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Research Article

Robust Monitoring of Simple Linear Profiles Using M-estimators

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Abstract

In many applications of statistical process control, the quality of a product or a process is described by the relationship between the response variable and one or more independent variables which is called a profile. A profile could be either linear or nonlinear. The control limits of a chart, used to monitor a profile, are functions of model parameters. The classical estimators used to estimate the parameters, are defined under certain hypotheses such as the normality of the error terms. Deviation from any of these assumptions may cause contamination. Whenever contamination exists, the classical estimators are not robust, and the resulting control charts are not accurate when monitoring the profiles. In this research, a robust estimator of the model error term variance is introduced and evaluated using MSE. Then the robust estimators of the slope and the intercept along with the robust estimator of the error term variance are used to define the control limits for the process profile under consideration. Simulation results indicate that the out of control ARL of the proposed control charts is smaller than the ARL of the classical control charts in the presence of contamination.

1. Introduction

In many applications of statistical process control (SPC), the quality of a product or a process regarding a random variable or a vector of random variables is well described by a univariate or multivariate distribution, respectively. However, in some cases the quality of a product or a process is well described by the relationship between a response variable and one or more independent variables. This relationship is usually called a profile which could be either linear or nonlinear.

A process modeled by a profile is being monitored in two phases. In phase I, the process comes under control and the parameters of the profile are estimated while in phase II the running process is monitored to keep it in control which is done by constructing control charts. The parameters of a simple linear profile including the intercept, the slope and the error term variance are usually estimated by the least square method of estimation. This classical method is defined under certain hypotheses, such as normality assumption. Deviation from any of such assumptions at any time is called contamination. When contamination exists, the classical estimators are not robust and the resulting control charts will not accurately control the profile in phase II. Thus, other estimation methods are required for estimating the profile parameters which perform well, not only when the process is in control but also when any contamination exists.

Kang and Albin introduced the concept of monitoring linear profiles for the first time [1]. Several authors have studied robust control charts. Most of them tried to provide

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methods for estimating process dispersion [2]. A robust estimator was presented for process standard deviation. Based on this estimator, a robust R control chart was proposed [3]. A robust estimator was introduced for estimating process dispersion in which interquartile range (IQR) used as a measure of dispersion within the subgroups [4]. Based on [4]'s method, another dispersion control charts was proposed by [5]. A robust estimator was used to estimate the process dispersion. In this method, median absolute deviation of observations about sample mean is used as a measure of dispersion within the subgroups [6]. A profile monitoring method was suggested when the error terms are correlated [7]. The median of subgroup ranges was used as an estimator of dispersion [8]. Two novel robust control charts for monitoring multiple linear profiles were proposed in [9]. Based on the robust estimators used by [9], a robust process capability indices was suggested for multiple linear profiles [10]. New optimizing methods for minimizing the objective function were presented in [11], [12], [13] which could be used in minimizing the loss function. Using novel machine learning methods in healthcare and AI, there exists a good opportunity to apply the profile monitoring [14], [15].

In this work, a robust estimator of the profile error term variance is introduced and evaluated using mean square error (MSE). Based on [16]; the M-estimators of the slope and the intercept of the model are robust and have better performance than the classical ones. The suggested robust estimator of the variance is used along with the M-estimators of the slope and the intercept to construct robust control chart.

The classical method of parameter estimation and the robust M-estimator method are presented in this introductory section. Methodology of the study is discussed in section 2. The robust estimation of dispersion for simple linear profiles and its evaluation is presented in section 3. Determination of the control limits for this robust control chart is provided in section 4. A simulation study for evaluating the suggested method of constructing robust control chart and its application in monitoring a simple linear profile is provided in section 5. The findings are discussed and conclusions are made in section 6.

