A Study of Method for Tracing State Transition on Time Series of Process Variance

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Abstract. Quality of items produced at a manufacturing process isn’t necessarily uniform. Quality characteristics of respective items have stochastic variability. Control charts are basic tools to detect a change in process condition using the quality data with the stochastic variability. The $\overline{x}$ and $s$ control charts are famous tools to monitor process mean and variance based on the fluctuations on the respective charts. In particular, the $s$ control chart is operated prior to the $\overline{x}$ control chart because a change of process variance affects the decision about a change of process mean based on the $\overline{x}$ control chart. On one hand, when an assignable change in the process condition was detected by a control chart, it is required to identify a time point of process change and search for assignable causes. Hence, some methods of estimating the time point of a change in process variance have been developed. Then, it is supposed in some previous researches that the process has just a single change point. However, the process may have multiple change points until a chart signals. In this study, we propose a method of identifying the respective time points of multiple changes and tracing state transition on time series of process variances. Then, we show the validity of our proposal in comparison to some traditional methods.

Keywords: Akaike information criterion (AIC), change point detection, dynamic programming, maximum likelihood theory, $s$ control chart

1. INTRODUCTION

Control charts play an important role in statistical process control (Montgomery, 2005). Control charts are used to distinguish whether the fluctuation of quality characteristics depends on chance or assignable causes. When a control chart signals that an assignable cause is present, process engineers must initiate a search for the assignable cause of the process disturbance. It is well known that a certain amount of time is needed until the Shewhart $\overline{x}$ control chart signals a change in a process mean after the change in the process mean actually occurred. Therefore, the process engineers should identify when the process has changed into an out-of-control condition first. Consequently, by identifying the point of change in the process condition, the search for the assignable cause can be simplified and then appropriate actions needed to improve quality can be implemented sooner (Samuel et al., 1998a).

In the statistical literature, there is a research area called change point detection (CPD) (Qui, 2014). Ali et al. (1997) have considered a method for estimating a change point in a process mean under the assumption that a process mean is changed once until a chart signals. Under same assumption, Samuel et al. (1998a) and Pignatiello and Samuel (2001) have proposed a CPD method for a single change point in a process mean using the maximum likelihood theory. Further, Hawkins (2001) has considered a multiple change-points model under the situation that a process mean is changed multiple times until a chart signals. Also, Perry and Pignatiello (2006) have considered a CPD method of a process mean under the assumption that a process mean is changed along a linear trend after a process changed to an out-of-control condition. Then, Takemoto
and Arizono (2009) have considered a CPD method under the situation that a process mean is changed continuously after a process changed to an out-of-control condition. Also, Noorossana and Shadman (2009) have investigated a CPD method in a process mean with a monotonic change. In a monotonic change, the type of change is unknown a priori, but the direction of shifts is the same, increasing or decreasing (Amiri and Allahyari, 2012). The researches described above are investigated based on the maximum likelihood theory. An overview of CPD literature shows that a maximum likelihood estimator (MLE) is one of the prominent approaches for CPD (Amiri and Allahyari, 2012). In recent years, some CPD methods have been proposed using some techniques in soft computing and machine learning (Ghasabadi et al., 2013; Kazemi et al., 2016).

On the other hand, Samuel et al. (1998b) have considered a CPD method in process variance using the maximum likelihood theory under the assumption that process variance is changed once until a chart signals. Then, Noorossana and Heydari (2009) have assumed that process variance is changed along a linear trend after a process changed to an out-of-control condition. Further, Noorossana and Heydari (2012) have considered a CPD method with a monotonic change of process variance. Further, Amiri, Niaki, and Moghadam (2015) have proposed a probabilistic neural network (PNN)-based procedure to estimate a change point in process variance.

