

Projections and the U^2 Multivariate Control Chart

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A projection approach to designing multivariate control schemes is used that simplifies the construction and understanding of these charts. The method is applied to construct charts that are sensitive to specific assignable causes such as a mean shift that affects only a subset of the variables and a model-fixed assignable cause that can occur when one variable causes another. The projection results in a chart that is easy to compute and design and it has greater sensitivity than a chi-square chart for the assignable cause under study. Furthermore, the chart can be analyzed using the convenient central and noncentral chi square distributions when the process is on-target and off-target, respectively.

Introduction

MULTIVARIATE statistical process control uses the relationships between variables to improve the detection of assignable cause in processes. An event might not be flagged as unusual from individual monitoring of several variables, but it can appear as quite unusual in a multivariate control chart. A projection approach to designing multivariate control schemes is presented to develop charts that are sensitive to assignable causes that shift the mean vector into a specific subspace, such as a mean shift that affects only a subset of the variables and a model-fixed assignable cause that can occur when one variable causes another. The projection results in a chart that is easy to understand, compute, design, and analyze.

Multivariate control charts such as chi-square charts, multivariate cumulative sum (CUSUM) charts, or multivariate exponentially weighted moving average EWMA charts are used to detect a shift in the mean vector of several variables. (See, for example, Crosier (1988), Hawkins (1991), Hawkins (1993), Lowry, Woodall, Champ, and Rigdon (1992), Pignatiello and Runger (1990), and Wade and Woodall (1993)). These charts are sensitive to shifts of the process mean vector in any direction from the target value. Let \mathbf{X} ($p \times 1$) denote the p variables measured from a process at time t . Suppose the variables are normalized such that $E(\mathbf{X}) = \mathbf{0}$, the zero vector, when the process is on target. Also, suppose

the covariance matrix is unknown, it would be estimated from data obtained during normal operating conditions. Montgomery (1991) provides guidance for estimation and charting in this case. If the mean vector of \mathbf{X} shifts to $\boldsymbol{\mu}$ then the average run length of a chi-square chart only depends on p (the number of variables) and on $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ only through $\lambda = \boldsymbol{\mu}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}$. The detection sensitivity increases with λ .

To reduce the dimensionality of the control problem, the method of principal components analysis has been recommended (see, e.g., Jackson (1991)). This generates a new set of variables, sometimes referred to as latent variables, that are linear combinations of the original variables. The first principal component variable is that linear combination of the original variables with greatest variance (for all coefficient vectors of unit length). The second principal component variable is that linear combination with greatest variance chosen from among coefficient vectors of unit length that are orthogonal to the first coefficient vector. Continuing in this manner, up to p latent variables can be constructed.

Although using all p latent variables does not provide a dimensional reduction, sometimes the data can be approximated as falling in a lower-dimensional subspace spanned by a few (say, three or fewer) latent variables. Then, the p -dimensional data set can be approximated with three or fewer variables. Let \mathbf{U} denote the vector of the first k principal component variables. If most of the variability in \mathbf{X} can be explained by the first k principal components variables, then a chi-square chart can be applied to \mathbf{U} . Of

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course, this chart is not sensitive to shifts of the process mean in directions orthogonal to the subspace of U . However, because the dimensionality has been reduced, this chart has greater sensitivity to shifts within the subspace defined by U .

The subspace defined by the principal components is just one approach to reducing the dimension of a multivariate control problem. Another approach is to sensitize a control chart to detect shifts in an arbitrary subspace of the variables. In some applications, knowledge of assignable causes suggests that shifts in the mean can only occur in a subset of the full set of variables. That is, a shift might occur only in the mean of X_1, \dots, X_k . The mean of variables $k+1$ to p are not affected by a specific assignable cause.

For example, the manufacturing of magnetic tape consists of wet processes that coat the web with a magnetic ink and dry processes that slit and test the tape. Typically, an assignable cause only affects the mean of either the wet or dry variables, although the variables are not necessarily independent. More specifically, an assignable cause might shift the means of all measurements across the tape approximately equally or an assignable cause might produce a difference in the means of measurements at opposite edges of the tape. A chart can be sensitized to specific assignable causes.