2. Methodology

2.1. Classical Method

According to [1], slope, intercept and standard deviation of a simple linear profile are estimated based on m subgroups of size n observations. Then, the profile parameters are estimated using the least square estimation (LSE) method for each subgroup. When the data are collected, the process may not be in control and outliers exist. So, the data used to estimate the model parameters in phase I must be first checked out which is done by constructing a T^2 control chart. Let the simple linear profile be represented as Eq. (1)

$$Y = \beta_0 + \beta_1 x + \varepsilon; \qquad \varepsilon \sim N(0, \sigma^2) \tag{1}$$

where β_0 and β_1 are the intercept and slope, respectively and σ^2 is the error term variance. They are the model parameters.

Then, T^2 is defined as:

$$T_j^2 = \frac{n}{n-1}\left(\boldsymbol{b}_j - \bar{\boldsymbol{b}}\right)' \boldsymbol{S}^{-1}\left(\boldsymbol{b}_j - \bar{\boldsymbol{b}}\right); \quad j = 1,2,\dots,m \tag{2}$$

where $\mathbf{b}_j = (b_{0j}, b_{1j})'$, $\bar{\mathbf{b}} = (\bar{b}_0, \bar{b}_1)'$, $\mathbf{S} = \begin{pmatrix} S_0^2 & S_{01} \\ S_{10} & S_1^2 \end{pmatrix}$ and $\mathbf{b}_j$ is the vector of estimated profile parameters for j^{th} subgroup, $\bar{\mathbf{b}}$ and $\mathbf{S}$ are the sample mean vector and the sample variance-covariance matrix of $\mathbf{b}_j$s over m subgroups, respectively.

[1] defined the upper control limit for T^2 control chart as:

$$UCL = 2F_{(2,n(n-2),\alpha)} \tag{3}$$

where $F_{(\nu_1,\nu_2,\alpha)}$ is the α-upper percentile of the F distribution with ν_1 and ν_2 degrees of freedom. Therefore, in this method T_j^2 is computed for all m subgroups. As long as a T_j^2 is smaller than *UCL*, given in equation (3) the profile is considered in control and b_{0j}, b_{1j} is a valid model parameter estimates. While, when a T_j^2 is larger than *UCL*, the profile is considered to be out of control, and its related b_{0j}, b_{1j} are not valid and discarded. This is done for all *m* subgroups. Finally, a simple average over all valid model parameter estimates, $\bar{\mathbf{b}} = (\bar{b}_0, \bar{b}_1)'$, is computed as the estimators of the intercept and the slope of the model, respectively.

2.2. M-estimate Method

The general linear profile is defined as:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \varepsilon; \qquad \varepsilon \sim N(0, \sigma^2) \tag{4}$$

Eq.(4) could be written as:

$$\boldsymbol{y} = \boldsymbol{x}'\boldsymbol{\beta} + \varepsilon \tag{5}$$

where, $\mathbf{x} = (1, x_1, \dots, x_k)'$ and $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_k)'$ are the vector of independent variables and model parameters, respectively and ε is the error term. The LSE method used to estimate the general linear profile model parameters in Eq. (5) is based on minimizing the quantity.

$$Q = \sum_{i=1}^{n} (Y_i - \mathbf{x}_i'\boldsymbol{\beta})^2 = \sum_{i=1}^{n} r_i^2 \tag{6}$$

where *r* is the residual.

There is another method for estimating the parameters of general linear profile called least absolute deviation (LAD) or L_1. In this method $\sum_{i=1}^{n} |r_i|$ is minimized. [16] showed that this method is robust against data contamination and presented an algorithm for estimating the model parameters. They introduced another estimator called M-estimator which uses L_1 as the initial value and is more robust to data contamination. The robust estimator of $\boldsymbol{\beta}$ is the solution of the equation:

$$\sum_{i=1}^{n} \psi_0\left(\frac{r_i(\hat{\boldsymbol{\beta}})}{\sigma}\right)\boldsymbol{x}_i = \mathbf{0} \tag{7}$$

in which:

$\psi_0 = \rho_0' = -\frac{f_0'}{f_0}$ and $\hat{\sigma} = \frac{1}{0.675} Median_i\{|r_i| \,; r_i \neq 0\}$.

where f_0 is the probability density function of the error terms and f_0' is its derivative. [16] recommended the iterative reweighed algorithm for solving Eq. (7) as the followings:

(1) Compute an initial L$_1$ estimate for $\widehat{\boldsymbol{\beta}}_0$ and then compute $\hat{\sigma}$

(2) For k = 0, 1, 2, … :

- Given $\widehat{\boldsymbol{\beta}}_{\mathrm{k}}$, for i = 1, 2, …, n. compute $r_{i,k} = Y_i - \mathbf{x}_i'\widehat{\boldsymbol{\beta}}_{\mathrm{k}}$ and $w_{i,k} = W(\frac{r_{i,k}}{\hat{\sigma}})$
- Compute $\widehat{\boldsymbol{\beta}}_{\mathrm{k+1}}$ by solving $\sum_{i=1}^{n} w_{i,k}\mathbf{x}_i(Y_i - \mathbf{x}_i'\widehat{\boldsymbol{\beta}}) = \mathbf{0}$

(3) Stop when $max_i(\frac{|r_{i,k} - r_{i,k+1}|}{\hat{\sigma}}) < tolerance$

Note that in this algorithm W(.) is a weight function which corresponds to ψ function. Using this ψ function, a special weight is assigned to each observation. Usually $W(x)$ is a non-increasing function of $|x|$ and thus the atypical observations receive less weight. There are different ρ, ψ and W functions.

According to [16] some of these functions are provided in Table 1. Huber functions and Bisquare functions perform well for k = 1.37 and k = 4.68, respectively.

In this research, a robust control chart for monitoring simple linear profile is proposed. So, the robust estimators of parameters of the profile $Y = \beta_0 + \beta_1 x + \varepsilon$, where εs are mixed normal, must be introduced. Robust estimators of the parameters β_0 and β_1 are obtained by the algorithm presented in the previous section. Robust estimator of the error term variance is suggested in the next section.

3. Robust Estimation of Error Term Variance in Simple Linear Profile

The estimate of error term variance is used to perform statistical analysis, design control charts and compute process capability indices. According to [16] the classical methods overestimate the error term variance when contamination exists. So, it is necessary to propose a robust method for estimating the error term variance. The robust error term variance estimator in linear profile model is not proposed in [16]. It is stated in Section 1 that the W(.) function allocates a weight to each observation to reduce the effects of outliers. Therefore, it is logical to estimate the error term variance by considering the weights. Let $\sigma^2 = \theta$, then θ may be estimated from Eq. (8).

Table 1. The Family of Huber and Bisquare Functions

Functions	Huber	Bisquare
$\rho_k(x)$	$\begin{cases} x^2 & if\ \lvert x\rvert \le k \\ 2k\lvert x\rvert - k^2 & if\ \lvert x\rvert > k \end{cases}$	$\begin{cases} 1-(1-(\frac{x}{k})^2)^3 & if\ \lvert x\rvert \le k \\ 1 & if\ \lvert x\rvert > k \end{cases}$
$\psi_k(x)$	$\begin{cases} x & if\ \lvert x\rvert \le k \\ sgn(x)k & if\ \lvert x\rvert > k \end{cases}$	$\begin{cases} x(1-(\frac{x}{k})^2)^2 & if\ \lvert x\rvert \le k \\ 0 & if\ \lvert x\rvert > k \end{cases}$
$W_k(x)$	$\min\{1, \frac{k}{\lvert x\rvert}\}$	$\begin{cases} (1-(\frac{x}{k})^2)^2 & if\ \lvert x\rvert \le k \\ 0 & if\ \lvert x\rvert > k \end{cases}$

$$\hat{\theta} = \frac{\sum_{i=1}^{n} w_i\, r_i^2}{n-2} \tag{8}$$

where $w_i = W(\frac{r_i}{\sqrt{\hat{\theta}}})$ is provided in Table 1.

