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A Self-Starting Control Chart for Linear Profiles

CHANGLIANG ZOU, CHUNGUANG ZHOU, and ZHAOJUN WANG

Nankai University, Tianjin, China

FUGEE TSUNG

Hong Kong University of Science and Technology, Kowloon, Hong Kong

A self-starting control chart based on recursive residuals is proposed for monitoring linear profiles when the nominal values of the process parameters are unknown. This chart can detect a shift in the intercept, the slope, or the standard deviation. Because of the good properties of the plot statistics, the proposed chart can be easily designed to match any desired in-control average run length. Simulated results show that our approach has good charting performance across a range of possible shifts when the process parameters are unknown and that it is particularly useful during the start-up stage of a process.

Key Words: Average Run Length; EWMA Charts; Markov Chain; Recursive Residuals.

STATISTICAL PROCESS CONTROL (SPC) has been widely used to monitor various industrial processes. Most research on SPC focused on the charting techniques and it was assumed that the quality of a process can be represented by the distribution of a quality characteristic. However, in some situations, the quality of a process is better characterized and summarized by a relationship between a response variable and one or more explanatory variables. In particular, most studies focused on the simple linear regression profiles (Woodall et al. (2004)).

In the literature, Phase I and Phase II control charts need to be distinguished. In Phase II monitoring, the process distribution is assumed to be completely known. However, the process distribution or the process parameters are often unknown in prac-

tice. Before Phase II monitoring, it is necessary to conduct Phase I analysis to ensure that the process is statistically in control and to estimate the parameters of the process. Mahmoud and Woodall (2004) studied a Phase I method for monitoring linear profiles. Mahmoud et al. (2007) proposed a change-point method, based on likelihood ratio statistics, to detect sustained changes in a linear profile data set in Phase I. They concluded that, to detect both sustained and randomly occurring unsustained shifts, one could employ the change-point method in conjunction with the methods proposed by Mahmoud and Woodall (2004). On the other hand, Kang and Albin (2000) proposed two control charts for Phase II monitoring of linear profiles. One is a multivariate T^2 chart and the other is the combination of the exponentially weighted moving average (EWMA) chart and the range (R) chart. In Kim et al. (2003), the method based on a combination of three EWMA charts was proposed for detecting a shift in the intercept, slope, and standard deviation simultaneously. Simulations showed that, in detecting the sustained shifts in the parameters, the three EWMA charts outperformed the methods in Kang and Albin (2000) in terms of average run length (ARL) and their methods also seemed more interpretable. An extensive discussion of research problems in monitoring linear profiles can be found in Woodall et al. (2004).

Mr. Zou is a Doctoral Student in the LPMC and School of Mathematical Sciences. His email is chlzhou@yahoo.com.cn.

Mr. Zhou is a Doctoral Student in the LPMC and School of Mathematical Sciences. His email is chgzhou@yahoo.com.cn.

Dr. Wang is a Professor in the LPMC and School of Mathematical Sciences. His email is zjwang@nankai.edu.cn.

Dr. Tsung is an Associate Professor in the Department of Industrial Engineering and Logistics Management. He is a Senior Member of ASQ. His email is season@ust.hk.

All the Phase II methods mentioned above assume that the parameters of the process are known. However, the process parameters, including the intercept, slope, and standard deviation of the linear profiles, are usually not exactly known, but estimated by m in-control (IC) historical samples of subgroup size n . Some authors have recommended using 20–30 samples with four to five observations each to estimate the process parameters for traditional control charts (see Montgomery (2005), Ryan (2000)). Quesenberry (1993) and Jones et al. (2001, 2004), among others, have investigated the effect of the estimated parameters on the performance of traditional control charts. A recent literature review by Jensen et al. (2006) provided a thorough discussion of the effects of parameter estimation on control-chart performance. They concluded that, when the number of reference samples is small, control charts with estimated parameters produce a large bias in the IC ARL and reduce the sensitivity of the chart in detecting process changes as measured by the out-of-control (OC) ARL. In fact, to attain performance similar to a chart with known parameters, 20 or 30 samples may be far from enough. For example, for the traditional EWMA chart with $\lambda = 0.2$, 300 samples of five observations are needed to achieve the desired level of IC performance (Jones et al. (2001)). In most cases, however, it may not be feasible to wait for the accumulation of sufficiently large subgroups because the users usually want to monitor the process at the start-up stages. Hence, many authors studied the design procedures of traditional control charts with estimated parameters, such as Hillier (1967, 1969), Yang and Hillier (1970), Nedumaran and Pignatiello (2001), and Jones (2002). Such a problem due to estimated parameters would be even more severe for profile monitoring, as the set-up of profile charting schemes requires many more parameter estimates (e.g. the intercept, slope, and standard deviation of a linear profile) than do traditional control charts.

To overcome the situation when sufficiently large samples for parameter estimation are unavailable, self-starting methods have been developed accordingly that update the parameter estimates along with new observations and simultaneous checks of the OC conditions (see Hawkins (1987), Hawkins and Olwell (1998), Quesenberry (1991, 1995), and Sullivan and Jones (2002)). In particular, Hawkins et al. (2003) and Hawkins and Zamba (2005a, 2005b) proposed a change-point model based on the likelihood ratio for on-line monitoring that can also be seen as a self-

starting method. However, no self-starting research has so far extended to the application of profile monitoring.

In this paper, a self-starting control chart based on recursive residuals is proposed for monitoring linear profiles when the process parameters are not known. This means that it is not necessary to assemble a large number of reference samples before the control scheme begins (although it is generally advisable to collect a few preliminary samples). The combination of two EWMA charts is used. These charts monitor the regression coefficients and the standard deviation. Given the desired overall IC ARL, the control limits of each chart can be obtained through the Markov-chain method. We also demonstrate the effectiveness of our proposed approach by the Monte Carlo method. In the remainder of this paper, we describe our work as follows: in the next section, we give a description and explain the design of our proposed control chart. Next, a semiconductor-manufacturing example is used to illustrate our proposed control chart. Then we assess the performance of the chart. Finally, we discuss the results and draw conclusions. Our derivations are presented in the Appendix.

The Self-Starting Chart for Linear Profiles

In this section, the linear-profile model and the recursive residuals are described. Also, the proposed self-starting control chart, its design, and some diagnostic aids are discussed.

The Linear Profile Model and Control Charts

Assume the j th random sample collected over time is (x_i, y_{ij}) . When the process is IC, the relationship between the response and the explanatory variables is assumed to be

$$y_{ij} = A_0 + A_1 x_i + \varepsilon_{ij}, \quad i = 1, 2, \dots, n, \quad (1)$$

where ε_{ij}/σ is an independent identically distributed (i.i.d.) standard normal random variable and the value of the explanatory variable X is assumed to be fixed at n . This is usually the case in many practical applications. such as in Kang and Albin (2000), Kim et al. (2003), and Mahmoud and Woodall (2004).