U^2 Chart

What is the appropriate multivariate control chart if only a subset of variables are affected by an assignable cause? This question is a special case of the more general question of the appropriate control chart for detecting a shift of the process mean to a particular subspace, say U , of p -dimensional space. The multivariate hypothesis test for a subspace alternative provides guidance. The more general question also applies to the case in which the means of some variables are determined (or caused) by others (see, e.g., Wade and Woodall (1993)). For example, if $Y = \beta X$, then a shift in the mean of X from 0 to μ results in a simultaneous shift in the mean of Y from 0 to $\beta\mu$. Consequently, the mean of the bivariate vector (X, Y) shifts along the vector $(1, \beta)$.

An appropriate control chart can be determined by an extension of the projection method used by Pignatiello and Runger (1990) to detect a shift along a specific vector. Let Z ($p \times 1$) denote a vector of independent and identically distributed (i.i.d.) standard

normal variables, so that $E(Z) = 0$ and the covariance matrix of $Z = I$, the $p \times p$ identity matrix. To detect a shift in the mean of Z from 0 along the unit vector ν , we should use a control chart based on the length of the orthogonal projection of Z onto ν .

The result is a control chart based on the statistic $\nu'Z$. Then, in general, to detect a shift of X from 0 to μ we can standardize by considering $Z = \Sigma^{-1/2}X$ and $\nu = \Sigma^{-1/2}\mu$ where $\Sigma^{-1/2}$ is the inverse of a symmetric square root of Σ . The projection method used results in the control statistic

$$\nu'Z = \mu'\Sigma^{-1}X. \quad (1)$$

For the one-dimensional case of detecting a shift along a single vector, this result also agrees with the recommendations given by Healy (1987) and Hawkins (1991).

Now consider the detection of a shift in the mean of X from 0 along an arbitrary vector in the k -dimensional subspace U . Let the columns of the $p \times k$ matrix U consist of a set of k orthonormal basis vectors for the subspace U . We can standardize to $Z = \Sigma^{-1/2}X$ and $V = \Sigma^{-1/2}U$. Then, the length squared of the orthogonal projection of Z onto V is

$$U^2 = Z'V(V'V)^{-1}V'Z \\ = X'\Sigma^{-1}U(U'\Sigma^{-1}U)^{-1}U'\Sigma^{-1}X \quad (2)$$

and this is referred to as the U^2 statistic.

Therefore, the recommended control statistic to detect a shift along a vector in U is a plot of U^2 over time. Although U^2 appears complex, it is the length of an orthogonal projection, and it can also be described as a quadratic form based on an idempotent matrix. Therefore, standard results can be applied. For example, U^2 has a chi-square distribution when the process is on target with degrees of freedom equal to the rank of the subspace V which equals the rank of the subspace U in all but trivial cases. Consequently, a control limit for the plot of U^2 can be selected from the 100α tail-percentage point of a chi-square distribution with k degrees of freedom.

Furthermore, if the mean of X shifts to the vector μ in the subspace U , then U^2 has a noncentral chi-square distribution with noncentrality parameter $\lambda = \mu'\Sigma^{-1}\mu$. Therefore, the performance of the U^2 chart is easily determined. The value of λ under a shift is the same for the U^2 chart as for a chi-square chart.

However, the important advantage of the U^2 chart is that the dimensionality has been reduced, with no reduction in the noncentrality parameter. Therefore, the performance of the U^2 chart can be contrasted to a chi-square chart by simply using a noncentral chi-square table with a different degrees of freedom. Table 1 illustrates that a large improvement in detection performance that can be obtained from the U^2 chart when it is applicable.

Healy's (1987) chart is used to detect a shift along a single vector in p -dimensional space. This reduces the multivariate control problem to the use of a single statistic that is a linear combination of the observed variables. The U^2 chart can be considered to be a generalization of Healy's method that accommodates shifts in a subspace of arbitrary dimension.

