A New Bootstrap Based Algorithm for Hotelling’s T2 Multivariate Control Chart

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Abstract

Normality is a common assumption for many quality control charts. One should expect misleading results once this assumption is violated. In order to avoid this pitfall, we need to evaluate this assumption prior to the use of control charts which require normality assumption. However, in certain cases either this assumption is overlooked or it is hard to check. Robust control charts and bootstrap control charts are two remedial measures that we could use to overcome this issue. In this paper, a new bootstrap algorithm is proposed to construct Hotelling’s T\textsuperscript{2} control chart. The performance of proposed chart is evaluated through a simulation study. Our results are compared to the traditional Hotelling’s T\textsuperscript{2} control chart results and the bootstrap results reported by Phaladiganon et al. \cite{13} using in-control and out-of-control average run lengths denoted by ARL\textsubscript{0} and ARL\textsubscript{1}, respectively. The latter case is obtained when the process mean is subject to sustained shifts. Numerical results indicate that the proposed algorithm performs better than the above mentioned methods. The new bootstrap algorithm is also applied to a real data set.

Keywords: Bootstrap; Hotelling’s T\textsuperscript{2}; Multivariate control charts; Average run length; Monte Carlo simulation.

Introduction

One of the major goals of quality control charts is to detect any variation or disturbances in the process as early as possible before many nonconforming products reach the final stage of production. Hence, control charts are widely used in statistical process control activities. In almost all products, quality depends on several quantitative characteristics which need to be controlled or monitored simultaneously. It is well known that when univariate control charts are used, the correlation structure between quality characteristics is ignored and under such condition one should expect misleading results. Multivariate control charts are used to monitor several quality characteristics simultaneously. In multivariate case, it is difficult to check the normality assumption prior to the use of parametric multivariate control charts. Under such condition, nonparametric control charts which have lower power in comparison to parametric methods are

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suggested.

However, a bootstrap method seems to be desirable because it does not require the normality assumption. Bajgier [1] introduced a univariate control chart whose control limits were estimated using a bootstrap method. Seppala et al. [18] proposed a subgroup bootstrap chart which uses the residuals, i.e. the difference between the mean of a subgroup obtained by bootstrap and each observation in the subgroup. In another study, Liu and Tang [10] suggested a bootstrap control chart that can monitor both independent and dependent observations. Moving block bootstrap was used to monitor the mean of dependent processes. Jones and Woodall [8] compared the performance of bootstrap control charts introduced by Bajgier [1], Seppala et al. [18], and Liu and Tang [10] in non-Normal situations. Polansky [15] used bootstrap method to estimate a discrete distribution, a density estimation method to obtain a continuous distribution, and established control limits. Lio and Park [9] proposed a bootstrap control chart based on Birnbaum-Saunders distribution. Chatterjee and Qiu [3] developed a class of nonparametric cumulative sum (CUSUM) control charts and used bootstrap to find their control limits. Park [12] proposed median control charts whose control limits were established by estimating the variance of the sample median via bootstrap method. Phaladiganon et al. [13] proposed $T^2$ multivariate control chart based on bootstrap. Noorossana and Ayoubi [11] proposed profile monitoring using nonparametric bootstrap $T^2$ control chart. Phaladiganon et al. [14] developed the principal component analysis of control charts for multivariate non-Normal distributions. They used bootstrap method to establish control limits. Psarakis et al. [16] investigated the impact of parameter estimation on the performance of different types of control charts. Faraz et al. [6] evaluated the in-control performance of the $S^2$ control chart with estimated parameters conditional on the phase I sample.

The use of bootstrap-based $T^2$ multivariate control chart was first introduced by Phaladiganon et al. [13]. They used bootstrap approach to determine control limits for a $T^2$ control chart in which observations did not follow a Normal distribution. Although the large sample size is not commonly used for the statistical process control, Phaladiganon et al. [13] applied the large sample size in their approach. While the essence of bootstrap method is based on resampling from original observations, they resampled using $T^2$ statistic.

In present paper, a bootstrap approach based on original observations is considered to obtain control limits. The proposed method allows one to use different sample sizes, while the fixed 1000 sample size was allowed by Phaladiganon’s method. Although the sample size is not essential to be large in the proposed algorithm, but to be able to compare the performances of our algorithm with the Phaladiganon’s algorithm we used the smaller sample sizes. Bootstrap definition (Efron and Tibshirani [5]) was used to create resample from the original data. Here, $ARL_1$ is also calculated for several defined distributions. Our simulation results are then compared to both traditional Hotelling’s $T^2$ and Phaladiganon methods.