When the parameters, A_0 , A_1 , and σ^2 , are unknown, a widely used method is to estimate them by historical data. Suppose that there are, in total, $m-1$ ($m \geq 2$) IC historical samples of size n $\{(x_i, y_{ij}), i = 1, 2, \dots, n, j = 1, 2, \dots, m-1\}$. The most often used unbiased estimators for A_0 , A_1 , and σ^2 are the

average of the $m-1$ least-square estimators, a_{0j} , a_{1j} , and MSE_j , which are given by

$$\begin{aligned} a_{0j} &= \bar{y}_j - a_{1j}\bar{x}, \\ a_{1j} &= \frac{S_{xy(j)}}{S_{xx}}, \\ MSE_j &= \frac{1}{n-2} \sum_{i=1}^n (y_{ij} - a_{1j}x_i - a_{0j})^2, \end{aligned}$$

where $\bar{y}_j = (1/n) \sum_{i=1}^n y_{ij}$, $\bar{x} = (1/n) \sum_{i=1}^n x_i$, $S_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2$, and $S_{xy(j)} = \sum_{i=1}^n (x_i - \bar{x})y_{ij}$.

After we determine the estimations, the parameters are assumed to be known and the monitoring could be started. Kim et al. (2003) used the coded explanatory values and obtained the following alternative form of the underlying model:

$$y_{ij} = B_0 + B_1 x_i^* + \varepsilon_{ij}, \quad i = 1, 2, \dots, n,$$

where $B_0 = A_0 + A_1\bar{x}$, $B_1 = A_1$, $x_i^* = (x_i - \bar{x})$ and $\bar{x} = (1/n) \sum_{i=1}^n x_i$. For the j th sample, the least square estimators for B_0 , B_1 , and σ^2 are

$$\begin{aligned} b_{0j} &= \bar{y}_j, \\ b_{1j} &= \frac{S_{xy(j)}}{S_{xx}}, \\ MSE_j &= \frac{1}{n-2} \sum_{i=1}^n (y_{ij} - b_{1j}x_i^* - b_{0j})^2. \end{aligned}$$

Note that these three estimators are independent. Thus, Kim et al. (2003) proposed using three EWMA charts ($EWMA_I$, $EWMA_S$, $EWMA_E$) to detect if the Y -intercept (B_0), the slope (B_1), and the standard deviation (σ) had changed, respectively. They are

$$\begin{aligned} EWMA_I(j) &= \theta b_{0j} + (1 - \theta)EWMA_I(j-1) \\ EWMA_S(j) &= \theta b_{1j} + (1 - \theta)EWMA_S(j-1) \\ EWMA_E(j) &= \max \left\{ \theta \ln(MSE_j) + (1 - \theta)EWMA_E(j-1), \right. \\ &\quad \left. \ln(\sigma^2) \right\}, \end{aligned}$$

where θ is a smoothing constant, $EWMA_I(0) = B_0$, $EWMA_S(0) = B_1$, and $EWMA_E(0) = \ln(\sigma^2)$. The three EWMA charts (denoted as the KMW charts hereafter) are used jointly. They signal an out-of-control condition as one of the charts triggers.

As more IC samples are obtained, one may wish to update the estimations and start monitoring again. However, the statistical properties of this procedure,

such as the IC ARL, cannot be obtained easily, so that the design of this procedure seems difficult. An alternative method to deal with the unknown parameters is to use a self-starting control chart, which has flexibility in updating the parameter estimates with new samples and in simultaneously checking for the OC conditions.

The Proposed Self-Starting Chart and Its Design

The proposed self-starting chart is based on recursive residuals that were first applied to a regression model by Brown et al. (1975). First, we pool all of the $m-1$ IC historical and future $m, m+1, \dots$ samples of size n into one sample, i.e., $\{(x_i, y_{ij}), i = 1, 2, \dots, n, j = 1, 2, \dots, m-1, m, m+1, \dots\}$. For convenience, let $y_{(j-1)n+i} = y_{ij}$, $i = 1, 2, \dots, n$, $j = 1, 2, \dots$. We can then define the standardized recursive residuals for the future samples as

$$\begin{aligned} e_{ij} &= (y_{(j-1)n+i} - \mathbf{z}_i' \boldsymbol{\beta}_{(j-1)n+i-1}) \\ &\quad \div [S_{(j-1)n+i-1} \\ &\quad \times (1 + \mathbf{z}_i' (\mathbf{X}_{(j-1)n+i-1}' \mathbf{X}_{(j-1)n+i-1})^{-1} \mathbf{z}_i)]^{1/2}, \\ &\quad i = 1, 2, \dots, n, \quad j = m, m+1, \dots, \end{aligned} \quad (3)$$

where

$$\begin{aligned} \mathbf{z}_i' &= (1, x_i), \\ \mathbf{y}_{(j-1)n+i-1}' &= (y_1, y_2, \dots, y_{(j-1)n+i-1}), \\ \mathbf{X}_{(j-1)n+i-1}' &= \overbrace{(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_n, \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_n, \dots)}^{(j-1) \times n}, \\ &\quad \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_{i-1}), \\ \boldsymbol{\beta}_t &= (\mathbf{X}_t' \mathbf{X}_t)^{-1} \mathbf{X}_t' \mathbf{y}_t \\ S_t &= \frac{1}{t-2} (\mathbf{y}_t - \mathbf{X}_t \boldsymbol{\beta}_t)' (\mathbf{y}_t - \mathbf{X}_t \boldsymbol{\beta}_t). \end{aligned}$$

Under the IC model (1), it is known that e_{ij} has a Student- t distribution with $(j-1)n+i-3$ degrees of freedom (see Brown et al. (1975) and Hawkins and Olwell (1998)). Using a lemma from Basu (Lehmann (1991)), we can show that the e_{ij} 's are statistically independent. Thus, through a transformation, we obtain the following statistic:

$$w_{ij} = \Phi^{-1} [T_{(j-1)n+i-3}(e_{ij})], \quad (4)$$

which is called the Q -statistic by Quesenberry (1991) (see also Hawkins (1987) and Hawkins and Olwell (1998)), where Φ^{-1} denotes the inverse of the cumulative distribution function (CDF) of the standard normal random variable, T_ν is the CDF of the Student- t distribution with ν degrees of freedom. Therefore, $\{w_{ij}, i = 1, 2, \dots, n, j = m, m+1, \dots\}$ is

a sequence of independent standard normal random variables.