Interpretation of a U^2 Chart

The interpretation of a signal from a U^2 chart is similar to the interpretation of a chi-square chart. However, the interpretation of a U^2 chart can sometimes benefit from a simplifying assumption. A U^2 chart is developed to detect an assignable cause that shifts the mean vector in a subspace of the variables. The subspace being monitored is best chosen based on process knowledge of anticipated (or potential) assignable causes. Consequently, a signal from a U^2 chart suggested that the anticipated assignable cause has occurred.

To reduce the dimension of the control problem, a consideration of the variables that can potentially be affected by a assignable cause is made during the development of a U^2 chart. Initiating the consideration

of potential assignable causes at the design of a chart has the benefit of addressing this important question early, at the phase-in of the control chart, rather than reacting much later to a signal. Data available at the time of a signal might confirm or contradict some of the early evaluations of assignable causes. In either case, both the knowledge of the process and the understanding of an appropriate control strategy will improve.

If there is knowledge that the mean of some, but not all variables will be affected by an assignable cause, then a subset chart of the type described below can be used. If process knowledge can only distinguish an important subset of variables, then the interpretation of the variables contributing to a signal is similar to the interpretation of a chi-square chart for this subset of variables. That is, the individual variables and their relationships at the time of the signal are studied for guidance. Methods proposed for interpreting a signal from a chi-square chart by Murphy (1987), Chua and Montgomery (1992), and Mason, Tracy, and Young (1995) should be adaptable to interpreting a signal from a U^2 chart.

Although the interpretation of a multivariate control chart signal can be difficult, it is often difficult to correct the signal from even a univariate control chart without adequate process knowledge. Consider a signal from a univariate control chart for a dimension of an injection molded part. There is rarely a machine control that affects only that dimension. Instead, there are pressure, temperature, and flow controls for the press, and changes to any one of the press settings can affect all the dimensions (as well as other characteristics of a molded part). One will investigate all the individual variables and their relationships to understand a signal from even a univariate control chart and to select the best corrective action from among choices that affect many of the variables.

More generally, a single measured variable does not often uniquely correspond to a single process or machine setting variable. However, the variables that contribute to a signal from a control chart are identified, the final corrective action is based on process knowledge and requires an understanding of the relationships between the process settings and all of the measured variables.

Subset Assignable Causes

It is useful to consider an important special case of the U^2 chart. Suppose that an assignable cause can

TABLE 1. Average Run Length Comparisons for χ^2 and U^2 Control Charts

Chart	UCL	No. of Variables	Dimension of Shift Subspace	λ			
				1	2	3	4
χ^2	40.00	20		117	74	49	34
U^2	25.19		10	93	51	31	21
U^2	18.55		6	74	37	22	14
U^2	12.84		3	52	24	14	9
χ^2	25.19	10		93	51	31	21
U^2	16.75		5	68	33	19	12
U^2	12.84		3	52	24	14	9
U^2	10.60		2	42	18	11	7

On-Target Average Run Length = 200.

only shift the mean of a subset of k variables. This is referred to as a subset assignable cause. Other than specifying the subset, the assignable cause is arbitrary. Let the variables in the subset be denoted as the $k \times 1$ vector \mathbf{X}_1 and let the remaining $p - k$ variables be denoted as \mathbf{X}_2 so that $\mathbf{X}' = (\mathbf{X}_1', \mathbf{X}_2')$. For example, in the manufacturing of magnetic tape \mathbf{X}_1 and \mathbf{X}_2 can denote subsets of wet and dry variables, respectively. An assignable cause that affects the mean vector of \mathbf{X}_1 is an example of a subset assignable cause.