This estimator of the error term variance is not necessarily unbiased. To obtain an unbiased estimator of σ^2, the estimator must be divided by I_n which depends on the sample size n. The I_n is estimated by $\frac{\bar{\bar{\theta}}}{\sigma^2}$ where $\bar{\bar{\theta}} = \frac{\sum_{i=1}^{m}\hat{\theta}_i}{m}$ and m is the number of subgroups. Then $I_n\sigma^2 = E(\hat{\theta})$ and $\hat{\sigma}^2 = \frac{\bar{\bar{\theta}}}{\hat{I}_n}$.

4. Computation of Robust Control Limits

Once the error term variance is estimated the control limits for the simple linear profile may be calculated. According to [17] control limits for the simple linear regression model are:

$$\begin{aligned} (UCL, LCL) &= \hat{Y} \pm t_{\left((mn-2),\frac{\alpha}{2}\right)}\sqrt{\hat{\sigma}^2\left(\frac{1}{m}+\frac{1}{n}+\frac{(x-\bar{x})^2}{S_{xx}}\right)} \\ &= \hat{\beta}_0 + \hat{\beta}_1 x \\ &\pm t_{\left((mn-2),\frac{\alpha}{2}\right)}\sqrt{\hat{\sigma}^2(\frac{1}{m}+\frac{1}{n}+\frac{(x-\bar{x})^2}{S_{xx}})} \end{aligned} \tag{9}$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are robust estimates of the model parameters, $\hat{\sigma}^2$ is robust estimate of the error term variance where these robust estimates are introduced in previous section, $t_{((mn-2),\frac{\alpha}{2})}$ is the upper $\frac{\alpha}{2}$-percentile of t distribution with $(mn-2)$ degrees of freedom, n is the number of levels of the independent variable, $S_{xx} = \sum_{i=1}^{n}(x_i - \bar{x})^2$ and m is the number of observations at each level of the independent variable. These limits are functions of *x*. The statistic being plotted on this chart is the sample mean of m new observations at any level of independent variable *x* denoted by $\bar{Y}$.

4.1. Example

An example presented in [1] is provided here to investigate and compare the results of the classical and the robust estimators. They suggested the use of a simple linear profile model of the form $Y = 3 + 2x + \varepsilon$ where ε is normally independently distributed with mean zero and variance σ^2.

Simulation studies are conducted in three stages to compare the classical and the robust estimators under the two scenarios absence and presence of contamination. In first simulation runs, ε is independent $N(0,1)$ variable when no contamination exists. While, in second simulation runs, 90% of εs are distributed $N(0,1)$and 10% of ε s are either distributed $N(1,5)$or $N(3,7)$to simulate two different contamination scenarios.

For each level of the independent variable $x = 2, 4, 6,$ and 8 random samples of size $n = 20$ responses are generated. Therefore, the number of observations in each run is 80. The simulation run is repeated 20,000 times using MATLAB software on personal computer model HP COMPAC 6520.

Huber and Bisquare functions are used as weight functions to compute the M-estimates of model parameters β_0, β_1 and σ. The correction coefficients for variance estimator for Bisquare function with $k = 4.68$ and for Huber function with $k = 1.37$ are calculated as $\hat{I}_n = 1.7108$ and $\hat{I}_n = 1.4279$, respectively.

The estimates of the model parameters including slope (β_0), intercept (β_1) and error term variance (σ^2) are computed by applying the classical method in absence and presence of contamination. Robust estimates of these three parameters are computed using the proposed method suggested in Section 2.

Table 2 shows the simulation results from different estimation methods in the absence of contamination and when there is a 10% contamination in each case.