When an assignable cause occurs after some subgroups, say τ subgroups, the distribution of Q -statistics $\{w_{ij}, i = 1, 2, \dots, n, j = \tau + 1, k + 2, \dots\}$ is different from that of $\{w_{ij}, i = 1, 2, \dots, n, j = 1, \dots, \tau\}$. The difference between them will be used in our method to detect the assignable cause.

For the transformed residuals $\{w_{ij}, i = 1, 2, \dots, n, j = m, m + 1, \dots\}$, let $\bar{w}_j = (1/n) \sum_{i=1}^n w_{ij}$ and $S_{w_j} = [1/(n-1)] \sum_{i=1}^n (w_{ij} - \bar{w}_j)^2$ denote, respectively, the sample mean and the variance of their j th subgroup. Define two EWMA statistics, EWMA_{IS} and EWMA _{σ} , as follows:

$$\begin{aligned} \text{EWMA}_{\text{IS}}(j) &= \lambda \sqrt{n} \bar{w}_j + (1 - \lambda) \text{EWMA}_{\text{IS}}(j - 1), \\ \text{EWMA}_{\sigma}(j) &= \max \left(0, \lambda \sqrt{\frac{n-1}{2}} (S_{w_j} - 1) \right. \\ &\quad \left. + (1 - \lambda) \text{EWMA}_{\sigma}(j - 1) \right), \end{aligned} \quad (5)$$

where $j = m, m + 1, \dots$, $\text{EWMA}_{\text{IS}}(m - 1) = \text{EWMA}_{\sigma}(m - 1) = 0$, and λ ($0 < \lambda \leq 1$) is a smoothing constant. Our proposed self-starting scheme (denoted as the SS chart hereafter) is defined to be the combination of the above two EWMA charts, i.e., an out-of-control signal is triggered as soon as $\text{EWMA}_{\text{IS}}(j) < \text{LCL}_{\text{IS}}$ or $\text{EWMA}_{\text{IS}}(j) > \text{UCL}_{\text{IS}}$ and/or $\text{EWMA}_{\sigma}(j) > \text{UCL}_{\sigma}$, where UCL_{IS} , LCL_{IS} , and UCL_{σ} are chosen to obtain the given specified IC ARL. Note that Hawkins (1991) also applied recursive residuals by using the cumulative sum in a fixed sample for assessing the leverage, mean compatibility, and influence of all excluded cases. There are two major differences between our proposed scheme and Hawkins' scheme (1991): First, our considered type of data set is a rational subgroup of size n , while the individual observations are investigated by Hawkins (1991). Another difference is Hawkins (1991) mainly focuses on the use of recursive residuals as a diagnostic of the regression, but this is not our concern in on-line SPC monitoring.

Note that the EWMA _{σ} chart in Equation (6) is a one-sided scheme that is used to detect the increase in process variance only. If one also wants to detect a decrease in variance, some other appropriate methods may be used, such as the method discussed by Acosta-Mejia et al. (1999). Crowder and Hamilton (1992) considered monitoring the logarithm of

the variance instead of the natural unit of the variance. However, our simulation study indicates that the chart directly using the variance performs slightly better than the logarithm-scale chart.

The smoothing constants, λ , in Equations (5) and (6) are set equal to 0.2, as in the EWMA chart used by Kang and Albin (2000) and Kim et al. (2003). We can certainly use different smoothing constants for each chart and, in general, smaller smoothing constants lead to quicker detection of smaller shifts, as shown by Lucas and Saccucci (1990).

From the definition, we know the EWMA_{IS} chart is used to monitor the change in the slope and intercept, while EWMA _{σ} is effective in monitoring the shift in the standard deviation of the process. Under the IC condition, because $w_{ij} \sim N(0, 1)$, the statistics $\sqrt{n} \bar{w}_j$ and $\sqrt{(n-1)/2} (S_{w_j} - 1)$ are independently distributed as a standard normal and a scaled χ^2 distribution, respectively. Hence, for each chart, the IC ARL properties can be easily obtained through a classical Markov-chain procedure (Brook and Evans (1972)). However, as these two charts are not irrelevant, the two-dimensional Markov-chain method is used to evaluate the IC ARL of our proposed chart (see the Appendix).

Here, we assume that these three parameters are equally important. Hence, the ratio of the EWMA _{σ} chart's IC ARL to that of the EWMA_{IS} chart is designated to be 2. For some given IC ARL and sample size $n = 3, 4, \dots, 10$ and 15, 20, the control limits for each chart are tabulated in Table 1 (note that $\text{LCL}_{\text{IS}} = -\text{UCL}_{\text{IS}}$). Other ratios can also be specified so that the charts can be more sensitive to certain parameters under the same overall false-alarm rate. A Fortran program that easily finds the control limits for each chart given a desired overall IC ARL, a smoothing constant, λ , and a proper ratio, is available from the authors.

The Diagnostic Aids and Implementation

In the practice of quality control, it is important to detect a process change quickly and it is also critical to diagnose the change and to identify which parameter or parameters have shifted after a signal occurs. Such a diagnostic aid is particularly important in profile monitoring, where there are more process parameters involved. The diagnostic aids to locate the change point in the process and to isolate the type of parameter change in a profile will help an engineer to identify and eliminate the root cause of a problem quickly and easily.

TABLE 1. The Control Limits of the Self-Starting Chart

IC ARL	200	300	370	400	500
$n = 3$					
UCL_{IS}	0.9250	0.9741	0.9982	1.0066	1.0320
UCL_{σ}	1.3596	1.4577	1.5064	1.5243	1.5769
$n = 4$					
UCL_{IS}	0.9276	0.9746	0.9978	1.0062	1.0302
UCL_{σ}	1.2959	1.3794	1.4214	1.4369	1.4812
$n = 5$					
UCL_{IS}	0.9271	0.9748	0.9985	1.0071	1.0313
UCL_{σ}	1.2530	1.3318	1.3717	1.3864	1.4280
$n = 6$					
UCL_{IS}	0.9268	0.9745	0.9986	1.0066	1.0311
UCL_{σ}	1.2235	1.2983	1.3372	1.3501	1.3895
$n = 7$					
UCL_{IS}	0.9270	0.9746	0.9985	1.0067	1.0310
UCL_{σ}	1.2021	1.2739	1.3107	1.3235	1.3615
$n = 8$					
UCL_{IS}	0.9271	0.9746	0.9983	1.0067	1.0310
UCL_{σ}	1.1856	1.2549	1.2902	1.3029	1.3397
$n = 9$					
UCL_{IS}	0.9271	0.9745	0.9982	1.0070	1.0311
UCL_{σ}	1.1720	1.2396	1.2739	1.2868	1.3233
$n = 10$					
UCL_{IS}	0.9270	0.9745	0.9982	1.0070	1.0311
UCL_{σ}	1.1607	1.2269	1.2605	1.2731	1.3078
$n = 11$					
UCL_{IS}	0.9270	0.9748	0.9982	1.0067	1.0310
UCL_{σ}	1.1236	1.1860	1.2168	1.2284	1.2601
$n = 12$					
UCL_{IS}	0.9268	0.9747	0.9982	1.0072	1.0313
UCL_{σ}	1.1035	1.1621	1.1918	1.2032	1.2340

