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ISSN 0940-5151

Economic Quality Control
Vol 21 (2006), No. 1, 143 – 153

Multivariate Diagnostic Tests: A Review of Different Methods

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Abstract: There are many instances where the quality of a product is determined by the joint level of several characteristics. Under these types of situations, one wishes to detect quickly any departure from a satisfactory level, while at the same time it is of interest to know which characteristic(s) is(are) responsible for the deviation. The most common and popular solution to the first query is to use a T^2 control chart which is an aggregate monitoring function, when the mean vector of the correlated characteristics is the major concern and the normal approximation may be used. However, the answer to the second query is not so easy. The lack of a simple method of selecting the 'out of control' variable has made the routine use of T^2 control chart impractical so far. This paper provides a review of different techniques available to identify the culprit variable(s), when a T^2 control chart gives an out-of-control signal.

1 Introduction

The use of multivariate control charts to monitor industrial process is increasingly popular. The quality of a product is often characterised by the joint level of p correlated variables. This suggests a multivariate approach for monitoring simultaneously several correlated variables. Among the multivariate control chart techniques, Hotelling T^2 statistic is the most popular one. It is often called a multivariate Shewhart control chart. A major advantage of Hotelling T^2 statistic is that, provided the normal approximation is permissible, it can be shown to be the optimal test statistic for detecting general shifts in the process mean vector for an individual multivariate observation (Hawkins [9]). Since the purpose of this paper is not to describe the T^2 control chart, it is worth while to mention here that the procedure of T^2 control chart (Phase-I, Phase-II) is elaborately described in the paper by Wierda [8]. A major drawback of this chart is that an out-of-control signal does not provide information about the variable(s), for which the out of control situation occurs. But a successful implementation of a T^2 control chart needs to address this problem, since this would be desirable for performing the necessary corrective action to bring the process back to the in-control.

Several recent papers address this problem and present different approaches for answering the question. This paper aims at summarizing the different approaches to identify the out-of-control variable(s) in the multivariate case and review their merits and demerits.

In the following section we will discuss the T^2 control chart and four techniques to identify the out of control variables, viz, the ranking technique proposed by Doganaksoy, Faltin and Tucker [1], the T^2 difference method proposed by Murphy [7], the MYT decomposition proposed by Mason, Tracy, Young [3], and the MSSD proposed by Holmes and Morgan [2].

1.1 Hotelling's T^2 Method

This is considered to be the most widely accepted method simply because of its simplicitly and more importantly, due to its similarity with the popular Shewhart control charts. It is assumed that the joint probability distribution of the p quality characteristics is the p-variate normal distribution. The test statistic plotted on the control chart for each sample is:

$$X_0^2 = n(\bar{X} - \mu)'\Sigma^{-1}(\bar{X} - \mu) \tag{1}$$

where, $\mu' = (\mu_1, \ldots, \mu_p)$ is the vector of in-control means for the quality characteristics, $X' = (X_1, \ldots, X_p)$ is the random vector describing a sample, and Σ is the covariance matrix of X.

The upper limit on the control chart UCL for specified significance level α is given by the upper quantile of order α of the χ^2-distribution with p degrees of freedom:

$$UCL = \chi_p^2(\alpha) \tag{2}$$

In practice, it is usually necessary to estimate μ and Σ by analyzing preliminary samples, taken when the process is assumed to be in control. Using the resulting estimates, $\bar{x}$ and s, the test statistic becomes:

$$T^2 = n(\bar{X} - \bar{x})'s^{-1}(\bar{X} - \bar{x}) \tag{3}$$

with the following upper control limit:

$$ULC_{T^2} = \frac{p(k-1)(n-1)}{k(n-1)-(p-1)} F_{p,k(n-1)-(p-1)}(\alpha) \tag{4}$$

where $F_{p,k(n-1)-(p-1)}(\alpha)$ is the upper quantile to the order α of the F-distribution with $(p, k(n-1)-(p-1))$ degrees of freedom.

However, the technique has several practical drawbacks. A major drawback is tha, when the T^2 statistic indicates that a process is out of control, it does not provide information about which variable(s) is(are) out of control. Further, it is difficult to distinguish location shifts from scale shifts, since the statistic is sensitive to both types of process changes.

