cyclic pattern, and the T^2 value (the statistical squared distance) would double the frequency of the periodic pattern. Thus, the T^2 chart will have twice as many cycles and thereupon, resembles repeated U-shape patterns for a shorter period.

One method for identifying the serial correlated variable is the MYT decomposition (Mason, Tracy, Young, 1997). With this procedure, a T^2 value is decomposed into two types of orthogonal components, an unconditional component and a conditional component. The unconditional component is used to check the operating range of individual variables. The conditional component is used to determine if an observation vector is satisfying the linear relationships among the variables based on the historical data set. Each conditional T^2 value is determined from the residuals of a conditional relationship of one variable conditioned on a subset of the remaining variables.

Suppose a process has several variables of interest, and the T^2 chart shows a cyclic pattern, then the time sequence of the conditional T^2 terms can be plotted to identify the cyclic variable. For instance, if the cyclic effect is observed in a time sequence plot of the T-component value for x_1 given x_2, while very little cyclic variation is observed in the one for x_1 given x_3, then x_3 is indicated to be the variable that is cyclic in nature.

Mixture Patterns

Another common pattern is a *mixture pattern*, which is due to the process data being sampled from two or more populations. Under this circumstance, there will be very few observations around zero in the T^2 chart, and clusters tend to show up near the estimated means of the individual populations instead of the overall mean. As the separation between the means of the different groups of population increases, the scale of the vertical values on the chart is expanded and the points move further away from zero. The mixture pattern can be removed by treating the data as separate batch processes and then performing separate analyses.

Trend Patterns

A *trend pattern* in a T^2 chart occurs where there is continuous upward or downward movement of some variable. An undesirable trend, such as linear trends in process variables, are usually caused by some type of process decay, such as the wearing out of a tool or the deterioration of a critical process component such as catalyst. The upward or downward trend is also detectable in a T^2 chart corresponding to the data.

Some trends and fluctuation are natural. For example, consider the T^2 values associated with observations taken on the rate of fuel consumed and the rate of electrical generation. Increase of fuel leads to the production of more electricity. As the observed values of the fuel consumed and electricity generated move further from the average

system load, the load is reduced toward the average when an increase in the T^2 values is noted.

Some trends, however, are abnormal. If the means of the observed values show a linear trend, and the corresponding T^2 values show a quadratic expression in i. then a bowl shaped pattern is observed in the T^2 control chart.

A continuous increase in T^2 values indicates some imbalance of the data. Combined with the past knowledge of the performance of the system, a trend can be spotted. The trend pattern in a T^2 chart can be remedied by removing the cause of trend.

Shifts in the level of a T^2 statistic are due to events such as change of machinery, change in operators, change in production rates, or the introduction of new technology. Shifts occur in a similar manner in a T^2 chart. The absence of values near zero is noted, so is the grouping of T^2 values where levels are changing. With abnormal shifts, an easier way to reveal the source of the problem is to check the individual variable charts respectively.

Autocorrelation occurs frequently for many processes used in the chemical industry also. A bowl-shape pattern might be observed in the T^2 chart. Even if the chart does not have a distinct "pattern", the large values tend to be followed by large values and similarly for small values.

Besides the knowledge of the non-random patterns above, we have to be aware that each process has its own individual signature for a T^2 chart. Any difference from this established pattern implies that the current operating conditions deviate from the standard situations. Overall, the non-random or abnormal patterns in the T^2 chart can be employed as aids to the practitioner in bringing a process into a state of statistical in-control.

EXAMPLE

Table 1 represents the data analyzed by Kenett and Zacks (1998) which gives the dimensions of aluminum pins in a production process. Suppose the data contains the preliminary samples taken from the production line every 10 minutes in order to derive the control limits.

If a multivariate procedure is selected, the resulting control chart using the data in Table 1 is presented in Figure 2. If individual variable control charts are used (rather than the multivariate control chart), we get the Shewhart charts for the four variables which are shown in Figure 3.