A method based on the maximum likelihood estimator of the change point is proposed to assist in the diagnosis of our self-starting chart. We assume that the chart signals at subgroup k , i.e., there are $m - 1$ historical IC samples and $k - m + 1$ future samples, and a shift in parameters occurred after the τ th sample ($m - 1 \leq \tau < k$). The classical likelihood ratio statistic is given by

$$lr(k_1n, kn) = kn \log[\hat{\sigma}_{kn}^2 (\hat{\sigma}_{k_1n}^2)^{-k_1/k} (\hat{\sigma}_{k_2n}^2)^{-k_2/k}]. \quad (7)$$

The expressions of $\hat{\sigma}_{kn}^2$, $\hat{\sigma}_{k_1n}^2$, $\hat{\sigma}_{k_2n}^2$ and the derivations are given in the Appendix. Our proposed estimator of the change point, τ , of a step shift in parameter(s) of the linear profile is given by

$$\hat{\tau} = \arg \max_{m-1 \leq k_1 < k} \{lr(k_1n, kn)\}. \quad (8)$$

Note that this is consistent with that in Pignatiello and Samuel (2001).

In addition, as Kim et al. (2003) pointed out, it is also necessary to justify which parameter or parameters have shifted after a signal occurs. Because their proposed chart is the combination of three EWMA charts and each chart detects the corresponding parameter, the diagnosis of any process change is easier than that of omnibus methods of Kang and Albin (2000). At first glance, our proposed method based on recursive residuals may seem an omnibus method and it might seem difficult to diagnose which parameter has shifted. In Mahmoud et al. (2007), a method of decomposing the likelihood ratio statistic into three parts was introduced to enhance the ability of their change-point approach in detecting where the shift occurred. As Reynolds and Stoumbos (2005) pointed out, the control charts used as diagnostic aids do not necessarily have to be the same control charts used to determine when to signal. After the SS chart signals, some other simple diagnostic aids may be used as auxiliary tools to determine which of the parameters has changed. For example, Hawkins and Zamba (2005b) suggested two conventional parametric tests, a two-sided F -test for detecting the changes in variance and an approximate t -test for detecting the changes in mean. Likewise, in this paper, assume that the SS chart signaled at the k th sample. After obtaining the change-point estimator, $\hat{\tau}$, using (8), we may consider the parameter test method as follows:

- The t -test for a Y -intercept change using degrees of freedom $(kn - 4)$ and test statistic

$$t_{B_0} = \frac{\sqrt{\frac{(k-\hat{\tau})\hat{\tau}n}{k}}(\hat{B}_0^{(1)} - \hat{B}_0^{(2)})}{\sqrt{\frac{\{(\hat{\tau}n-2)\hat{\sigma}_{(1)}^2 + [(k-\hat{\tau})n-2]\hat{\sigma}_{(2)}^2\}}{(kn-4)}}}.$$

- The t -test for a slope change using degrees of freedom $(kn - 4)$ and test statistic

$$t_{B_1} = \frac{\sqrt{\frac{(k-\hat{\tau})\hat{\tau}S_{xx}}{k}}(\hat{B}_1^{(1)} - \hat{B}_1^{(2)})}{\sqrt{\frac{\{(\hat{\tau}n-2)\hat{\sigma}_{(1)}^2 + [(k-\hat{\tau})n-2]\hat{\sigma}_{(2)}^2\}}{(kn-4)}}}.$$

- The F -test for a standard deviation change using degrees of freedom $\hat{\tau}n - 2$ and $(k - \hat{\tau})n - 2$. The test statistic is $F_\sigma = \hat{\sigma}_{(1)}^2 / \hat{\sigma}_{(2)}^2$,

where

$$\begin{aligned}\hat{B}_0^{(1)} &= \frac{1}{\hat{\tau}n} \sum_{j=1}^{\hat{\tau}} \sum_{i=1}^n y_{ij} \\ \hat{B}_0^{(2)} &= \frac{1}{(k-\hat{\tau})n} \sum_{j=\hat{\tau}+1}^k \sum_{i=1}^n y_{ij} \\ \hat{B}_1^{(1)} &= \frac{1}{\hat{\tau}S_{xx}} \sum_{j=1}^{\hat{\tau}} \sum_{i=1}^n x_i^* y_{ij} \\ \hat{B}_1^{(2)} &= \frac{1}{(k-\hat{\tau})S_{xx}} \sum_{j=\hat{\tau}+1}^k \sum_{i=1}^n x_i^* y_{ij} \\ \hat{\sigma}_{(1)}^2 &= \frac{1}{\hat{\tau}n-2} \sum_{j=1}^{\hat{\tau}} \sum_{i=1}^n (y_{ij} - \hat{B}_0^{(1)} - \hat{B}_1^{(1)} x_i^*)^2 \\ \hat{\sigma}_{(2)}^2 &= \frac{1}{(k-\hat{\tau})n-2} \\ &\quad \times \sum_{j=\hat{\tau}+1}^k \sum_{i=1}^n (y_{ij} - \hat{B}_0^{(2)} - \hat{B}_1^{(2)} x_i^*)^2.\end{aligned}$$

Moreover, it seems that our proposed method requires a lot of computations, such as the inverse matrix in Equation (3). In fact, the calculations of the e_{ij} 's can be considerably simplified by the following recursive formulas:

$$\begin{aligned}(\mathbf{X}'_t \mathbf{X}_t)^{-1} &= (\mathbf{X}'_{t-1} \mathbf{X}_{t-1})^{-1} \\ &\quad - \frac{(\mathbf{X}'_{t-1} \mathbf{X}_{t-1})^{-1} \mathbf{z}_i \mathbf{z}'_i (\mathbf{X}'_{t-1} \mathbf{X}_{t-1})^{-1}}{1 + \mathbf{z}'_i (\mathbf{X}'_{t-1} \mathbf{X}_{t-1})^{-1} \mathbf{z}_i},\end{aligned}\quad (9)$$

$$\beta_t = \beta_{t-1} + (\mathbf{X}'_t \mathbf{X}_t)^{-1} \mathbf{z}_i (\mathbf{y}_t - \mathbf{z}'_i \beta_{t-1}), \quad (10)$$

$$(t-2)S_t = (t-3)S_{t-1} + (e_{ij})^2, \quad (11)$$

where $t = (j-1)n + i$.