Table 2. Results of Classical and Robust Estimates of the Parameters for Profile $Y = 3 + 2x + \varepsilon$

Estimation Method	Estimators	0% contamination	10% contamination with N(1,3)	10% contamination with N(1,5)	10% contamination with N(3,5)	10% contamination with N(3,7)
M-estimate method with Bisquare function	b_0	3.0052	3.003	3.0102	2.9968	2.9968
	b_1	2.0004	2.0003	1.9998	2.0001	2.0002
	$\tilde{\sigma}^2$	0.584501	1.148537	1.103535	1.116742	1.076633
	$MSE(\tilde{\sigma}^2)$	0.543	0.080852	0.0644	0.068992	0.0553
M-estimate method with Huber function	b_0	3.06	2.9969	2.9968	2.9968	2.9968
	b_1	2.0003	2.0002	2.0002	2.0002	2.0002
	$\tilde{\sigma}^2$	0.700306	1.22636	1.252954	1.297465	1.285407
	$MSE(\tilde{\sigma}^2)$	0.2199	0.113248	0.1323	0.165995	0.158
Classical Control Chart	b_0	3.3001	3.1054	3.099	3.001	2.9967
	b_1	1.9998	2.0004	2.0005	2.0004	2.0003
	$\hat{\sigma}^2$	0.998014	1.8652276	3.396795	4.112972	6.416103
	$MSE(\hat{\sigma}^2)$	0.019975	1.437778	7.481249	8.210812	37.43541

Figure 1 compares the results of the three estimation methods for estimating the error term variance.

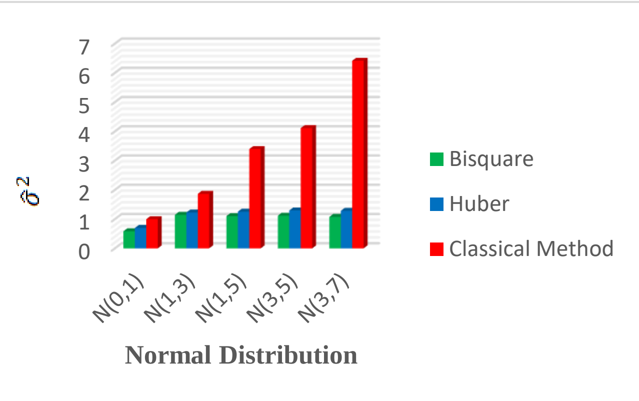


Figure 1. Comparison of Estimated Variances by Classical and Robust Methods

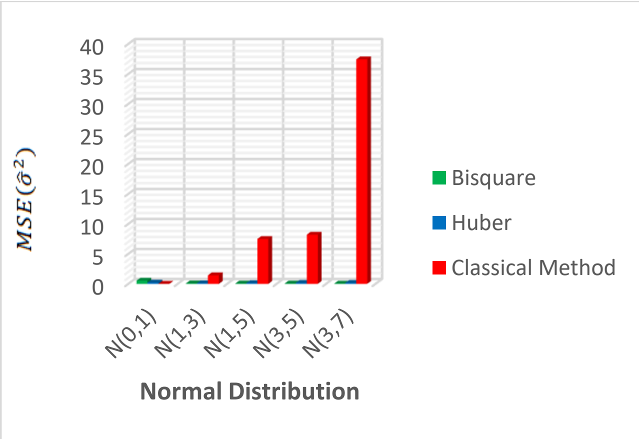


Figure 2. Comparison of MSE of Error Term Variance Estimators for Estimation Methods

For comparing the efficiency of the estimators, the value of $MSE(\hat{\sigma}^2)$ are computed for the three methods and are displayed in Figure 2. Investigation of Table 2 and Figures 1 and 2 show that the classical method introduces estimators with better performance in absence of contamination. While, in presence of contamination, the two robust estimators have better performances than the classical estimator. By applying the proposed method of estimating the error term variance, the value of $MSE(\hat{\sigma}^2)$ remains within an acceptable limits, and the estimated error term variance is close to its actual value. However, the estimated variance using the classical method is far from the actual value of the error term variance.