1.2 Ranking Technique

The following procedure, developed by Doganaksoy, Faltin, Tucker [1] aims

1. at providing a ranking of the components of the observation vector according to how likely each is to have participated in the change, and

2. at indicating whether there is sufficient evidence in hand to identify definitively which attributes have changed.

The procedure can be described by the following five steps.

Step 1:
Conduct a T^2 test with a specified nominal significance level α. If an out of control condition is signaled then continue.

Step 2:
Calculate for each of the p variables the realization of the associated univariate t statistic:

$$t = \frac{\bar{x}_{i,new} - \bar{x}_{i,ref}}{\sqrt{\left(\frac{1}{n_{new}} + \frac{1}{n_{ref}}\right) s_{ii}^2}} \tag{5}$$

where:

$$\bar{x}_{i,new} = \text{new sample mean of the } i\text{th variable} \tag{6}$$

$$\bar{x}_{i,ref} = \text{reference sample mean of the } i\text{th variable} \tag{7}$$

$$s_{ii}^2 = \text{estimate of the variance of the variable from the reference sample} \tag{8}$$

Step 2 is used to rank the components according to their influence towards the shift. This ranking, however, provides only a relative, not an absolute, measure about which variables are particularly highly suspicious.

Step 3: For each variable calculate the smallest confidence level β_{ind} that would yield an individual confidence interval for $\mu_{i,ref} - \mu_{i.new}$, $(i = 1, \ldots, p)$ that contains zero. For this let t be the calculated value of the univariate t statistic for a variable and $T(t; d)$ be the cumulative distribution function of the t-distribution with d degrees of freedom. Then

$$\beta_{ind} = |2T(t, n_{ref} - 1) - 1| \tag{9}$$

The variables with larger β_{ind} values are the ones, which require closer investigation, as they are possibly among those components, which have undergone a change.

Step 4 : Compute the confidence level

$$\beta_{bonf} = \frac{p + \beta_{sim} - 1}{p} \tag{10}$$

where β_{sim} is the confidence level of the Bonferroni type simultaneous confidence intervals for $\mu_{i,ref} - \mu_{i.new}$, $(i = 1, \ldots, p)$.

Step 5: Components having $\beta_{ind} > \beta_{bonf}$ are classified as being those which are most likely to have changed.

This approach is based on intrinsically meaningful process/product attributes and provides a priority ranking of attributes to be investigated even in instances where no unambiguous source identification is feasible. In addition, it is intuitively sound and easy to implement using standard statistical methods.

1.3 T^2 Difference Method

This approach was proposed by Murphy [7] and is based on principal component analysis. The used statistic T^2 is written as

$$T^2 = \sum Z_i^2 \tag{11}$$

where the principal components Z_i are independent.

When an out of control signal x^* is obtained, the vector x^* is divided into two parts $x* = (x^*_{(1)}, x^*_{(2)})$, where $x^*_{(1)}$ contains those p_1 of the p variables, which are suspected to be the cause of the out-of-control signal, and $x^*_{(2)}$ consists of the remaining $p_2 = p - p_1$ variables. Then let $T^2_{p_1}$ denote the reduced T^2-distance corresponding to the p_1 variables:

$$T^2_{p_1} = n(\mu_0^{(1)} - x^*_{(1)})'\Sigma_{11}^{-1}(\mu_0^{(1)} - x^*_{(1)}) \tag{12}$$

with $\mu_0^{(1)}$ and Σ_{11} being those parts of $\mu : 0$ and Σ, which belong to $x^*_{(1)}$.

Next, consider the difference $D = T^2 - T^2_{p_1}$. The test of the null-hypothesis

$$H_0 : \quad D = 0 \tag{13}$$

is equivalent to testing that the p_1 variables discriminate just as well as the full set of p variables. Under H_0 the difference D is χ^2-distributed with p_2 degrees of freedom.

1.4 Mason-Young-Tracy (MYT) Decomposition Method

Mason, Tracy and Young [4] suggested to decompose the statistic T^2 into p orthogonal components as:

$$T^2 = T_1^2 + T_{2.1}^2 + \ldots + T^2_{p.1,2,\ldots,p-1} \tag{14}$$

T_1^2 is an unconditional Hotelling's T^2 for the first variable of the observation vector. The remaining terms are called conditional terms, their general form is derived in [4].