An Illustrative Example

In this section, we adopt a semiconductor manufacturing example described by Kang and Albin (2000). In the example, a semiconductor wafer is put into a chamber and exposed to gases that etch away the photoresist and generate a specified pattern for the chips, where the etching quality mainly depends on the mass flow controller (MFC) performance. To monitor MFC, we have y , which is the measured pressure in the chamber, and x , which is the set point for MFC flow, where their functional relationship is known to be linear. For more background about this example, please refer to Kang and Albin (2000), Sheriff (1995), and references therein. Here, we demonstrate how to implement our proposed self-starting control chart to monitor and diagnose such a process.

In this example, according to Kang and Albin (2000), the underlying in-control linear profile model is $y_{ij} = 3 + 2x_i + \varepsilon_{ij}$, where the ε_{ij} s are i.i.d. normal random variables with zero mean and unit variance. The explanatory variable takes the values of 2, 4, 6, 8. Obviously, $\bar{x} = 5$, $S_{xx} = 20$. There are five IC historical samples of size $n = 4$, which are given in the first five rows in Table 2. Suppose that the intercept, A_0 , has shifted from 3.0 to 3.8 after the 15th future sample. For given overall IC ARL = 200, the control limits of EWMA_{IS} and EWMA_σ charts are, respectively, 0.9276 and 1.2959. The statistics \bar{w}_j , S_{w_j} , EWMA_{IS}, and EWMA_σ for $j = 6, 7, \dots, 28$ are tabulated in Table 2. Figure 1 and Figure 2 give the charts of EWMA_{IS} and EWMA_σ, respectively, along with the corresponding control limits.

We can see that the EWMA_{IS} chart signals a shift at the 28th sample (i.e., $j = 28$). Then, by looking at the values of $lr(jn, 28n)$ for $j = 5, 6, \dots, 27$, tabulated in the last column of Table 2, we can find that its maximum occurs at $j = 20$ with $lr(20n, 28n) = 14.87$. This maximum indicates precisely the change-point location, τ , of the shift. Moreover, by computing the test statistics, t_{B_0} , t_{B_1} , and F_σ , we obtain $t_{B_0} = -3.42$, $t_{B_1} = -1.22$, and $F_\sigma = 0.64$. Considering a significant level, $\alpha = 0.05$, it follows that $t_{B_0} < t(0.025; 28n-4) = -1.98$, $|t_{B_1}| < |t(0.025; 28n-4)| = 1.98$, and $F_\sigma < F(0.95; 20n-2; 8n-2) = 1.71$, where $t(0.025; 28n-4)$ and $F(0.95; 20n-2; 8n-2)$ are the lower percentiles of the Student- t distribution with $(28n-4)$ degrees of freedom and of the F -distribution with $(20n-2)$ and $(8n-4)$ degrees of freedom. Hence, our diagnosis concludes that there is a shift in the intercept after sample 20, which is a correct finding.

TABLE 2. Data for Example with a Shift in the Intercept after 20th Sample

j	y_{ij}				\bar{w}_j	S_{w_j}	EWMA _{IS}	EWMA _{σ}	$lr(jn, kn)$
1	7.29	10.46	13.14	20.88					
2	7.65	10.39	15.89	20.19					
3	7.37	11.88	14.54	20.33					
4	7.39	13.34	13.92	18.92					
5	5.64	11.06	15.47	19.33					1.39
6	6.63	11.51	15.66	18.42	−0.18	0.43	−0.07	0.00	2.56
7	8.16	12.12	16.27	19.83	0.79	0.10	0.26	0.00	1.85
8	5.90	11.21	16.45	18.71	−0.26	1.04	0.10	0.01	2.70
9	6.49	12.56	15.78	20.42	0.49	0.69	0.28	0.00	3.03
10	8.69	11.87	17.46	18.92	0.83	1.45	0.56	0.11	1.37
11	6.05	12.61	14.09	18.44	−0.61	1.51	0.20	0.21	1.20
12	7.88	10.02	16.02	18.39	−0.30	1.05	0.04	0.18	1.79
13	9.27	12.31	14.34	17.91	0.08	2.39	0.06	0.49	2.61
14	7.91	10.68	16.15	18.46	−0.07	0.62	0.02	0.30	3.95
15	7.43	11.62	14.82	20.34	0.18	0.40	0.09	0.09	4.34
16	6.53	10.08	15.92	19.04	−0.47	0.62	−0.11	0.00	5.24
17	6.77	11.76	13.86	18.48	−0.61	0.61	−0.34	0.00	7.98
18	5.66	10.98	15.00	20.18	−0.34	1.05	−0.40	0.01	8.59
19	7.39	10.13	15.94	19.00	−0.18	0.59	−0.39	0.00	11.00
20	5.96	11.75	14.81	18.64	−0.49	0.55	−0.51	0.00	14.87
21	4.41	12.28	17.02	20.02	0.29	1.82	−0.29	0.20	14.07
22	8.85	10.99	19.13	21.25	1.32	1.20	0.29	0.21	8.04
23	7.47	10.62	17.28	21.33	0.68	0.64	0.51	0.08	6.95
24	8.46	8.92	13.08	21.56	−0.09	2.26	0.37	0.37	7.84
25	4.24	12.00	16.58	19.53	−0.03	1.31	0.28	0.37	11.45
26	6.54	12.39	17.33	20.32	0.63	0.42	0.48	0.16	12.64
27	10.23	13.70	15.63	18.29	0.80	1.71	0.70	0.30	8.16
28	10.33	13.67	14.58	23.51	1.40	1.69	1.12	0.41	
							UCL _{σ} = 1.2959		
							UCL _{IS} = 0.9276		

Performance Comparisons

In this section, we assess the performance of our proposed self-starting control chart through comparisons with other methods in terms of ARL. For the known parameters, Kim et al. (2003) showed that the KMW charts outperform the methods in Kang and Albin (2000) in terms of detecting the sustained shifts in the parameters. Therefore, we compare our proposed self-starting method with KMW only. However, there is in fact no standard alternative because other methods rely on the availability of the values of the IC parameters. Hence, we assess the OC ARL performance of the proposed self-starting chart for different numbers of τ of IC samples (including his-

torical samples and future monitored IC samples) before a shift occurs.