Therefore, the efficiency of the robust estimators is much better than the classical estimators. It can also be noted that the two robust estimators have almost the same performance in presence and absence of contamination.

5. Construction of Robust Control Chart for Phase II Monitoring

In this section robust control chart, based on robust estimates of the model parameters, are constructed and their performances are compared with the classical control chart. Control limits for profile $Y = 3 + 2x + \varepsilon$ is obtained by substituting robust and classical estimates of the parameters obtained in phase I in Eq. (9). Table 3 provides upper and lower control limits for the simple linear profile under consideration obtained from the three methods.

Table 3. Control Limits for Profile $Y = 3 + 2x + \varepsilon$

Estimation Method	Lower Control Limit	Central Line	Upper Control Limit
Robust Method with Huber Function	$3.06 - 3.1\left(\sqrt{1.13376\left(0.35 + \frac{(x-5)^2}{20}\right)}\right) + 2.0003x$	$3.06 + 2.0003x$	$3.06 + 3.1\left(\sqrt{1.13376\left(0.35 + \frac{(x-5)^2}{20}\right)}\right) + 2.0003x$
Robust Method with Bisquare Function	$3.0052 - 3.1\left(\sqrt{1.03761\left(0.35 + \frac{(x-5)^2}{20}\right)}\right) + 2.0004x$	$3.0052 + 2.0004x$	$3.0052 + 3.1\left(\sqrt{1.03761\left(0.35 + \frac{(x-5)^2}{20}\right)}\right) + 2.0004x$
Classical Control Chart	$3.3001 - 3.355\left(\sqrt{3.85\left(0.35 + \frac{(x-5)^2}{20}\right)}\right) + 1.9998x$	$3.3001 + 1.9998x$	$3.3001 + 3.355\left(\sqrt{3.85\left(0.35 + \frac{(x-5)^2}{20}\right)}\right) + 1.9998x$

Table 3 shows that the central lines for the three methods are approximately similar. While *LCL* and *UCL* are different due to different methods of estimating the error term variance. It is notable that *LCL* and *UCL* for the two robust methods are very similar. The three control charts are illustrated in Figures 3, 4 and 5. Also, the comparison of the three control charts are shown together in Figure 6.

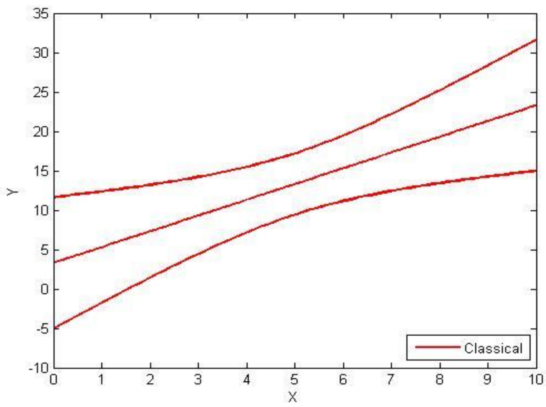


Figure 3. Classical Control Limits for Profile $Y = 3 + 2x + \varepsilon$

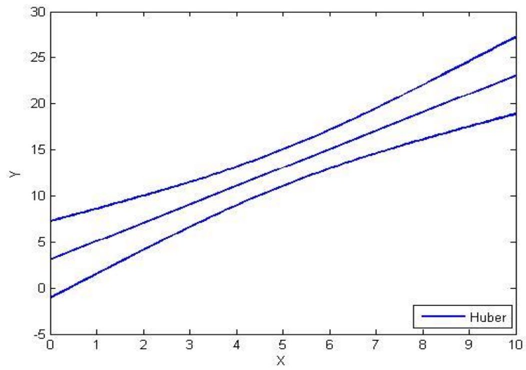


Figure 4. Robust Control Limits with Huber Function for Profile $Y = 3 + 2x + \varepsilon$

