Control Charts with Estimated Control Limits

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Abstract. The Shewhart control charts are the most widely used tools for monitoring industrial processes. For normal data, and when it is not necessary to estimate the control limits, a situation that rarely happens in practice, these charts present a high performance in the detection of moderate up to large changes in the process parameters. However, when the under control target mean value and/or the target standard deviation are not fixed given values or when we have non-normal data, the performance of these charts may be adversely affected. Here we present a simulation study to compare the performance of various control charts, with true and estimated limits. The estimation of the target values is based on m initial subgroups of size n, taken when the process is considered to be stable. To describe the model underlying these subgroups, and apart from the standard normal distribution, we shall consider contaminated normal distributions. To estimate the target mean value and standard deviation, we shall consider, apart from the most common estimators, a few robust estimators. The results of this study lead us to conclude that the robust estimation of the target values reduces the differences between the performance of the charts with estimated and fixed limits. The behaviour of the charts under study is also illustrated with an application to a set of real data, and the conclusions are similar to the ones obtained through the simulation Monte Carlo study.

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1 Introduction

In all industrial processes there is always some variability that can be due either to random or to deterministic causes. When there is only random variability, inherent to any production process, we say that the process is in-control (state IN). If there is another kind of variability, associated to deterministic causes, we say that the process is out-of-control (state OUT). One of the main objectives of Statistical Quality Control (SQC) is to distinguish these two kinds of variability, and the control charts are basic tools for this purpose. A control chart is a graphical representation that allows us to decide whether an industrial process is IN or OUT, and may be regarded as a test on the process parameters, performed along time.

Let us generally denote the control chart statistic by W and the region of the chart associated to the IN-control state by C (*Continuation Region*). The W-chart plots for each sampling point t, the value of the statistic W_t. For the implementation of the most common control charts, the samples are taken at regular fixed intervals of time. These charts are called FSI control charts, from *Fixed Sampling Intervals*. They are the ones we shall consider in this paper. The values W_t are compared, in general, with two lines, the lower and the upper control limits of the chart, generically denoted by LCL_W and UCL_W. If W_t falls in the region C, we decide that the process is in-control; otherwise, we decide that the process is out-of-control, and we must then detect and alter the deterministic causes of such an occurrence.

General details about control charts may be found, for instance, in Montgomey (1996) and in Ryan (2000). In Section 2 we try motivating the use of control charts with robust estimated control limits, and we also present some background information. In Section 3 we describe the methodology used to carry out the simulation study in this paper, and advance with some considerations about the estimation of the process target values, necessary to set up the control limits of the different charts. In Section 4 we describe the simulation experiment and we present the simulated output. In Section 5 we apply the control charts under study to a set of real data, and we comment the results. Finally, in Section 6 we present some overall conclusions.

2 Motivation and some background information

The most commonly used charts for monitoring industrial processes, or more precisely, a certain quality characteristic X, at the targets μ_0 and σ_0, the mean value and the standard deviation of the process X, respectively, are the Shewhart Control Charts with 3-sigma Control Limits. These charts usually assume independent and normally distributed observations, and have control limits of the form,

$$LCL_{W} = E(W) - 3\sqrt{Var(W)}, \qquad UCL_{W} = E(W) + 3\sqrt{Var(W)}$$

where W, $E(W)$ and $Var(W)$ denote the control statistic of the chart, its expected value and its variance, respectively. More precisely, to monitor the process mean value, it is common to implement a two-sided sample mean chart, $\overline{X}$, also denoted M-chart, with control limits given by

$$LCL_{M} = \mu_0 - 3\sigma_0/\sqrt{n}, \qquad UCL_{M} = \mu_0 + 3\sigma_0/\sqrt{n}. \tag{2.1}$$

To monitor the process standard deviation, it is usual to implement one of the following upper control charts: the sample standard deviation chart (S-chart), with upper control limit

$$UCL_S = \left(c_4 + 3\sqrt{1-c_4^2}\right)\sigma_0 \tag{2.2}$$

or the sample range chart (R-chart), with upper control limit

$$UCL_R = (d_2 + 3d_3)\,\sigma_0, \tag{2.3}$$

where c_4, d_2 and d_3 are tabulated for normal data and for the most common sample sizes n. For $n = 5$, the size of the rational subgroups considered, $c_4 =$???, $d_2 = 2.326$ and $d_3 = 0.864$.