In common, it has been insisted that the $\tau$ and $s$ control charts are used together. One of the reasons is that a change of process variance affects the decision about a change of a process mean based on the $\tau$ control chart. By contraries, a change of a process mean doesn’t affect the decision about a change of process variance based on the $s$ control chart. Therefore, the inference of change points in process variance should be considered separately from a change of a process mean. However, Samuel et al. (1998b), Noorossana and Heydari (2009, 2012), and Amiri, Niaki, and Moghadam (2015) have assumed that a process mean always maintains an in-control condition. Hence, an estimator of process variance has been given as a departure from an ideal process mean in the in-control condition. This estimator is different from plotted statistics in the $s$ control chart, that is, a common unbiased estimator of process variance.

Also, Samuel et al. (1998b), Noorossana and Heydari (2009, 2012), and Amiri, Niaki, and Moghadam (2015) have assumed the single change-point model for estimating a change point in process variance. In this case, the process keeps being in a particular out-of-control condition until the chart signals after the process shifted to an out-of-control condition. However, it shall be common that a process condition is getting worse as time progresses. Therefore, Noorossana and Heydari (2009, 2012) have investigated a linear trend change and a monotonic change model in process variance. However, their studies have assumed some specified pattern of change in process variance. On one hand, Hawkins (2001) has considered a multiple change-points model in a process mean. Then, a multiple change-points model in process variance is worth investigating.

On the other hand, on considering a multiple change-points model, it is sometimes assumed that the number of change points is known (Qiu, 2014). Alternatively, there are some studies in which the number of change points is treated as one of unknown parameters that should be estimated. For example, Lavielle and Moulines (2000), and Lebarbier (2005) have applied the least square method and its related method to estimation of an unknown number of shifts in a time series.

In this paper, we consider a multiple change-points model with respect to a change of process variance. Then, a new CPD method is proposed. Also, in the traditional literature, the stochastic properties in the observations before and after the change point are specified in the statistical model. Hence, the probability density function of the observations has been utilized on constructing a log-likelihood function in a statistical model. On one hand, in this study, we don't assume that a process mean always maintains the in-control condition. In this case, we utilized the unbiased estimator of process variance associated with a charting statistic in the $s$ control chart. Therefore, the stochastic property in the unbiased estimator of process variance before and after the change point is specified in the statistical model. The unbiased estimator of process variance is independent of a process mean and obeys a chi-square distribution. Hence, the probability density function of the chi-square distribution is utilized on constructing a log-likelihood function in the statistical model. Further, we apply Akaike Information Criterion (AIC) to determination of the number of change points because AIC is closely connected with the maximum likelihood theory. Then, the usefulness of our proposal is shown in comparison to some traditional methods through a numerical example.

2. TRADITIONAL RESEARCHES

In this section, we introduce the following traditional researches about CPD for process variance: Samuel et al. (1998b) and Noorossana and Heydari (2009). We first show some assumptions and notations. The respective quality characteristics of $j$th item $j = 1, \ldots, n$ in $i$th sampling, $x_{ij}, j = 1, \ldots, n$, are normally distributed, where $n$ is the number of samples in every sampling. Then, denote the normal distribution with mean $\mu$ and variance $\sigma^2$ by $N(\mu, \sigma^2)$. Further, the probability density function of the
normal distribution $N(\mu, \sigma^2)$ is defined as $f_n(x; \mu, \sigma^2)$. The respective quality characteristics of items $x_i$ are also independently and identically distributed in every sampling. The following $i$th statistic with respect to the process variance is plotted on the $s$ control chart:

$$s_i = \sqrt{\frac{1}{n-1} \sum_{j=1}^{n} (x_j - \bar{x})^2},$$

where

$$\bar{x} = \frac{1}{n} \sum_{j=1}^{n} x_j.$$  

Then, control limits on the $s$ control chart are defined according to a basic discipline (Montgomery, 2005).