For simplicity, we only consider the case of overall IC ARL = 200. The underlying IC model is the same as that in Kang and Albin (2000): that the parameters in the in-control model are $A_0 = 3$, $A_1 = 2$, and $\sigma^2 = 1$, $x_i = 2, 4, 6, 8$. In Kim et al. (2003), the control limits are set to be 3.0156, 3.0109, and 1.3723 for the three EWMA charts, EWMA_I, EWMA_S, EWMA_E, respectively, when the smoothing constant, λ , is chosen to be 0.2. In the case of known parameters, this design has an overall IC ARL of roughly 200 and the IC ARL of each chart is about 584. Although the IC ARL of our proposed

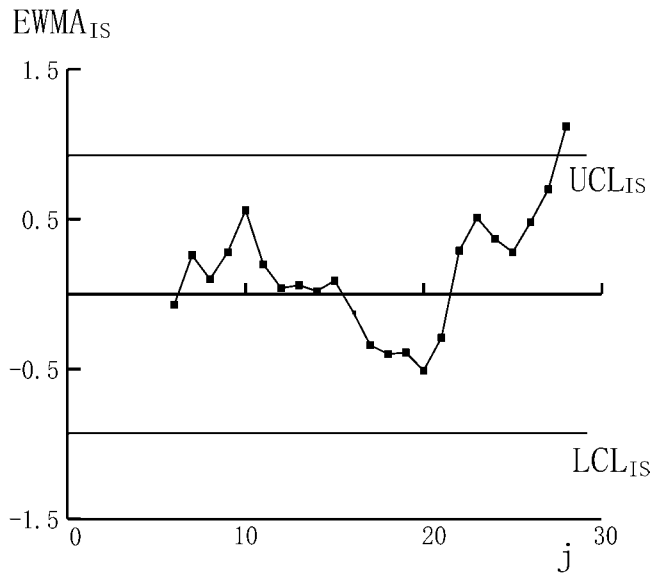


FIGURE 1. The Self-Starting EWMA_{IS} Chart for the MFC Example.

self-starting chart can be evaluated by the Markov-chain procedure, the OC ARL is rather difficult to calculate by the Markov chain-method due to the intricacy of OC distribution. Therefore, the results in this section are evaluated by 10,000 simulation runs. Moreover, the types of shifts considered in this paper are the same as those in Kim et al. (2003), although some other scales, instead of the scale σ , can be used to measure the size of shifts in all parameters. The OC ARLs of the SS chart with $\tau = 20, 50, 100, 300$, and 500 and the ARLs of KMW charts with the true values of parameters are tabulated in Table 3.

Table 3 shows that the proposed SS chart performs almost equally well for all values of τ when detecting a large shift. Naturally, the OC ARL will be affected by the number of reference samples gathered before a shift actually occurs. Yet the benefit is much more obvious in the case of detecting a small or moderate shift than in detecting a large shift. Because the SS chart updates the parameter estimations with new samples, the more IC future samples one collects, the more sensitive the EWMA chart is to a small or moderate shifts.

We also found that, when $\tau = 500$, for the detection of the shift in slope A_1 , the SS chart has almost the same performance as the KMW charts with known parameters, while for shifts in the intercept or standard deviation, our approach performs nearly uniformly better than the KMW charts.

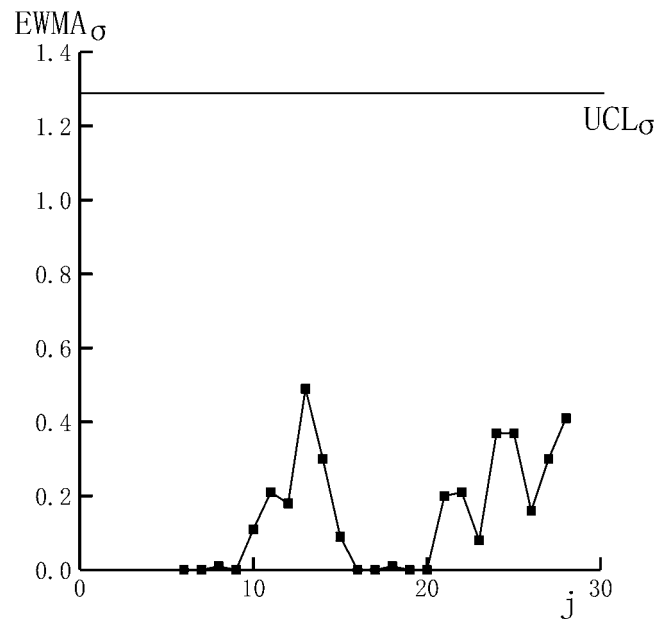


FIGURE 2. The Self-Starting EWMA_{σ} Chart for the MFC Example.

Table 4 shows a comparison between an SS chart with $m = 500$ IC historical samples and the KMW charts with known parameters when there is a step shift in the parameter B_1 of model (2). We observed that the KMW charts have better ARL performance than the SS chart for a small δ . The two methods perform similarly for the moderate-to-large shift sizes. The KMW charts are, in general, more effective than our approach in this case.

Conclusions and Considerations

Based on the recursive residuals, we proposed a self-starting control chart to detect shifts in the intercept, slope, and standard deviation for the linear profile. This chart can be easily designed, and it performs well in the case when process parameters are unknown but some historical samples are available. We also gave a useful tool based on the maximum likelihood ratio to diagnose the position of shift. In practical applications, if one wants to get information about which parameter(s) has (have) been changed, three parameter tests can then be applied to aid the proposed chart.

In this paper, we only consider detecting increases in the error variance to be consistent with Kim et al. (2003) and Kang and Albin (2000), so that our results are comparable with theirs under the same cri-

TABLE 3. Out-of-Control ARLs of SS Chart with Different Values of τ and KMW Chart with True Parameters