The ability of a FSI control chart to detect process changes is usually measured by the expected number of samples taken before the chart signals, i.e., by its ARL (*Average Run Length*), or alternatively, by its power function. When the sucessive values of the control statistic are independent, the ARL is given by

$$ARL_W(\theta) = \frac{1}{1 - P(W \in C\,|\,\theta)} =: \frac{1}{\pi_W(\theta)},$$

where θ denotes the parameter to be controlled at $\theta = \theta_0$, with $\pi_W(\theta)$ the power function of the W-chart. Depending on the distribution underlying the data and on the functional expression of the control statistic W, we may be able obtain the exact value of the ARL, or only an approximated value (by simulation, for instance). Assuming that the process changes from the in-control state, $\theta = \theta_0$, to an out-of-control state, θ, a value in the space parameter, the power function of the chart is the probability of detection of that change in any arbitrary rational subgroup. When the process is in-control, the power function gives us the *false alarm rate* of the chart, also called the α-risk and given by

$$\alpha = P\left(W \notin C \vert\ IN\right) = P\left(W \notin C \vert\ \theta = \theta_0\right). \tag{2.4}$$

The control limits of a W-chart are usually determined in order to have a chart with a small fixed false alarm rate (a large in-control ARL) and we hope to obtain high power function values (small out-of-control ARL) for the shifts the chart must detect.

For normal data, and when it is not necessary to estimate the control limits, the Shewhart 3-sigma control charts present a reasonable high performance in detecting moderate-to-large changes in the process parameters. Then, the α-risk in (2.4), associated with the M, S and R charts, with control limits given in (2.1), (2.2) and (2.3), is given by 0.0027, 0.0046 and 0.0039, respectively.

However, the sets of data related to the most diversified processes, from areas like telecommunications, insurance, finance and reliability, among others, may exhibit a significant correlation, with an asymmetric heavy-tailed underlying model. The assumptions associated to the usual control charts rarely hold true in practice, and these charts must be carefully used. It is thus important to advance with “robust” control charts to monitor the process parameters, so that we do not have either a very high or a very low false alarm rate whenever the parameters to be controlled are close to the target values, μ_0 and σ_0, although the data is no longer normal. Details about the effect of non-normality in the performance of the usual control charts and the design of some “robust” control charts can be found in Schilling and Nelson (1976), Balakrishnan and Kocherlakota (1986), Amin and Lee (1999), Borror et it al. (1999) and Figueiredo and Gomes (2004, 2005), among others. Some considerations about “robust” estimation as well as different approaches to determine robust control limits can be found in Lax (1985), Rocke (1989,1992), Tatum (1997), Nedumaran and Pignatiello (2001), Wilcox and Keselman (2002), Champ and Chou (2003), Chan and Heng (2003), Figueiredo (2003), Champ and Jones (2004). **(Tentar cortar alguns)**

The performance of the Shewhart control charts can also be adversely affected when, even for normal data, the target values, μ and σ, are not fixed given values. To obtain charts with estimated control limits, with properties similar to the ones with true limits, some authors have recommended the evaluation of these limits in a "resistant" way, and there has been an agreement on the use of a reasonably large number of initial subgroups, to perform this estimation. Some of them have recommended the collection, whenever the process is stable and in-control, of 20 or 30 subgroups of size $n = 4$ or 5 **(???, ???)**. Others suggest the consideration of at least $m = 400/(n-1)$ subgroups **(???, ???)**. Langenberg and Iglewicz (1986) and Chan et *al.* (1988) provide some corrections to the control limits of the usual charts in order to maintain the expected false alarm rate when monitoring non-normal data. However these corrections must be done case-to-case, and given the huge number of different situations we may have in practice, this approach does not seem the most appropriate.

In this paper we shall adress the problem of estimation of the control limits of the traditional M, S an R Shewhart control charts, but with the possible use of robust estimation of both μ and σ. Apart from normal processes we shall also consider contaminated normal processes, with low degrees of contamination. The comparison of the different estimators used in this study, as well as the choice of an adequate value for m, the number of initial subgroups on which we base the estimation, has been done on the basis of the behaviour of confidence intervals of the simulated α-risk, in (2.4).