The ordering of the p components in the observation vector is, of course, not unique. Each of the $p!$ possible orderings generates the same overall T^2 value, but provides a distinct partitioning of T^2 into p-orthogonal terms, with

$$T_1^2 \sim \chi_1^2 \tag{15}$$

$$T^2_{j.1,\ldots,j-1} \sim \frac{n+1}{n} F_{1,n-1} \tag{16}$$

B means of the orthogonal terms, one can compare each of the variables for deciding when a term is considered to be significant. An advantage of this method is its ability to consolidate past research findings about the interpretation of a T^2 signal. Note that imbedded in this partitioning are the regression adjusted variables of Hawkins [9], the T^2 difference of Murphy [7], as well as the standardized t value of Doganaksoy, Faltin and Tucker [1].

1.5 Mean Square Successive Differences (MSSD) Method

The following procedure for identifying the sources for out of control signals was proposed by Holmes and Mergen [2].

Step 1: Construct standardized variables for each of the p variables:

$$Z_{i,j} = \frac{X_i - \frac{1}{n}\sum X_{i,j}}{S_j} \tag{17}$$

where X_i is the ith variable and $X_{i,j}$ is the mean square successive difference estimator and

$$S_j = \frac{1}{1-\frac{3}{8n}}\sqrt{\frac{1}{2(n-1)}\sum\left(X_{i+1,j} - X_{i,j}\right)^2} \tag{18}$$

Step 2: The control limits are calculated by the Bonferroni approach which says that effective value of α risk may be approximated by $\alpha = p\alpha_i$, where α_i is the risk associated with the ith variable. If a certain $Z_{i,j}$ lies beyond the corresponding limit, the corresponding variable X_j is considered to be the aberrant one.

2 Performance Analysis of the Methods Under Different Correlation Structures

The sensitivity of the proposed methods is analyzed by generating data through simulation under different conditions. For simplicity, we consider the number of variables, p, to be two. It is assumed that the original process follows a bivariate normal distribution with both the means being zero and both the variance one, and correlation coefficients ρ.

Thus we have for the in-control process variable X:

$$X \sim N_2(\mu_1, \mu_2, \sigma_1, \sigma_2, \rho) \tag{19}$$

where $\mu_1 = 0$, $\mu_2 = 0$, $\sigma_1 = 1$, and $\sigma_2 = 1$.

The data were generated by shifting the mean from 0 to k_1 and k_2, respectively.

Under the changed scenario (when an assignable cause has occurred) the distribution of the process variable X is:

$$X \sim N_2(\mu_1', \mu_2', \sigma_1, \sigma_2, \rho) \tag{20}$$

where

$$\mu_1' = \mu_1 + k_1\sigma_1 \tag{21}$$
$$\mu_2' = \mu_2 + k_2\sigma_2 \tag{22}$$

100 observations were generated from the changed distribution for different values of k_1 and k_2. In each case, it was tested whether the T^2 statistics was able to detect the shift. If the shift was detected then by the four methods described above an attempt was made to find out which of the variables had caused the shift. The number of signals in each case was recorded. Hence % of correct diagnosis were recorded under different situations.

The values of k_1 and k_2 considered for the study were as follows: $0, \pm 0.5, \pm 1.0, \pm 1.5, \pm 2.0$. The above described analysis was repeated for different values of ρ, namely $\rho = \pm 0.4, \pm 0.8$. The results are summarized in the tables below.