### 2.1 Research in Samuel et al. (1998b)

Samuel et al. (1998b) have assumed that the process variance is changed once until the chart signals. This is called a single change-point model. In the detail, denote the in-control and out-of-control condition by $N(\mu_0, \sigma_0^2)$ and $N(\mu_1, \sigma_1^2)$, respectively. Note that the process mean isn’t changed in their model. Then, the following statistical model is considered:

$$\begin{cases} (\mu_0, \sigma_0^2), & i = 1, \ldots, \tau, \\ (\mu_1, \sigma_1^2), & i = \tau + 1, \ldots, T, \end{cases}$$

where $\tau$ and $T$ express the last point of the in-control condition and the signal point on the control chart. For this statistical model, a log-likelihood function is given as follows:

$$\ell_s(\tau) = \sum_{i=1}^{\tau} \log f_s(x_i; \mu_0, \sigma_0^2) + \sum_{i=\tau+1}^{T} \log f_s(x_i; \mu_1, \sigma_1^2)$$

$$= -\frac{n_1}{2} \log 2\pi\sigma_1^2 - \frac{1}{2\sigma_1^2} \sum_{t=1}^{\tau} (x_t - \mu_0)^2 - \frac{1}{2\sigma_1^2} \sum_{t=\tau+1}^{T} (x_t - \mu_1)^2$$

For a given $\tau$, Samuel et al. have the following maximum log-likelihood estimator (MLE) $\hat{\tau}$ for $\sigma_1^2$ by differentiating $\ell_s(\tau)$ with respect to $\sigma_1^2$:

$$\hat{\tau} = \frac{1}{T - \tau} \sum_{i=1}^{\tau} (x_i - \mu_0)^2.$$  

By inserting $\hat{\tau}$ in eq.(5) into $\ell_s(\hat{\tau})$ in eq.(4), Samuel et al obtain the following maximum log-likelihood $\ell_s(\hat{\tau})$ for a given $\tau$:

$$\ell_s(\hat{\tau}) = -\frac{n(T - \tau)}{2} \left(1 + \log \frac{\sigma_1^2}{\sigma_0^2} - \frac{\sigma_1^2}{\sigma_0^2} \right).$$  

Further, the maximum log-likelihood $\ell_s(\hat{\tau})$ is maximized in $\tau$ for the purpose of obtaining the estimator of $\tau$. The estimator $\hat{\tau}$ is obtained as follows:

$$\hat{\tau} = \arg \max_{\tau} \ell_s(\hat{\tau}).$$

### 2.2 Research in Noorossana and Heydari (2009)

Noorossana and Heydari (2009) have assumed that the process variance is changed along a linear trend after the process changed to an out-of-control condition. This is called a linear trend change model. In the detail, the following statistical model is considered:

$$\begin{cases} (\mu_0, \sigma_0^2), & i = 1, \ldots, \tau, \\ (\mu_0, \sigma_1^2), & i = \tau + 1, \ldots, T, \end{cases}$$

where

$$\sigma_i^2 = \sigma_0^2 + \beta(i - \tau).$$

$\beta$ is a magnitude of changes in unit time. Note that the process mean isn’t also changed in their model. For this statistical model, a log-likelihood function is given as follows:

$$\ell_s(\beta) = \sum_{i=1}^{\tau} \log f_s(x_i; \mu_0, \sigma_0^2) + \sum_{i=\tau+1}^{T} \log f_s(x_i; \mu_0, \sigma_1^2)$$

$$= -\frac{n_1}{2} \log 2\pi\sigma_1^2 - \frac{1}{2\sigma_1^2} \sum_{t=1}^{\tau} (x_t - \mu_0)^2 - \frac{1}{2\sigma_1^2} \sum_{t=\tau+1}^{T} (x_t - \mu_0)^2$$