3 Description of the methodology

To monitor the mean value and the standard deviation of an industrial process, we are going to implement $M \equiv \overline{X}$, S and R charts, with 3-sigma estimated control limits, for a sample size $n = 5$. To estimate the chart control limits, we collect $m = 20,\ 50,\ 100$ and 200 initial subgroups of size $n = 5$, taken when the process is considered to be stable and in-control. To analyze the in-control performance of the implemented charts, we obtain their false alarm rates α, in (2.4), through Monte Carlo simulation techniques, and we compare those simulated α-risks with the expected value of α.

3.1 Models underlying the initial subgroups and the process

To describe the data of the underlying process X, we have considered the following set-ups:

1. The initial samples upon which we base the estimation of μ and σ, as well as the samples generated to estimate the α-risks, come from a standard normal distribution, $N(0, 1)$.
2. The initial samples come from a N(0,1) model, but the other ones come from a contaminated standard normal distribution, with 1% (or 5%) of contamination, i.e., 1% (or 5%) of the observations come from a normal distribution with a larger standard deviation, more precisely, from a $N(0, 3)$ model.
3. All generated samples come from 1 of the contaminated normal models in 2.

Remark 3.1. *We have also used set-ups similar to the ones described in 2. and 3., working with samples from a standard normal distribution, but with one outlier, from a $N(0, 3)$ distribution, every 100 observations. Since there were practically no significant differences, we shall no longer refer this situation.*

3.2 Estimators used for the in-control target values

On the basis of a sample $(X_1, \cdots, X_n)$ taken from the process, we shall consider the usual estimator $\overline{X}$, and a robust estimator, the trimmed mean T, for the mean value μ of the process. To estimate the standard deviation σ of the process, we have used the classical estimators, R (sample range) and S (standard deviation), as well as the median absolute deviation (MAD), described later on in this subsection.

We shall also use alternative estimators, based on the bootstrap sample, $(X_i^*,\ 1 \le i \le n)$, obtained from the observed values $(x_1, \cdots, x_n)$, through a sampling with replacement. To be more precise, X_i^*, $1 \le i \le n$, is a random sample of independent, identically distributed (i.i.d.) replicates from a random variable (r.v.)

X^*, with distribution function (d.f.) equal to the empirical d.f. of our observed sample, i.e., given by

$$F_n^*(x) = \frac{1}{n} \sum_{i=1}^{n} I_{\{x_i \le x\}}, \quad \text{with } I_A = \begin{cases} 1 & \text{if } A \text{ occurs} \\ 0 & \text{otherwise} \end{cases}$$

the indicator function of the set A. Let us denote $X_{i:n}$, the i-th ascending order statistics (o.s.) associated to the sample X_i, $1 \le i \le n$. We shall consider the median of the bootstrap sample, denoted BMd, i.e.,

$$BMd := \begin{cases} X^*_{m:n} & \text{if} \quad n = 2m-1 \\ \\ \frac{X^*_{m:n}+X^*_{m+1:n}}{2} & \text{if} \quad n = 2m \end{cases}, \quad m = 1, 2, 3, \cdots .$$

For $1 \le i \le j \le n$, the probabilities $\alpha_{ij} = P\left(BMd = (x_{i:n} + x_{j:n})/2\right)$ and $\beta_{ij} = P\left(X^*_{n:n} - X^*_{1:n} = x_{j:n} - x_{i:n}\right)$ have been explicitly obtained in Figueiredo and Gomes (2004) and Figueiredo (2003), respectively. The total median statistic, TMd, is the linear combination $TMd := \sum_{i=1}^{n} \sum_{j=i}^{n} \alpha_{ij} \ (X_{i:n} + X_{j:n})/2$ and the total range statistic, TR, is defined by $TR := \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} \left(X_{j:n} - X_{i:n}\right)$. These statistics can also be written as a linear combination of the sample o.s., in the form

$$TMd := \sum_{i=1}^{n} a_i X_{i:n}, \quad a_i = \frac{1}{2} \left(\sum_{j=i}^{n} \alpha_{ij} + \sum_{j=1}^{i} \alpha_{ji} \right). \tag{3.1}$$