Let the covariance matrix of \mathbf{X} be partitioned similarly into Σ_{11} and Σ_{22} . Let \mathbf{I} denote a $k \times k$ identity matrix and $\mathbf{0}$ denote a $(p - k) \times k$ zero matrix. Then, a convenient orthonormal basis for the space of off-target means is $\mathbf{U}' = (\mathbf{I}, \mathbf{0})$. It is shown in the appendix that in this case

$$U^2 = \mathbf{X}'\Sigma^{-1}\mathbf{X} - \mathbf{X}_2'\Sigma_{22}^{-1}\mathbf{X}_2. \quad (3)$$

That is, U^2 is the remainder after the chi-square statistic applied to \mathbf{X}_2 is subtracted from the full chi-square statistic. This form is quite simple for computations. Note that, in general, U^2 in (3) is not equal to $\chi_1^2 = \mathbf{X}_1'\Sigma_{11}^{-1}\mathbf{X}_1$. The covariances between \mathbf{X}_1 and \mathbf{X}_2 are used in the computation of U^2 .

Furthermore, U^2 has a convenient chi-square distribution with k degrees of freedom when the process is on target. If the process mean shifts to a vector in the subspace of \mathbf{U} , then $\boldsymbol{\mu}' = (\boldsymbol{\mu}_1', \mathbf{0})$ for an arbitrary k -dimensional vector $\boldsymbol{\mu}_1$ and U^2 has a noncentral chi-square distribution with noncentrality parameter $\lambda = \boldsymbol{\mu}'\Sigma^{-1}\boldsymbol{\mu}$. This is the same noncentrality parameter as the chi-square statistic applied to the full set of p variables.

If one uses the statistic $\chi_1^2 = \mathbf{X}_1'\Sigma_{11}^{-1}\mathbf{X}_1$ to detect the shift to $\boldsymbol{\mu}' = (\boldsymbol{\mu}_1', \mathbf{0})$, then the dimension of the control statistic is also reduced to k . However, if the noncentrality parameter for the off-target distribution of χ_1^2 is denoted as λ_1 , then it is shown in the appendix that

$$\lambda_1 \leq \lambda. \quad (4)$$

That is, the sensitivity of U^2 to shifts is always as large or larger than the sensitivity of χ_1^2 .

In the special case that \mathbf{X}_1 and \mathbf{X}_2 are independent,

$$\mathbf{X}'\Sigma^{-1}\mathbf{X} = \mathbf{X}_1'\Sigma_{11}^{-1}\mathbf{X}_1 + \mathbf{X}_2'\Sigma_{22}^{-1}\mathbf{X}_2 \quad (5)$$

and $U^2 = \chi_1^2$.

Hawkins (1991, 1993) proposed solutions for detecting a shift in the mean of one of several variables. The U^2 chart for a subset assignable cause is designed to detect a shift in the mean vector of a subset of the variables. Consequently, the objectives of the procedures are somewhat different. Hawkins' (1991) method does not distinguish between the measured variables that can and cannot experience a shift in mean. Simultaneous univariate CUSUM control charts are used to detect a shift in the mean of a single variable in \mathbf{X} . Each variable is regression adjusted for the others. Although this method effectively detects a shift in the mean of a single variable, an adjustment to all variables in \mathbf{X} can result in control chart gaps in which assignable causes that shift the means of more than one variable in \mathbf{X} are not easily detected. Also, correlations between the simultaneous univariate charts complicate the selection of control limits and the evaluation of performance. Simulations have been used to study these charts.

Hawkins (1993) distinguishes between the measured variables that can and cannot experience a shift in mean. The method uses simultaneous univariate CUSUM control charts on the variables in \mathbf{X}_1 that are regression adjusted for the variables in \mathbf{X}_2 to detect a shift in the mean of a single variable in \mathbf{X}_1 . Correlations between the simultaneous univariate charts complicate the selection of control limits and the evaluation of performance. Simulations have been used to study these charts. In the case in which the mean of any variable in \mathbf{X} can potentially shift, Hawkins' (1993) method results in simultaneous univariate CUSUM charts on each measured variable (unadjusted). In this case, the control procedure is the same as ones considered by Woodall and Ncube (1985) and the correlations between the variables are ignored.