- **The case $\rho = 0.4$:**

Table 1: Results for a shift in the same direction for $\rho = 0.4$.

k_1	k_2	MYT	T^2 diff	Ranking	MSSD
-0.5	-0.5	100%	71%	100%	100%
-1.0	-1.0	100%	100%	100%	86%
-0.5	-1.0	100%	60%	100%	80%
0.5	0.5	50%	100%	50%	50%
1.0	1.0	100%	100%	100%	75%
0.5	1.0	100%	100%	100%	34%
-2.0	-2.0	100%	100%	100%	100%
2.0	2.0	100%	100%	100%	93%
1.5	2.0	81%	100%	100%	73%

Table 2: Results for a shift in the opposite direction for $\rho = 0.4$.

k_1	k_2	MYT	T^2 diff	Ranking	MSSD
-0.5	+0.5	86%	100%	57%	43%
-1.0	+1.0	100%	100%	75%	60%
-0.5	+1.0	100%	100%	43%	29%
-1.5	+1.5	100%	100%	77%	63%
-2.0	+2.0	100%	100%	96%	71%
-1.5	+2.0	100%	100%	92%	67%

Table 3: Results for a shift in one direction for $\rho = 0.4$.

Deviation k_1 in one variable	MYT	T^2 diff	Ranking	MSSD
-0.5	80%	40%	72%	60%
-1.0	100%	60%	87%	60%
-1.5	100%	100%	100%	70%
-2.0	100%	100%	100%	85%
0.5	80%	50%	50%	20%
1.0	100%	70%	60%	40%
1.5	100%	100%	100%	60%
2.0	100%	100%	100%	80%

1. From the empirical results we conclude that the MYT decomposition, the T^2 difference method and the ranking technique perform equally well in detecting the source of variation when an out-of-control signal is released by the T^2 statistic, if the shifts have the same direction. The ranking method does not performs well, when the shift occurs in the opposite direction. Both T^2 difference method and ranking technique performs worse than MYT decomposition, when a shift occurs only in one variable and with a low magnitude.

2. MSSD perform worse than the other three methods for almost all cases considered.

- **The case $\rho = -0.4$:**

Table 4: Results for a shift in the same direction for $\rho = -0.4$.

k_1	k_2	MYT	T^2 diff	Ranking	MSSD
-0.5	-0.5	90%	100%	100%	60%
-1.0	-1.0	100%	100%	100%	80%
-0.5	-1.0	100%	100%	100%	57%
0.5	0.5	100%	100%	100%	100%
1.0	1.0	100%	100%	100%	83%
0.5	1.0	100%	100%	100%	71%
-2.0	-2.0	100%	100	100%	82%
2.0	2.0	100%	100%	100%	80%
1.5	2.0	100%	100%	100%	70%

Table 5: Results for a shift in the opposite direction for $\rho = -0.4$.

k_1	k_2	MYT	T^2 diff	Ranking	MSSD
-0.5	+0.5	87%	88%	100%	67%
-1.0	+1.0	100%	100%	100%	100%
-0.5	+1.0	100%	100%	100%	75%
-1.5	+1.5	100%	100%	100%	87%
-2.0	+2.0	100%	100%	100%	100%
-1.5	+2.0	100%	100%	100%	100%

Table 6: Results for a shift in one direction for $\rho = -0.4$.

Deviation k_1 in one variable	MYT	T^2 diff	Ranking	MSSD
-0.5	100%	75%	100%	50%
-1.0	100%	80%	100%	60%
-1.5	100%	100%	100%	65%
-2.0	100%	100%	100%	83%
0.5	100%	80%	100%	60%
1.0	100%	100%	100%	70%
1.5	100%	100%	100%	70%
2.0	100%	100%	100%	85%

1. The MYT decomposition and the T^2 difference method and the ranking technique perform similar and detect the source of variation in most of the cases when an out-of-control signal is released by the T^2 statistic. T^2 difference method performs worse than MYT decomposition, when a shift occurs in one variable and with low magnitude.
2. MSSD performs well below the other two in almost all cases considered.

Table 7: Results for a shift in the same direction for for $\rho = 0.8$.

k_1	k_2	MYT	T^2 diff	Ranking	MSSD
-0.5	-0.5	60%	20%	33%	33%
-1.0	-1.0	80%	33%	33%	57%
-0.5	-1.0	72%	72%	72%	57%
0.5	0.5	75%	75%	75%	40%
1.0	1.0	100%	33%	100%	100%
0.5	1.0	75%	75%	25%	25%
-2.0	-2.0	100%	85%	100%	100%
2.0	2.0	100%	80%	100%	100%
1.5	2.0	90%	75%	90%	70%

Table 8: Results for a shift in the opposite direction for for $\rho = 0.8$.

k_1	k_2	MYT	T^2 diff	Ranking	MSSD
-0.5	+0.5	100%	100%	43%	29%
-1.0	+1.0	100%	100%	44%	50%
-0.5	+1.0	100%	100%	30%	12%
-1.5	+1.5	100%	100%	73%	50%
-2.0	+2.0	100%	100%	53%	77%
-1.5	+2.0	100%	100%	80%	63%

Table 9: Results for a shift in one direction for $\rho = 0.8$.