In this paper, Hotelling’s $T^2$ multivariate control charts for monitoring mean of the process have been reviewed. The proposed bootstrap approach for multivariate control charts is then introduced. A simulation study using $ARL_0$ and $ARL_1$ assuming multivariate Normal, multivariate $t$, multivariate skew-Normal and multivariate lognormal distributions is then performed. Finally, an application to a real data set is presented.

**Multivariate Control Charts for Process Mean**

Let a random vector $X$ have a $p$-dimensional Normal distribution, denoted by $N_p(\mu_0, \Sigma_0)$. It is well known that the statistic

$$T^2 = (X - \mu_0)' S^{-1} (X - \mu_0),$$

can be used to construct a control chart. The $T^2$ statistic follows a chi-square distribution with $p$ degrees of freedom. Hence, $L_u = \chi^2_{p, 1-\alpha}$ is the upper control limit for the control chart when the vector mean $\mu_0$ and covariance matrix $\Sigma_0$ are known. This control chart is called a phase II chi-squared control chart. In practice, however, $\mu_0$ and $\Sigma_0$ are unknown and should be estimated using sample mean vector $\overline{X}$ and sample covariance matrix $S$, respectively. The sample mean vector and sample covariance matrix are estimated using the random sample $X_1, \ldots, X_m$ from $N_p(\mu_0, \Sigma_0)$ in phase I. If $X$ is a new observation in phase II, we compute

$$T^2 = (X - \overline{X})' S^{-1} (X - \overline{X}),$$

where $c T^2$ has an $F$ distribution with $p$ and $m-p$ degrees of freedom where $c = m (m-p)/p (m^2 - 1)$. Thus the upper control limit of a multivariate control chart for the process mean, with unknown parameters can be written as $L_u = c^{-1} F_{1-\alpha, p, m-p}$. When process
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is in control and \( \mu_0 \) and \( \Sigma_0 \) are known, then average run length of the multivariate control chart is \( ARL_0 = 1/\alpha \), where \( \alpha \) is the probability of \( T^2 \) exceeding \( L_u \). From practical point of view, it is better to use the fundamental definition of ARL, the average number of observations required for the control chart to detect a change under the in-control process (Woodall and Montgomery [20]). Furthermore, the out of control ARL \( (ARL_1) \) of the multivariate chart depends on the mean vector only through the non-centrality parameter defined as \( \lambda^2 (\mu_1) = m \delta' \Sigma_0^{-1} \delta \), where \( \mu_1 = \mu_0 + \delta \) is a specific out of control mean vector. Thus, \( ARL_1 \) is a function of \( \lambda^2 (\mu_1) \) and can be calculated using \( ARL_1 = 1/(1 - \beta) \), where \( \beta \) is the probability of an in-control observation while process is indeed out of control.

A New Bootstrap Approach

In order to construct a \( T^2 \) control limit for the mean of a process, we have introduced a new algorithm. First, Phaladiganon Bootstrap (PB) algorithm is explained (Figure 1).

1. Compute \( T^2 \) in equation (1) using \( m \) in-control observations.
2. Let \( T_i^{2(i)}, \ldots, T_m^{2(i)} \) be a set of \( m \) values from the \( i \)th bootstrap sample \( (i = 1, \ldots, B) \) randomly drawn from the initial \( T^2 \) statistic with replacement.
3. In each of \( B \) bootstrap samples, determine the \( m(1 - \alpha) \) th percentile value given a specified value of \( \alpha \).
4. Determine the control limit by taking the average of \( Bm(1 - \alpha) \) th percentile values \( L_u^* = \frac{1}{B} \sum_{i=1}^{B} T_i^{2(i)}[m(1-\alpha)] \).
5. If an observed statistic exceeds \( L_u^* \), we conclude that process is out of control.

PB algorithm requires a large sample size for calculating the percentiles \( T_i^{2(i)} \), i.e. \( m \) must be large enough for small \( \alpha \). We assume that \( X_1, \ldots, X_m \) is a random sample in phase I from unknown distribution and \( \bar{X} \) and \( S \) are the sample mean vector and covariance matrix, respectively.