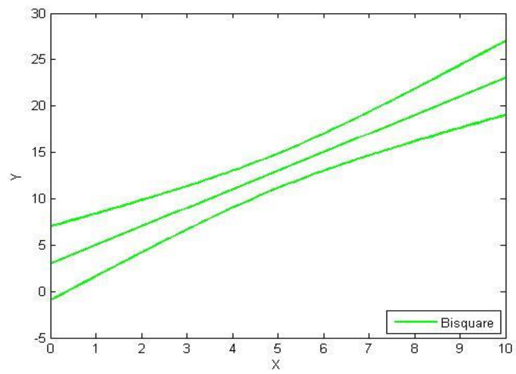


Figure 5. Robust Control Limits with Bisquare Function for Profile $Y = 3 + 2x + \varepsilon$

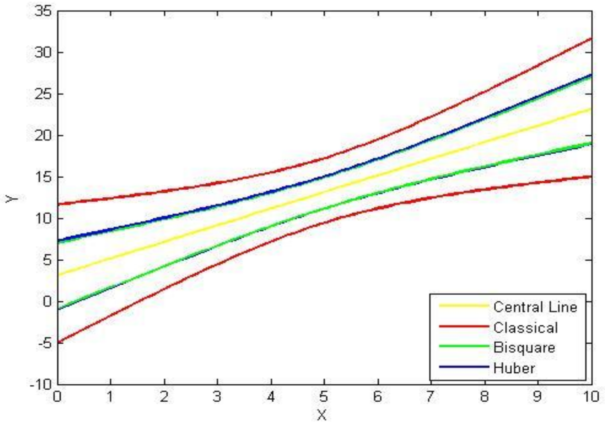


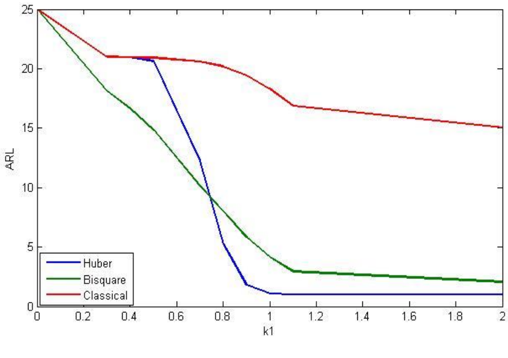
Figure 6. Comparison of Robust and Classical Control Limits for Profile $Y = 3 + 2x + \varepsilon$

All control limits are hyperbola shaped. It is obvious that the robust control charts are more sensitive than the classical one since its limits are wider than the robust control limits.

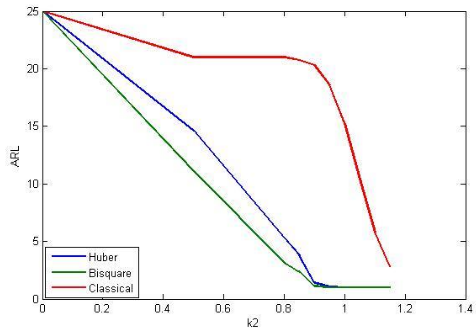
A simulation study is performed to compare the performances of the suggested robust control charts with the classical one by means of Average Run Length (ARL). In this study, the three control charts are constructed such that the in control ARL is 25. For each level of the independent variable, random samples of size 10 are generated from the model $Y = (3 + k_1\sigma) + (2 + k_2\sigma)x + N(0, (k_3\sigma)^2)$, in which k1, k2 and k3 are the sizes of the shift in units of the error term standard deviation. Needless to say that only one parameter is shifted at a time. The value of $\bar{Y}$ is computed for each run and is plotted on the chart. MATLAB software is used to generate data over 20,000 runs. Simulation results for different shifts in the intercept, slope and error term standard deviation for $x = 4$ are shown in Table 4 and are illustrated on Figure 7. The results for the other values of the independent variable may be obtained from the corresponding author.