		SS					KMW
δ		$\tau = 20$	$\tau = 50$	$\tau = 100$	$\tau = 300$	$\tau = 500$	
$A_0 + \delta\sigma$	0.2	161.2	125.4	94.8	59.9	53.8	59.1
	0.4	80.2	30.0	18.2	14.6	14.1	16.2
	0.6	22.6	8.7	7.7	7.1	7.1	7.9
	0.8	7.1	5.1	4.9	4.7	4.6	5.1
	1.0	4.3	3.7	3.6	3.5	3.5	3.8
	1.2	3.2	3.0	2.9	2.8	2.8	3.1
	1.4	2.7	2.5	2.5	2.4	2.4	2.6
	1.6	2.3	2.2	2.2	2.1	2.1	2.3
	1.8	2.1	2.0	2.0	1.9	1.9	2.1
	2.0	1.9	1.8	1.8	1.8	1.8	1.9
$A_1 + \delta\sigma$	0.025	181.7	166.9	152.3	117.3	108.3	101.6
	0.05	144.9	95.4	62.6	38.7	34.5	36.5
	0.075	92.4	37.3	22.0	16.6	15.8	17.0
	0.1	46.6	14.5	10.7	9.6	9.4	10.3
	0.125	19.7	7.9	7.1	6.7	6.6	7.2
	0.15	9.0	5.6	5.3	5.1	5.1	5.5
	0.175	5.8	4.5	4.3	4.1	4.1	4.5
	0.2	4.3	3.7	3.6	3.5	3.5	3.8
	0.225	3.6	3.2	3.1	3.0	3.0	3.3
	0.25	3.1	2.8	2.8	2.7	2.7	2.9
$\delta\sigma$	1.2	116.5	73.3	49.0	33.0	31.2	33.5
	1.4	49.0	18.5	12.1	10.3	9.9	12.7
	1.6	18.1	7.1	6.1	5.6	5.5	7.2
	1.8	7.4	4.4	4.0	3.8	3.8	5.1
	2.0	4.3	3.3	3.0	2.9	2.9	3.9
	2.2	3.1	2.6	2.5	2.4	2.4	3.2
	2.4	2.5	2.2	2.1	2.1	2.1	2.8
	2.6	2.2	1.9	1.9	1.8	1.8	2.5
	2.8	1.9	1.7	1.7	1.7	1.6	2.3
	3.0	1.7	1.6	1.6	1.5	1.5	2.1

TABLE 4. ARL Comparisons for B_1 to $B_1 + \delta\sigma$ in model (2) (IC ARL = 200)

Chart	δ								
	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
KMW chart	13.1	6.6	4.4	3.3	2.7	2.3	2.1	1.9	1.7
SS chart	111.5	33.3	10.8	5.6	3.6	2.7	2.0	1.6	1.4

teria. Usually a decrease in the variance would correspond to an improvement in the measurement process as long as the other parameters do not change. Thus, in some applications, detecting decreases in standard deviation is also desired. For such a case, we may need to combine another one-sided EWMA chart to detect such a shift.

After the values of statistics \bar{w}_j and S_{w_j} are computed, instead of using the combination of two EWMA charts, we can actually chart these two statistics in any other convenient way, such as with Shewhart or CUSUM charts, if one prefers. However, for charting the statistic \bar{w}_j , the CUSUM scheme requires two one-sided charts so that the design and implementation will be more complicated than when using the EWMA chart.

Moreover, the proposed approach can be easily generalized to multiple linear-regression profiles. However, it could be difficult to analyze the relative contribution of each parameter to the shift, which warrants future research.

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Appendix

The Markov Chain Approach for Evaluating the IC ARL of the SS Chart

Similar to the procedure proposed by Brook and Evans (1972), the formula to evaluate the IC ARL of the self-starting scheme can be obtained by approximating the combination of two EWMA charts with a Markov chain.

The transition probability matrix, $\mathbf{P} = (p_{ij \rightarrow kl})$, is partitioned into the following form:

$$\begin{pmatrix} \mathbf{R} & (\mathbf{I} - \mathbf{R})\mathbf{1} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}$$

where the submatrix, \mathbf{R} , is the transition-probability matrix for in-control states; \mathbf{I} is the identity matrix, and $\mathbf{1}$ is a column vector of ones. Let t_1 and

t_2 be given integers, $w_1 = 2\text{UCL}_{\text{IS}}/(2t_1 + 1)$ and $w_2 = 2\text{UCL}_{\sigma}/(2t_2 - 1)$. A pair of integers (i, j) is denoted as a state of the two EWMA charts, where $i = -t_1, \dots, 0, \dots, t_1$, $j = 0, 1, \dots, t_2 - 1$, and $(0, 0)$ denotes the initial state of the self-starting chart. The transition probability that the plot statistics of $\text{EWMA}_{\text{IS}}(q)$ and $\text{EWMA}_{\sigma}(q)$ go from state (i, j) to state (k, l) is denoted by $R_{ij \rightarrow kl}$, which is calculated by

$$\begin{aligned} R_{ij \rightarrow k0} &= \Pr\{(\text{EWMA}_{\text{IS}}(q), \text{EWMA}_{\sigma}(q)) = (k, 0) \mid \\ &\quad (\text{EWMA}_{\text{IS}}(q-1), \text{EWMA}_{\sigma}(q-1)) \\ &\quad = (i, j)\} \\ &= \Pr\left\{(k-i+\lambda i-0.5)\frac{w_1}{\lambda} \leq \sqrt{n}\bar{w}_q \right. \\ &\quad \left. < (k-i+\lambda i+0.5)\frac{w_1}{\lambda}, \right. \\ &\quad \left. (n-1)S_{w_q} < (n-1) \right. \\ &\quad \left. \cdot \left[\sqrt{\frac{2}{n-1}}(-j+\lambda j+0.5)\frac{w_2}{\lambda} + 1\right]\right\} \\ &= \left\{\Phi\left[(k-i+\lambda i+0.5)\frac{w_1}{\lambda}\right] \right. \\ &\quad \left. - \Phi\left[(k-i+\lambda i-0.5)\frac{w_1}{\lambda}\right]\right\} \\ &\quad \cdot \chi_{n-1}^2\left((n-1) \right. \\ &\quad \left. \cdot \left[\sqrt{\frac{2}{n-1}}(-j+\lambda j+0.5)\frac{w_2}{\lambda} + 1\right]\right) \\ R_{ij \rightarrow kl} &= \Pr\{(\text{EWMA}_{\text{IS}}(q), \text{EWMA}_{\sigma}(q)) = (k, l) \mid \\ &\quad (\text{EWMA}_{\text{IS}}(q-1), \text{EWMA}_{\sigma}(q-1)) \\ &\quad = (i, j)\} \\ &= \Pr\left\{(k-i+\lambda i-0.5)\frac{w_1}{\lambda} \leq \sqrt{n}\bar{w}_q \right. \\ &\quad \left. < (k-i+\lambda i+0.5)\frac{w_1}{\lambda}, \right. \\ &\quad \left. (n-1)\left[\sqrt{\frac{2}{n-1}}(l-j+\lambda j-0.5)\frac{w_2}{\lambda} + 1\right] \right. \\ &\quad \left. \leq (n-1)S_{w_q} < (n-1) \right. \\ &\quad \left. \cdot \left[\sqrt{\frac{2}{n-1}}(l-j+\lambda j+0.5)\frac{w_2}{\lambda} \right. \right. \\ &\quad \left. \left. + 1\right]\right\} \\ &= \left\{\Phi\left[(k-i+\lambda i+0.5)\frac{w_1}{\lambda}\right] \right. \end{aligned}$$