1. Draw a bootstrap sample \( X^* \) from the observed data \( X_1, \ldots, X_m \) with replacement.
2. Compute bootstrap statistic \( T^* \) using
   \[
   T^* = (X^* - \bar{X})'S^{-1}(X^* - \bar{X}).
   \]
3. Repeat steps 1 and 2, \( B \) times to produce \( T_1^*, \ldots, T_B^* \).
4. Determine \( B(1 - \alpha) \) th percentile values \( T^* \) as the upper control limit \( L_u^* = T_{[B(1-\alpha)]}^* \).

We use the established control limit to monitor new observations. That is, if the monitoring statistic of the new observations exceeds \( L_u^* \), we declare those observations as out-of-control signals.

The New Bootstrap (NB) algorithm is applicable for all sample sizes. Therefore, it can be stated that this algorithm is more efficient than the PB algorithm when the sample size is less than 1000. In this algorithm, resampling is done from the main sample not from the observed statistic \( T^2 \). This method requires \( B \) iterations but the PB algorithm needs to be repeated \( mB \) times, thus the new algorithm runs faster than PB algorithm.

The proposed algorithm is illustrated in Figure 2.
Simulation Study

In this section, a simulation study is performed to evaluate the performance of the proposed algorithm. Notice that there are two considerable ideas in the proposed algorithm.

1. NB algorithm runs faster than PB algorithm. Simulation studies are performed to investigate the performance of our algorithm and compare it to the traditional control chart and PB algorithm.

2. Its efficiency is high even if the sample size is less than 1000.

A total of \(m=100\), 500, and 1000 observations were generated from multivariate Normal (MN), multivariate t (Mt), multivariate skew-Normal (MSN) and multivariate lognormal (MLN) distributions. The distributions MN and Mt are symmetric while MSN and MLN are asymmetric. Each data set contains three variables \((p=3)\). In the simulation, we let \(\mu=[1\ 1\ 1]'\) for MLN distribution and \(\mu=[0\ 0\ 0]'\) for other distributions and the following covariance matrix was considered for MLN distribution:

\[
\Sigma = \begin{bmatrix}
1 & 0.7 & 0.6 \\
0.7 & 1 & 0.1 \\
0.6 & 0.1 & 1 \\
\end{bmatrix}
\]

This matrix was also used somehow for data generating from the other distributions Mt, MSN, and MLN.

Figures 3 and 4 show the boxplot and cumulative density function (CDF) for \(T^2\) given in Equation (1) using exact distribution, simulated data from F distribution with \(p\) and \(m-p\) degrees of freedom, and \(T^2^*\) based on NB method for all four distributions. It is not possible to compute distribution of \(T^2\) by PB method because it gives only one upper bound. To draw Figures 3 and 4, we generated \(m=100\) observations from each distribution with 1000 Monte Carlo simulation replications.

Figure 4 clearly shows that when distribution is not Normal, the CDF of the NB algorithm is closer to the CDF of \(T^2\) than F distribution. In other words, the proposed NB algorithm provides a more accurate density estimation for \(T^2\).

Comparison of control limits

We generated \(m=100\) in-control observations in phase I. The first set of observations was used to determine control limits for \(T^2\) control charts using PB and NB methods. The performance of the control charts is evaluated by generating new observations until the \(T^2\)

![Figure 3. Boxplot of \(T^2\) values based on exact distribution, F distribution, and NB algorithm](image-url)
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statistic exceeds control limits obtained in phase I. Figure 5 represents $T^2$ control charts from the 100 in-control observations. The false alarm rate was specified at $\alpha = 0.05$.

Figure 5 shows that, upper control limits of all three approaches are similar for MN distribution. It also

Figure 4. CDF of $T^2$ based on exact distribution, F distribution, and NB algorithm

Figure 5. Control limits of $T^2$ control charts established by F-distribution, PB and NB algorithms with $m=100$, $B=3000$, and $\alpha=0.05$ in phase I and 100 new observations in phase II
shows that all three approaches produce comparable control limits for MN case. When the distribution is not Normal, control limits from traditional $T^2$ tend to generate higher false alarm rates. The control limits for the traditional Hotelling’s $T^2$ is not accurate which leads to deviation of rate $\alpha = 0.05$ from the false alarm. The result for NB and PB algorithms control limits are also close together.