The U^2 chart can be designed to detect an arbitrary shift in the mean vector of \mathbf{X}_1 (as well as a shift in other types of subspaces) and it is particularly simple to select control limits for and analyze the U^2 chart. In the case in which the mean of any variable in \mathbf{X} can potentially shift, the U^2 chart reduces to the chi-square control chart applied to \mathbf{X} and uses the correlations between the variables in the control algorithm. Although we have been discussing a Shewhart version of the U^2 chart, the statistic can easily be incorporated into a multivariate EWMA or a multivariate CUSUM chart.

Control charts should be based on process knowledge of potential assignable causes. Variables are

best subsetted based on physical process characteristics and anticipated assignable causes. In the magnetic tape example, a slitting problem affects the means of the dry variables only. A U^2 chart developed to detect a subset shift in the means of the dry variables would be useful in this case. Any variables that could suffer a mean shift from the slitting problem would be included in X_1 . The remaining process variables would be included in X_2 . The U^2 chart is most useful when there is a natural partitioning of variables based on physical characteristics of the process. Further research on using statistical information to subset variables and to manage charts for different subsets in the same process is needed.

Model-Fixed Assignable Causes

In the case above, the mean vector of X_1 can shift without a corresponding change in the mean vector of X_2 . In other processes, the mean vector of X_1 is determined by X_2 . For simplicity, we consider just two variables X_1 and X_2 with

$$X_1 = \beta X_2 + e \quad (6)$$

where β is a known parameter, the variance of X_2 is σ^2 , and e follows the usual regression assumptions. That is, e is normally distributed, independent of X_2 , with mean 0 and variance σ_e^2 .

Suppose a shift in the mean of X_2 to μ results in a shift in the mean of X_1 to $\beta\mu$ so that the model is preserved under the impact. Then, these assignable causes result in a shift of (X_1, X_2) along the vector $U' = (\beta, 1)$. We refer to these types of shifts as *model-fixed* assignable causes to contrast them with the other case considered above. Shifts along a vector other than $(\beta, 1)$ might then be called *model-void* assignable causes.

Now, let $W = (X_1, X_2)'$. The covariance matrix of W is

$$\sigma^2 \begin{bmatrix} \beta^2 + \sigma_e^2/\sigma^2 & \beta \\ \beta & 1 \end{bmatrix}.$$

It is easily shown that $U'\Sigma^{-1} = (0, \sigma^{-2})$. Furthermore, using the definition of U^2 , it is a direct computation to show that in this case

$$U^2 = \frac{X_2^2}{\sigma^2}. \quad (7)$$

Consequently, we obtain the interesting result that if X_1 is caused by X_2 and the model persists after the assignable cause (model-fixed), then there

is no benefit from including X_1 in the control algorithm, regardless of the strength of the relationship between X_1 and X_2 . The benefits of this result are simpler charts with improved performance. Consequently, when there are causal relationships between variables, it is important to specify the anticipated impact of assignable causes in the system. The next obvious step suggested by this result is to supplement the U^2 chart by an additional control chart (or several) that is sensitive to assignable causes that change the model between X_1 and X_2 . The finite intersection tests proposed by Timm (1996) might be combined with U^2 statistics to sensitize a control strategy to a number of specific assignable causes.

Example

In a process 20 variables are being monitored. However, the assignable cause anticipated only shifts the mean of 6 of the variables. As an example, the 6 variables are dry process measurements in the manufacturing of magnetic tape. Let the 20×1 vector X denote the 20 process variables and let the 14×1 vector X_2 denote the 14 variables with means unchanged by the assignable cause. Then, a control chart that plots

$$U^2 = X'\Sigma^{-1}X - X_2'\Sigma_{22}^{-1}X_2$$

over time is recommended (Σ_{22} is the 14×14 submatrix of Σ). The control limit is obtained from the $100\alpha\%$ tail-area of a chi-square distribution with 6 degrees of freedom. If the size of the shift is $\lambda = 3$, then from Table 1 the average run length to detect the shift is 22 points. A chi-square chart requires 49 points, on average, to detect the same shift. Knowledge of the type of assignable cause expected can improve the multivariate control scheme.