and

$$TR := \sum_{i=1}^{n} b_i X_{i:n}, \quad b_i = \tag{3.2}$$

where the coefficients a_i and b_i, independent of the underlying model F, are presented in Table 1 for values from $n = 1$ until $n = 10$. Note that

$$a_i = a_{n-i+1}, \quad 1 \le i \le n, \quad 0 < a_1 \le a_2 \le \cdots \le a_{[n/2]}, \quad \sum_{i=1}^{n} a_i = 1.$$

and

$$b_i = ????.$$

The statistics TMd and TR are resistant to changes in the underlying model, and are similar to a special trimmed-mean, also used in this simulation study, where **(but?)** the ideal percentage of trimming does not depend on the data distribution. The distributional behaviour of the estimators in (3.1) and (3.2)

Table 1: Values of the coefficients a_i/b_i, for the most common sample sizes n.

i	1	2	3	4	5	7	10
1	1.000/????	0.500/????	0.259/????	0.156/????	0.058/????	0.010/????	0.001 /????
2			0.482	0.344	0.259	0.098	0.019
3					0.366	0.239	0.078
4						0.306	0.168
5							0.234
6							

has already been investigated, and these statistics have revealed to be efficient and robust estimators of the mean value and the standard deviation, respectively. Details about these estimators can be found in Cox and Iguzquiza (2001), Figueiredo (2003) and Figueiredo and Gomes (2004, 2005).

To estimate the mean value μ and the standard deviation σ of X, we have carried out the following procedure: from m=20, 50, 100 and 200 initial subgroups of size $n = 5$, we compute m partial estimates, $\widehat{\mu}_{0i}$ and $\widehat{\sigma}_{0i}$, $i = 1, \cdots, m$, and then the overall estimates $\widehat{\mu}_0 = \sum_{i=1}^{m} \widehat{\mu}_{0i}/m$ and $\widehat{\sigma}_0 = \sum_{i=1}^{m} \widehat{\sigma}_{0i}/m$, to be used in the control limits. To obtain the partial estimates $\widehat{\mu}_{0i}$, we have considered:

M1. the *sample mean*, $M \equiv \overline{X}=\frac{1}{5}\sum_{i=1}^{5} X_i$,

M2. the *total median*, $TMd = 0.058\,(X_{1:5} + X_{5:5}) + 0.366X_{3:5} + 0.259\,(X_{2:5} + X_{4:5})$, and

M3. the *trimmed-mean*, $T(5\%) = \frac{1}{4}\,(X_{1:5} + X_{5:5}) + \frac{2}{9}\,(X_{2:5} + X_{3:5} + X_{4:5})$.

To obtain the partial estimates $\widehat{\sigma}_{0j}$, unbiased whenever the underlying model is normal, we consider the following statistics divided by the scale constant c (into brackets):

S1. the *sample range*, $R = X_{5:5} - X_{1:5}$ $\quad (c = 2.326)$,

S2. the *sample standard deviation*, $S = \sqrt{\frac{1}{4}\sum_{i=1}^{5}\left(X_i - \overline{X}\right)^2}$ $\quad (c = 0.940)$,

S3. the *median absolute deviation from the median*, a common estimator for the standard deviation in robustness studies. Denoting the sample median by Md, we have $MAD = Md\,|X_i - Md|$ $\quad (c = 0.555)$, S4. the *total range*, $TR = 0.737\,(X_{5:5} - X_{1:5}) + 0.263\,(X_{4:5} - X_{2:5}) \quad (c = 1.801)$, and

S5. a *modified version of* S, defined by $S^{*} = \sqrt{\sum_{i=1}^{5} a_i\,(X_{i:5} - TMd)^2} \quad (c = 0.585)$, where a_i are the coefficients of the sample o.s. in the total median estimator, presented in Table 1.