Table 1: Data from Kenett and Zacks (1998)

	x1	x2	x3	x4		x1	x2	x3	x4
1	10.00	14.99	49.92	60.03	21	10.00	14.99	49.90	59.96
2	10.00	15.00	49.93	60.03	22	10.01	15.00	49.85	59.93
3	10.00	14.99	49.91	60.02	23	10.00	15.00	49.83	59.98
4	10.00	14.99	49.92	60.02	24	10.01	14.99	49.90	59.98
5	10.00	14.99	49.92	60.00	25	10.01	15.00	49.87	59.96
6	10.00	15.00	49.94	60.05	26	10.00	15.00	49.87	60.02
7	10.00	15.00	49.89	59.98	27	9.99	14.98	49.92	60.03
8	10.00	14.99	49.93	60.01	28	9.99	14.99	49.93	60.03
9	10.00	14.99	49.94	60.02	29	9.99	14.99	49.89	60.01
10	10.00	15.00	49.86	59.96	30	10.00	14.99	49.89	60.01
11	10.00	14.99	49.90	59.97	31	9.99	15.00	50.02	60.09
12	10.00	14.99	49.92	60.00	32	10.00	14.99	49.84	60.03
13	10.00	14.98	49.91	60.00	33	10.00	14.99	49.89	60.01
14	10.00	15.00	49.93	59.98	34	10.00	15.00	49.88	60.01
15	10.00	14.98	49.90	59.98	35	10.00	14.99	49.90	60.04
16	9.99	14.99	49.88	59.98	36	9.99	14.98	49.99	60.10
17	10.01	15.01	49.87	59.97	37	10.00	15.00	49.91	60.04
18	10.00	14.99	49.81	59.91	38	9.99	14.98	49.92	60.04
19	10.01	15.01	50.02	60.10	39	10.01	15.00	49.88	60.00
20	10.01	15.00	49.93	60.00	40	10.00	14.99	49.95	60.10

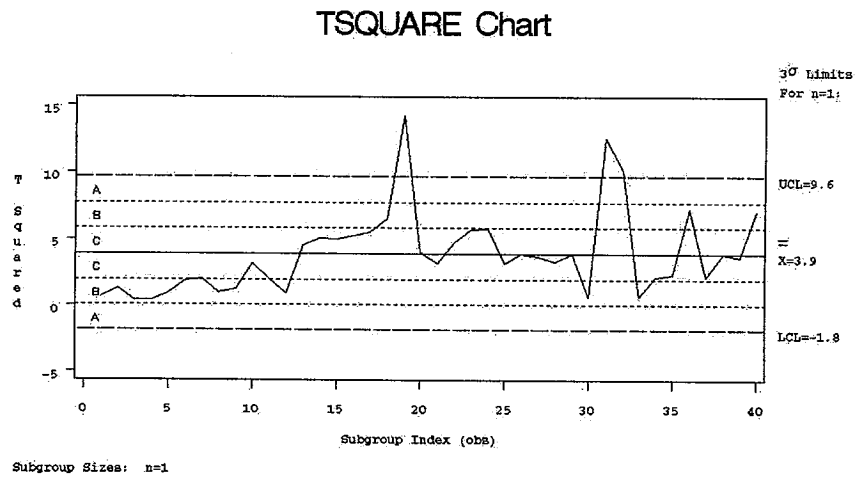**Figure 2**: The Multivariate T^2 Control Chart for the Example Data
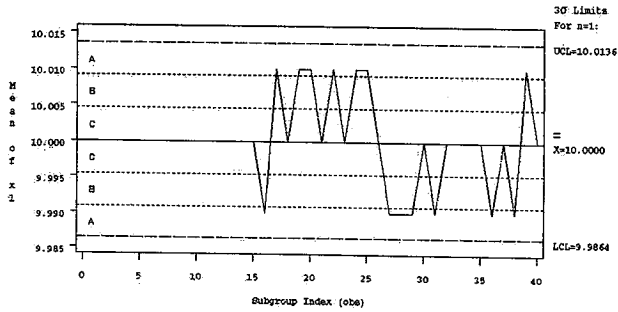

TSQUARE Chart
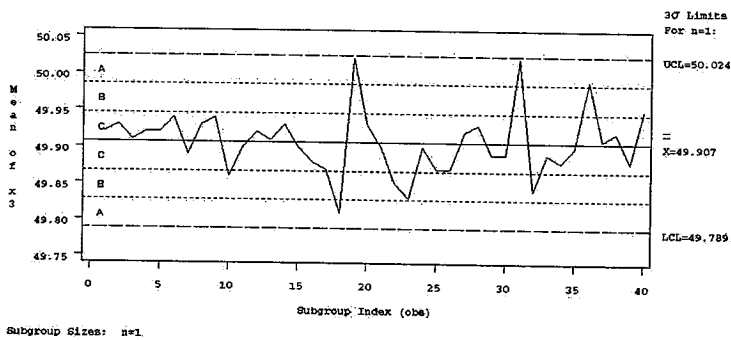
Figure 3: Individual Variable Control Charts for the Example Data