$$\begin{aligned}
& -\Phi\left[(k-i+\lambda i-0.5)\frac{w_1}{\lambda}\right] \Bigg\} \\
& \cdot \left\{ \chi_{n-1}^2 \left((n-1) \right. \right. \\
& \quad \cdot \left[\sqrt{\frac{2}{n-1}}(l-j+\lambda j+0.5)\frac{w_2}{\lambda} \right. \\
& \quad \quad \left. \left. +1 \right] \right) \\
& - \chi_{n-1}^2 \left((n-1) \right. \\
& \quad \cdot \left[\sqrt{\frac{2}{n-1}}(l-j+\lambda j-0.5)\frac{w_2}{\lambda} \right. \\
& \quad \quad \left. \left. +1 \right] \right) \Bigg\},
\end{aligned}$$

where $\Phi(\cdot)$ and $\chi_{n-1}^2(\cdot)$ are the CDFs of the standard normal distribution and the chi-square distribution with $n-1$ degrees of freedom. Following the procedure of Brook and Evans (1972), the ARL of the self-starting chart with initial state $(0,0)$ hence is given by

$$\mathbf{l}_0(\mathbf{I} - \mathbf{R})^{-1}\mathbf{1},$$

where $\mathbf{l}_0 = (\mathbf{0}, \dots, \mathbf{1}, \dots, \mathbf{0})$ is a row vector with 1 in the $(t_1 \times t_2 + 1)$ th element. To increase the accuracy of our method, the following extrapolation is used:

$$ARL(t) = ARL + B/t + C/t^2, \quad (12)$$

where $ARL(t)$ denotes the value of ARL calculated by $t_1 = t_2 = t$ states and $t = 10, 15, 20$ are used for Table 1.

The Approximate Calculation of the Control Limits

Let $ARL_{IS\sigma}(UCL_{IS}, UCL_{\sigma})$, $ARL_{IS}(UCL_{IS})$, and $ARL_{\sigma}(UCL_{\sigma})$ denote the ARL functions evaluated by the Markov-chain procedure for the combination of the two EWMA charts, the EWMA_{IS}, and EWMA _{σ} charts, respectively. Given an overall IC ARL_0 , the values of UCL_{IS} and UCL_{σ} can be found by solving the following equations:

$$\begin{cases} ARL_{IS\sigma}(UCL_{IS}, UCL_{\sigma}) = ARL_0 \\ ARL_{IS}(UCL_{IS}) = 0.5ARL_{\sigma}(UCL_{\sigma}). \end{cases}$$

The dichotomy method is used to search for the values.

The Derivation of Equation (7)

Let $\{(x_i, y_{ij}), i = 1, 2, \dots, n, j = 1, 2, \dots, k\}$ denote all the historical and collected future samples, $\bar{y}_{kn} = (1/kn) \sum_{j=1}^k \sum_{i=1}^n y_{ij}$, $\bar{x} = (1/n) \sum_{i=1}^n x_i$,

$S_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2$, and $S_{xy(kn)} = \sum_{j=1}^k \sum_{i=1}^n (x_i - \bar{x})y_{ij}$. Then, the logarithm of the likelihood function is given by

$$-\frac{1}{2} \sum_{j=1}^k \sum_{i=1}^n \left[\log(2\pi\sigma_j^2) + \frac{(y_{ij} - A_{0j} - A_{1j}x_i)^2}{\sigma_j^2} \right].$$

If the data are collected under in-control conditions, the maximum value of the logarithm of likelihood function is

$$l_0 = -\frac{kn}{2} \log(2\pi) - \frac{kn}{2} \log(\hat{\sigma}_{kn}^2) - \frac{kn}{2},$$

where

$$\hat{\sigma}_{kn}^2 = \frac{1}{kn} \sum_{j=1}^k \sum_{i=1}^n (y_{ij} - \hat{A}_{0(kn)} - \hat{A}_{1(kn)}x_i)^2,$$

with

$$\hat{A}_{1(kn)} = \frac{S_{xy(kn)}}{kS_{xx}}, \quad \hat{A}_{0(kn)} = \bar{y}_{kn} - \hat{A}_{1(kn)}\bar{x}.$$

Similarly, let

$$\bar{y}_{k_1n} = \frac{1}{k_1n} \sum_{j=1}^{k_1} \sum_{i=1}^n y_{ij},$$

$$S_{xy(k_1n)} = \sum_{j=1}^{k_1} \sum_{i=1}^n (x_i - \bar{x})y_{ij},$$

$$\bar{y}_{k_2n} = \frac{1}{k_2n} \sum_{j=k_1+1}^k \sum_{i=1}^n y_{ij},$$

$$S_{xy(k_2n)} = \sum_{j=k_1+1}^k \sum_{i=1}^n (x_i - \bar{x})y_{ij}.$$

When there is a step shift after the k_1 th sample, the corresponding maximum value is

$$\begin{aligned} l_1 = & -\frac{kn}{2} \log(2\pi) - \frac{k_1n}{2} \log(\hat{\sigma}_{k_1n}^2) \\ & - \frac{k_2n}{2} \log(\hat{\sigma}_{k_2n}^2) - \frac{kn}{2}, \end{aligned}$$

where

$$\hat{\sigma}_{k_1n}^2 = \frac{1}{k_1n} \sum_{j=1}^{k_1} \sum_{i=1}^n (y_{ij} - \hat{A}_{0(k_1n)} - \hat{A}_{1(k_1n)}x_i)^2,$$

$$\hat{A}_{1(k_1n)} = \frac{S_{xy(k_1n)}}{k_1S_{xx}},$$

$$\hat{\sigma}_{k_2n}^2 = \frac{1}{k_2n} \sum_{j=k_1+1}^k \sum_{i=1}^n (y_{ij} - \hat{A}_{0(k_2n)} - \hat{A}_{1(k_2n)}x_i)^2,$$

$$\hat{A}_{1(k_2n)} = \frac{S_{xy(k_2n)}}{k_2S_{xx}},$$

$$\hat{A}_{0(k_1n)} = \bar{y}_{k_1n} - \hat{A}_{1(k_1n)}\bar{x},$$

$$\hat{A}_{0(k_2n)} = \bar{y}_{k_2n} - \hat{A}_{1(k_2n)}\bar{x}.$$

Thus, the classical likelihood ratio statistic is defined by

$$\begin{aligned} lr(k_1n, kn) &= -2(l_0 - l_1) \\ &= kn \log[\hat{\sigma}_{kn}^2 (\hat{\sigma}_{k_1n}^2)^{-k_1/k} (\hat{\sigma}_{k_2n}^2)^{-k_2/k}]. \end{aligned}$$

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