Deviation k_1 in one variable	MYT	T^2 diff	Ranking	MSSD
-0.5	70%	65%	75%	50%
-1.0	80%	75%	80%	65%
-1.5	100%	100%	100%	80%
-2.0	100%	100%	100%	95%
0.5	65%	80%	80%	60%
1.0	70%	90%	90%	70%
1.5	100%	100%	100%	85%
2.0	100%	100%	100%	95%

1. The MYT decomposition method gives uniformly better results than the other techniques.
2. The T^2 difference method performs better than ranking technique, when shift is in opposite directions.
3. MYT decomposition, T^2 difference method and ranking technique do not perform well, when a shift is in one variable and with low magnitude.
4. MSSD performs quite poorly, compared with the other methods in almost all considered cases.

- **The case** $\rho = -0.8$**:**

Table 10: Results for a shift in the same direction for for $\rho = -0.8$.

k_1	k_2	MYT	T^2 diff	Ranking	MSSD
-0.5	-0.5	100%	100%	42%	43%
-1.0	-1.0	100%	100%	85%	42%
-0.5	-1.0	100%	100%	56%	43%
0.5	0.5	100%	100%	66%	66%
1.0	1.0	100%	100%	52%	32%
0.5	1.0	100%	100%	50%	31%
-2.0	-2.0	100%	100%	96%	87%
2.0	2.0	100%	100%	96%	87%
1.5	2.0	100%	100%	83%	73%

Table 11: Results for a shift in the opposite direction for for $\rho = -0.8$.

k_1	k_2	MYT	T^2 diff	Ranking	MSSD
-0.5	+0.5	100%	50%	100%	66%
-1.0	+1.0	100%	66%	100%	100%
-0.5	+1.0	100%	80%	80%	80%
-1.5	+1.5	100%	41%	100%	100%
-2.0	+2.0	100%	73%	100%	100%
-1.5	+2.0	100%	50%	100%	100%

Table 12: Results for a shift in one direction for $\rho = -0.8$.

Deviation k_1 in one variable	MYT	T^2 diff	Ranking	MSSD
-0.5	70%	65%	75%	50%
-1.0	80%	75%	80%	65%
-1.5	100%	100%	100%	80%
-2.0	100%	100%	100%	95%
0.5	65%	80%	80%	60%
1.0	70%	90%	90%	70%
1.5	100%	100%	100%	85%
2.0	100%	100%	100%	95%

1. The MYT decomposition method gives uniformly better results than other techniques.
2. The ranking technique performs worse than the T^2 difference method, when the shifts are in the same direction. When the shifts are in opposite directions the reverse is true.
3. The MYT decomposition, the T^2 difference method and the ranking technique do not perform well when there is a shift only in one variable and with low magnitude.
4. MSSD performs worse than the other in almost all considered cases.

3 Summary

Following conclusions were obtained from the simulation study:

1. The MYT decomposition seems to be the best amongst the four diagnostic techniques discussed, as, under all conditions, it is able to detect the source of variation whenever an alarm is triggered by the T^2 statistic. But it does not perform well when correlation is high and shift occurs in one variable.
2. The T^2 difference method performs similar to the MYT decomposition technique under almost all conditions, except for the cases when:
   (a) the shift is in one variable and with low magnitude,
   (b) the variables have a high negative correlation with the shift in opposite direction.
3. Ranking technique does not perform well:
   (a) when correlation is low and the shifts are in opposite directions and
   (b) the shift occurs for one variable only and with low magnitude.

4. The MSSD technique is outperformed by the other three techniques in almost all considered situations.

For the future work, the study should be extended to cover a larger number of variables under different correlation structures. In this paper, the performance of different technique was judged by its ability to detect the shift. However, it could also be checked through the ARL values.

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