Remark 3.2. *The interquartile-range, defined by* $IQR = X_{4:5} - X_{2:5}$*, for samples of size* $n = 5$*, is also a common robust estimator for the standard deviation. However, we think that its use to determine the control limits of the chart is not at all convenient, due to the large amount of information lost.*

4 Simulation Study and Results

4.1 The simulation experiment

To compute the false alarm rates of the charts under study we have carried out a multi-sample Monte Carlo simulation experiment of size $r \times k$. This technique is very common in simulation when we want to estimate measures of dispersion. In a multi-sample simulation of size $r \times k$, instead of generating a sample of a very large size (say, $N = r \times k$) of observed values of a statistic, we collect k observations of the statistic on each of the r independent replications of the experiment. The value of k also needs to be large enough to reduce the bias, and provide asymptotic normality. We next take as an overall estimate of the parameter of interest the average of the r corresponding estimates computed on the independent replications. Then, under very broad conditions, that overall estimator (which is a sample mean) converges to normality as r increases. Moreover, we may estimate the standard error of this overall estimate, and thus derive a confidence interval for the parameter of interest. For details see Fishman (1972).

Here the parameter of interest is the false alarm rate α of the different charts. To obtain an estimate for α, associated to a control statistic generically denoted W, we use a multi-sample Monte Carlo simulation with $r = 50$ replicates of size $k = 3,000,000$, described in the following algorithm:

1. For each replicate $j = 1, 2, \cdots, r$, $r = 50$, we generate m rational subgroups of size $n = 5$, and establish the control limits of the W-chart, $(LCL_W(j; m),\ UCL_W(j; m))$, taking into account the estimates for μ and σ, obtained through the different estimation procedures described in subsection 3.2; next, we generate a sample of $k = 3,000,000$ values of the control statistic, W. For each value of (j, m), we compute partial estimates for the false alarm rate α, i.e., we simulate the samples $\widehat{\alpha}_j(m),\ 1 \le j \le r$, $m = 20$, 50, 100 and 200.

2. Next, for any value of m, the estimate of α is the overall mean of the previous r partial estimates, i.e.

$$\widehat{\alpha}(m) = \frac{1}{r}\sum_{j=1}^{r}\widehat{\alpha}_j(m),$$

   with an associated standard error given by

$$s.e_{\widehat{\alpha}}(m) = \left(\frac{1}{r(r-1)}\sum_{i=1}^{r}\left(\widehat{\alpha}_j(m) - \widehat{\alpha}(m)\right)^2\right)^{1/2}.$$

   We then easily get a 95% confidence interval (c.i.) for the false alarm rate α.

3. Finally, we compute three different indicators,

$$I_1(m) := \text{Distance of } \widehat{\alpha}(m) \text{ to the target } \alpha = |\widehat{\alpha}(m) - \alpha|$$

$$I_2(m) := \text{Size of the 95\% confidence interval} = 2 \times 1.96 \times s.e_{\widehat{\alpha}}(m)$$

$$I_3(m) := \max\left(|\widehat{\alpha}(m) + 1.96 \times s.e_{\widehat{\alpha}}(m) - \alpha|\,,\ |\widehat{\alpha}(m) - 1.96 \times s.e_{\widehat{\alpha}}(m) - \alpha|\right)$$

   (maximum distance to α of any point in the 95% c.i.).

Ideally, we thus want small values for $I_1(m)$, $I_2(m)$ and $I_3(m)$.

4.2 The simulation output

We have run a FORTRAN program, to carry out the simulation. The large size of simulation allows us to evaluate the overall estimates for the false alarm rates and their standard errors with a precision of four decimal figures, and to present 95% confidence intervals for α with a reasonable length. For the different set-ups described before in subsection 3.1, we have carried out the algorithm described in subsection 4.1 for each pair of statistics $(M_i,\ S_j)$, $1 \le i \le 3$, $1 \le j \le 5$, provided in subsection 3.2.

In Table 2, for each value of m, the number of initial subgroups considered, and each chart type (M, S and R), we next present, in 3 different rows, associated with the set-ups 1., 2. and 3., respectively, described in subsection 3.1, the pair of statistics leading to the minimum I_2 indicator, given that the target α belongs to the 95% simulated confidence interva.