Comparison of in-control out-control average run length

ARL is the most widely used performance measure for control charts. In this study, we emphasize on the in-control ARL (ARL$_a$), which is defined as the average number of observations required until an out of control observation is detected under the in-control process. Furthermore, out of control ARL (ARL$_1$) was investigated when the process mean vector was contaminated. To calculate ARL$_1$, we changed the mean of the process using $\mu = [1 \ 1]^T$ for MN, Mt, MSN distributions, and set $\mu = [2 \ 2]^T$ for MLN distribution. ARL$_1$ value is calculated as the average number of observations needed for a control chart to alarm an out of control condition when the process is indeed out of control. Therefore, the corresponding control chart can give better control limits than the other ones, because if ARL$_1$ value is smaller than the deviations of the mean values of the process, we can be detected sooner. Geometric method is employed to calculate ARL$_0$ and ARL$_1$ while Phadadigon et al. [13] have used binomial method. In the binomial method, first, we generate $m$ data and compute $\alpha$, the percentage of

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Table 1. ARL$_0$ and ARL$_1$ from $T^2$ chart with control limits constructed using F-distribution, PB, and NB algorithms with $B=3000$ from 20000 simulation runs based on different distributions.
corresponding $T^2$ that is greater than the upper control limit, then calculate $ARL_0 = 1/\alpha$.

The values of $ARL_0$ and $ARL_1$ were calculated using 20000 simulation runs. When the distribution of the data is MN, the specified $ARL_0$ and the actual $ARL_0$ for $T^2$ control chart is expected to be close. Table 1 shows that for the Normal case, based on $ARL_0$ criterion, the classical Hotelling’s $T^2$ performs better than the other two methods but the results show that in all, except two cases, $ARL_1$ for the NB algorithm is smaller than F and PB algorithm. In Table 1, for Mt distribution in comparison with PB algorithm, the performance of the

Figure 6. Boxplot of $ARL_0$ when simulations are established by F-distribution, PB and NB algorithms with nominal $ARL_0=20, B=3000$ and $\alpha=0.05$
NB method is better for $\text{ARL}_0$ criterion except in one case. Also, $\text{ARL}_1$ criterion for NB algorithm is relatively better than the other methods. Table I shows that for the MSN distribution, the traditional Hotelling’s $T^2$ does not perform as expected. In almost all cases, $\text{ARL}_1$ for NB algorithm are less than the $\text{ARL}_1$ of PB algorithm. Also for MLN, the NB algorithm performs better than the PB algorithm based on the $\text{ARL}_0$ criterion, except for one case. NB algorithm has a better performance than PB algorithm based on $\text{ARL}_1$ criterion.

All $\text{ARL}_0$ values obtained in the simulation study are shown in Figures 6 and 7 for $\alpha = 0.05$ and $\alpha = 0.1$, respectively. Looking at both figures, it can be concluded that, in general, all methods have outlier observations and dispersion of $\text{ARL}_0$ values are different.

Figure 7. Boxplot of $\text{ARL}_0$ when simulations are established by F-distribution, PB and NB algorithms with nominal $\text{ARL}_0=10$, $B=3000$ and $\alpha=0.1$
An Application to Real Data

In this section, we consider an example associated with aluminum smelting data. A dataset consisting of 189 observations on 3 variables are collected over time. To assess the multivariate normality of observations, we conducted Royeston’s H test [17]. The p-value of less than 0.001 indicates that this data set does not follow a multivariate Normal distribution (Figure 8). Figure 9 shows the $T^2$ control chart whose control limits were estimated by F-distribution, PB, and NB algorithms with false alarm rate $\alpha = 0.01$. The actual ARL$_0$ for NB algorithm is 105 which is similar to the nominal ARL$_0$. In other words, upper control limit from NB method is more accurate than PB method for calculating ARL$_0$. Aluminum smelting is an energy intensive, continuous process, and cannot easily be stopped and restarted. In view of the possible lack of normality of the data and considering the enormous cost of process failure, it is worthwhile to monitor processes using the NB algorithm.

Results and Discussion

In this paper, we proposed a new bootstrap algorithm in order to obtain the control limits for a control chart which uses observations with unknown distribution because bootstrap method does not require a pre-specified distribution. In comparison to the Phaladiganon’s method, the new bootstrap method proposed in this article is easier to carry out, faster to run, and more accurate in estimation of the density of $T^2$. For non-Normal distributions, the Phaladiganon method can be used to determine the limit for $T^2$ control chart. The Phaladiganon method requires a large sample size, i.e. $m = 1000$, to have a reasonable performance while our new proposed algorithm works well with $m < 1000$. Furthermore, it is easier to implement. Our simulation results showed that the proposed algorithm is more efficient than the traditional $T^2$ control chart and Phaladiganon method for both Normal and non-Normal cases.

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References