Table 4. Comparison of ARLs for Control Charts

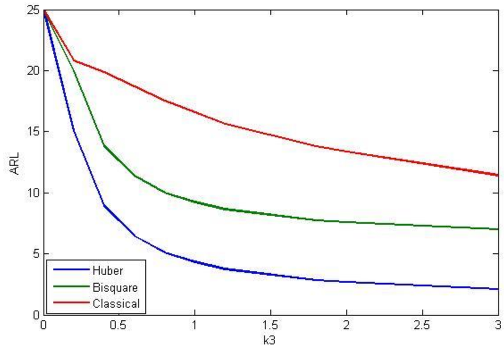
β_0 shifted to $\beta_0 + k_1\sigma$				β_1 shifted to $\beta_1 + k_2\sigma$				σ shifted to $\sigma + k_3\sigma$			
k_1	Huber	Bisquare	Classical Method	k_2	Huber	Bisquare	Classical Method	k_3	Huber	Bisquare	Classical Method
0	25	25	25	0	25	25	25	0	25	25	25
0.3	20.99	18.134	20.982	0.5	14.631	11.096	20.998	0.2	15.09	19.989	20.853
0.4	20.97	16.669	20.973	0.8	5.273	3.114	20.981	0.4	8.94	13.839	19.859
0.5	20.63	14.843	20.936	0.85	3.791	2.368	20.753	0.6	6.469	11.368	18.708
0.7	12.261	10.126	20.582	0.9	1.404	1.113	20.298	0.8	5.108	10.007	17.516
0.8	5.259	7.983	20.178	0.95	1.075	1.012	18.591	1	4.337	9.236	16.57
0.9	1.796	5.814	19.43	1	1.007	1.002	15.272	1.2	3.738	8.637	15.627
1	1.063	4.17	18.292	1.05	1	1	10.442	1.8	2.843	7.742	13.799
1.1	1.003	2.948	16.877	1.1	1	1	5.805	2	2.68	7.579	13.375
2	1	2.077	15.037	1.15	1	1	2.796	3	2.116	7.015	11.432



7- (a)



7- (b)



7- (c)

Figure 7. Comparison of ARLs for Control Charts for x=4: (a) β_0 is shifted (b) β_1 is shifted (c) σ is shifted

Investigation of Figure 7- (a) indicates that the robust control charts detect the shifts in parameters more quickly than the classical control chart. This result suggests that the robust estimator of a profile parameters is more reliable for monitoring profile in both presence and absence of contamination. It is also obvious that M-estimate method with Huber function has better performance than the M-estimate with Bisquare function when estimating the model parameters and constructing control charts.

6. Conclusions

In this research, an unbiased robust estimator of the error term variance in a simple linear profile is proposed, and the robust M-estimate method with Huber and Bisquare functions are applied to estimate the model parameters of a simple linear profile. These estimates are then compared with the classical estimates of the parameters in an extensive simulation study. The simulation results show that the robust estimates are not affected by contaminations and suggest better estimates than the classical ones. The MSE criterion indicates that the robust error term variance estimator is more accurate than the classical estimator when contaminations exist. The control limits constructed based on the robust estimates of the simple linear profile parameters detect any out of control situation more rapidly than the control chart established based on the classical estimates which are investigated by means of ARLs. The robust control charts have less ARL for the shifts in the intercept, the slope, and the error term variance. It is notable that M-estimate of the simple linear profile parameters with Huber function has better performances than the Bisquare function. Simultaneous shifts in model parameters two and three at a time are areas for further investigations. Thus, we recommend the use of the suggested robust estimates of a simple linear profile parameter when constructing control chart. The use of other robust estimators such as S, MCD and MVE for estimating the profile parameters are areas for further research.

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