Table 2: Pairs of statistics M_i/S_j, leading to the smallest value for the indicator I_1.

m	M-chart	S-chart	R-chart
20	$(M_1,\ S_2)$??	???	???
50			
100			
200			

(Com a ideia de ver se se conseguem tirar conclusões)

Remark 4.1. *The three location statistics, $\overline{X}$, TMd and $T(5\%)$, have provided similar alarm rates. This is the reason why in the following figures we have restricted to the classical statistic $M \equiv \overline{X}$.*

We next picture the confidence intervals for the false alarm rates of the M charts with control limits, $\widehat{\mu} \pm 3\, \widehat{\sigma}/\sqrt{5}$, and for the R and S charts with upper control limit, $(d_2 + 3d_3)\ \widehat{\sigma} = 4.9183\ \widehat{\mu}$ and $\left(c_4 + 3\sqrt{1 - c_4^2}\right) \widehat{\sigma} = 1.9635\ \widehat{\sigma}$, respectively. These charts are implemented under different conditions relatively to the estimation of the target values and, in Figures 2, 3 and 4, the data are generated according to the set-ups 1., 2. and 3., respectively, described in subsection 3.1. To estimate μ we have consider the $M \equiv \overline{X}$ statistic, and to estimate σ we have considered the statistics S, R, S^*, TR and MAD. From these figures we observe that the behaviour of the different charts depends on the number of initial subgroups, on the type of data we are dealing with, and on the estimates used to set-up the control limits.

From Figure 2 we observe that when we consider a small-to-moderate number of initial subgroups of $N(0, 1)$ data to estimate the in-control target values, like the value $m = 20$, we obtain charts with alarm rates very different from the expected value α, associated to fixed norms μ_0, σ_0. The correspondent confidence intervals have a large length, and even so, they usually do not include the expected value α.

If we increase the number of initial subgroups, i.e., if we consider $m = 50$, the alarm rates are closer to the expected value, and the associated confidence intervals have a much smaller size. On the basis of that size we are inclined to choose the estimate **??**. When we further increase m, the gain is not at all significant, and we are inclined to advise the choice $m = 50$ for the number of initial rational subgroups.

(A partir daqui já não fiz emendas, mas vou-te passar a pasta)

Figures 3 and 4 show that the behaviour of the different charts is not very different from the one observed in the case of normal data.Thus, we continue to advise the use of a large of number of subgroups to estimate the in-control target values as well as the use of robust statistics. More specifically, we can draw the following conclusions. The presence of outliers as well as the existence of some contamination in the distribution of the data of the initial subgroups has also a significant effect on the performance of the charts; in general, we obtain estimates for the standard deviation greater than the true value σ_0, and consequently, the control limits are set-up further apart than usual and we obtain charts that present smaller alarm rates than the expected value. As a result, these charts perform poorly and fail to detect changes in the process parameters. As expected, the behaviour of these charts becomes worse with the increase of the percentage of subgroups with outliers or contamination, but the effect of having contaminated data is less significant if we consider a small number of initial subgroups instead of a large number. The charts with σ_0 estimated in a robust way are the ones that present the best performance. In this study the MAD statistic usually lead us to obtain confidence intervals with large length, and thus we suggest the use of the TR or of the S^* statistic to estimate the target values, μ_0 and σ_0.

5 Illustrating example with real data

Here we are going to implement the previous charts to a set of real data.

6 Some overall conclusions

Form this study we conclude that the properties of the charts with estimated limits may differ markedly from the ones with true limits, depending on the type of data we have in the initial subgroups. The usual $\overline{X}$, R and S charts, present alarm rates very different from the expected values, unless we consider a large number of initial subgroups (say $m > 100$) of normal data. The presence of outliers or contaminated data in the initial subgroups has a significant effect on the performance of the charts. Even for a large number of initial subgroups, the estimated control limits are set-up wider (because we obtain estimates for the standard deviation greater than the true value σ_0), and consequently, we obtain charts that present smaller alarm rates than the expected value. If we have non-normal data in the initial subgroups, the robust estimation of the parameters μ_0 and σ_0 reduce the differences between the performance of the charts with estimated limits and the performance of the charts with true limits, compared to the classic estimation.

Thus, the use of these charts deserves more careful study. In addition, it is very important to propose charts with modified control limits for use in the beginning of the process control until we have an adequate number of initial subgroups for the estimation of unknown parameters, or alternatively, we can use the bootstrap methodology to improve the accuracy of the estimates.

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