Conclusions

Multivariate control schemes can be designed to be sensitive to specific assignable causes by a simple projection method. The projection approach simplifies the construction, explanation, and interpretation of multivariate control schemes. The results illustrate that the type of assignable cause that is anticipated is crucial to the design of a multivariate control scheme. Schemes can be tuned to be sensitive to specific process anomalies and the projection approach can clarify the different alternatives.

The concept of controlling for a shift in the plane of the first few principal components can be extended

to more general subspaces of p -dimensional space and the resulting statistic can be both easy to compute and interpretable. Furthermore, a causal relationship between variables can result in a control scheme that is sensitive to model-fixed assignable causes that ignores the dependent variable and simplifies to only include the independent variables.

In some cases, a few of these sensitized schemes can be combined to simultaneously monitor for a few assignable causes. The multiple comparison problem can be offset with slightly increased control limits selected by a simple Bonferroni approach. With a few sensitized schemes, the increased detection ability can more than compensate for the wider control limits resulting in improved performance and better process control.

Software that includes matrix multiplications can be used to calculate an arbitrary U^2 control chart. A statistical software package that computes a covariance matrix from process data would be helpful. Then any spanning vectors for the subspace of the assignable cause can be used as the columns of the matrix U to generate the U^2 statistic. In the special case of a subset assignable cause, the U^2 statistic can be computed more easily as the difference between two chi square statistics as in (3). In this important special case, any software package that includes a chi-square control chart can be suitably modified.

Appendix

Derivation of the U^2 Statistic for a Subset Assignable Cause

Partition Σ^{-1} into components of size k and $p-k$ such that

$$\Sigma^{-1} = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}.$$

Let $U' = (I, 0)$ then,

$$\begin{aligned} U^2 &= X' \Sigma^{-1} U (U' \Sigma^{-1} U)^{-1} U' \Sigma^{-1} X \\ &= X' \begin{bmatrix} B_{11} B_{11}^{-1} \\ B_{21} B_{11}^{-1} \end{bmatrix} [B_{11} B_{12}] X \\ &= X' \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{21} B_{11}^{-1} B_{12} \end{bmatrix} X. \end{aligned}$$

Using the formula for the inverse of a partitioned matrix

$$B_{21} B_{11}^{-1} B_{12} = B_{22} - \Sigma_{22}^{-1}.$$

Therefore,

$$\begin{aligned} U^2 &= X' \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} - \Sigma_{22}^{-1} \end{bmatrix} X \\ &= X' \Sigma^{-1} X - X'_2 \Sigma_{22}^{-1} X_2. \end{aligned}$$

Derivation of the Noncentrality Parameters for a Subset Assignable Cause

The notation for partitioned matrices from the first part of this appendix is also used here. The noncentrality parameter of the U^2 chart for detecting a shift to $\mu' = (\mu'_1, 0)$ is

$$\begin{aligned} \lambda &= \mu' \Sigma^{-1} \mu \\ &= \mu'_1 B_{11} \mu_1. \end{aligned}$$

The noncentrality parameter for the statistic $\chi^2_1 = X'_1 \Sigma_{11}^{-1} X_1$ is

$$\lambda_1 = \mu'_1 \Sigma_{11}^{-1} \mu_1.$$

From the results for the inverse of a partitioned matrix

$$\begin{aligned} B_{11} &= (\Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21})^{-1} \\ &= \Sigma_{11}^{-1} + \Sigma_{11}^{-1} \Sigma_{12} (\Sigma_{22}^{-1} \\ &\quad - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12})^{-1} \Sigma_{21} \Sigma_{11}^{-1} \end{aligned}$$

therefore,

$$\begin{aligned} \lambda - \lambda_1 &= \mu'_1 \Sigma_{11}^{-1} \Sigma_{12} (\Sigma_{22}^{-1} \\ &\quad - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12})^{-1} \Sigma_{21} \Sigma_{11}^{-1} \mu_1 \\ &\geq 0. \end{aligned} \quad (A1)$$

Last inequality in (A1) follows from the fact that the covariance matrix of X_2 given X_1 is $\Sigma_{22}^{-1} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$. Consequently, (A1) is a quadratic form of a positive semidefinite matrix and is nonnegative.

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