XBAR Chart for x1

Subgroup Sizes: n=1

XBAR Chart for x2

Subgroup Sizes: n=1

XBAR Chart for x3

Subgroup Sizes: n=1

XBAR Chart for x4

Subgroup Sizes: n=1
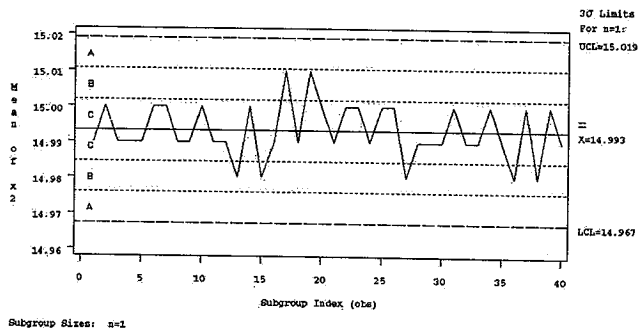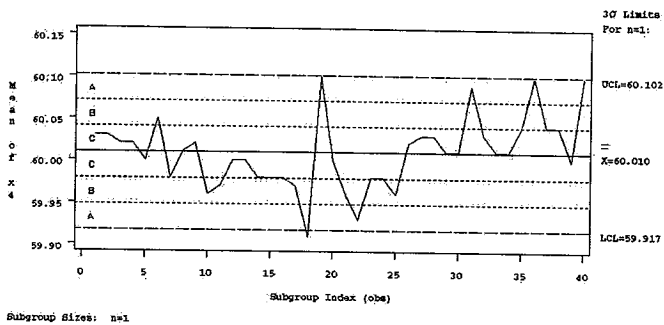
The univariate $\bar{x}$ charts provides no out-of-control signals, while the T^2 control chart represents three out-of-control signals for observation 19, 31 and 32. It is hard to interpret the status of the three observations by looking at the univariate $\bar{x}$ charts, so decomposition can help us to understand the situations.

Assume that the estimates of the in-control value of the process mean and the covariance matrix are very close to the true parameters. Consider the following summary:

Obs #	Observation Vector	T^2	$T^2_{(1)}$	$T^2_{(2)}$	$T^2_{(3)}$	$T^2_{(4)}$	d_1	d_2	d_3	d_4
19	(10.01,15.01,50.02,60.10)	14.19	12.28	12.91	12.31	13.72	1.91	1.28	1.88	0.47
31	(9.99,15.00,50.02,60.09)	12.51	7.89	8.40	8.83	11.94	4.62	4.11	3.68	0.57
32	(10.00,14.99,49.84,60.03)	10.13	9.69	9.76	0.61	2.61	0.44	0.37	9.52	7.52

Runger, Alt, and Montgomery (1996) suggest that an approximate cutoff for the magnitude of an individual d_i is $\chi^2_{\alpha,1}$. If α =0.01 is selected, any d_i exceeding $\chi^2_{0.01,1}$=6.63 would be considered a large contributor to the out-of-control signal. Thus, observation 32 signals because its value of x_3 and x_4 have shifted from the mean. For observations 19 and 31, no specific variables lead to a large T^2 statistic, yet the relationships between the four characters of interest might have changed.

CONCLUSIONS

Multivariate Statistical Process Control (MSPC) reduces the information contained in the data collected on production process variables down to a single statistic. It is also one of the most rapidly developing research areas in statistical process control. (Woodall and Montgomery, 1999). In addition to the T^2 control chart discussed in this article, the Multivariate Cumulative Sum Chart (MCUSUM) and the Multivariate Exponentially Weighted Moving Average (MEWMA) control chart have been developed to improve the sensitivity to small and moderate shifts in the mean vector.

The problem of interpreting an out-of-control signals needs to be researched further in the domain of multivariate SPC. Robust design of control charts and nonparametric control charts are also promising tasks. Multivariate control charting for attributes data is an open area for which more extensive investigations are neeeded.

REFERENCES

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