For a given $\tau$, we have the following equation about the MLE $\hat{\beta}$ for $\beta$ by differentiating $\ell_s(\beta)$ with respect to $\beta$:

$$\frac{d\ell_s(\beta)}{d\beta} = \frac{1}{2} \sum_{t=1}^{\tau} \frac{(i - \tau)(x_t - \mu_0)^2}{(\sigma_0^2 + \beta(i - \tau))^2} - \frac{n}{2} \sum_{t=\tau+1}^{T} \frac{(i - \tau)}{\sigma_0^2 + \beta(i - \tau)}.$$  

As shown in eq.(11), it is impossible to obtain the MLE of $\beta$ which satisfies $d\ell_s(\beta)/d\beta = 0$ as an explicit function. Noorossana and Heydari (2009) have proposed a numerical
search for $\beta$ which satisfies $d \ell_c(\beta)/d \beta = 0$. In their proposal, the MLE of $\beta$, $\hat{\beta}$, is obtained from the following iterative calculations:

$$
\hat{\beta}_{k+1} = \hat{\beta}_k - 
\frac{1}{2} \sum_{i=1}^{T} \sum_{j=1}^{n_i} \frac{(i-\tau) \left( x_{ij} - \mu_i \right)^2}{\left( \sigma_i^2 + \hat{\beta}_k (i-\tau) \right)^2} \frac{n}{2} \sum_{i=1}^{T} \frac{i-\tau}{\sigma_i^2 + \hat{\beta}_k (i-\tau)} 
- \sum_{i=1}^{T} \sum_{j=1}^{n_i} \frac{(i-\tau) \left( x_{ij} - \mu_i \right)^2}{\left( \sigma_i^2 + \hat{\beta}_k (i-\tau) \right)^2} \frac{n}{2} \sum_{i=1}^{T} \frac{(i-\tau)^2}{\sigma_i^2 + \hat{\beta}_k (i-\tau)}.
$$

(12)

This procedure is based on Newton's method. Then, they obtain the maximum log-likelihood $\ell_c(\hat{\beta})$ for a given $\tau$ by inserting $\hat{\beta}$ derived from eq.(12) into $\ell_c(\beta)$ in eq.(10). Further, the maximum log-likelihood $\ell_c(\hat{\beta})$ is maximized in $\tau$ for the purpose of obtaining the estimator of $\tau$. The estimator $\hat{\tau}$ is obtained as follows:

$$
\hat{\tau} = \arg \max_{\tau} \ell_c(\hat{\beta}).
$$

(13)

3. PROPOSED METHOD

In this study, we propose a method of detecting change points under the following situations:

(i) The process mean does not always maintain the in-control condition until the chart signals.

(ii) The process variance is changed multiple times until the chart signals, that is, multiple change-points model.

As described in the previous section, the traditional researches have assumed that the process mean isn’t changed in their model. Hence, the log-likelihood function is formed using the probability density function of the normal distribution. When the observations $x_{ij}, j=1,\cdots,n_i$ are given as the normal distribution $N(\mu, \sigma_i^2)$, the statistic $(n-1)\hat{\sigma}_i^2/\sigma_i^2$ obeys the chi-square distribution with $n-1$ degree of freedom. From this fact, the distribution of $\hat{\sigma}_i^2$ has the following probability density function:

$$
f_{\hat{\sigma}_i^2}(\hat{\sigma}_i^2; \sigma_i^2) = \frac{1}{\Gamma\left(\frac{n-1}{2}\right)} \left( \frac{n-1}{2} \right)^{\frac{n-1}{2}} \left( \hat{\sigma}_i^2 \right)^{\frac{n-1}{2} - 1} e^{-\frac{n-1}{2} \frac{1}{\sigma_i^2} \hat{\sigma}_i^2}. 
$$

(14)

Then, the following statistical model is considered since the process variance is changed multiple times until the chart signals:

$$\begin{align}
\sigma_0^2, \ i = 1, \ldots, r_0, \\
\sigma_1^2, \ i = r_0 + 1, \ldots, r_1, \\
\vdots \\
\sigma_k^2, \ i = r_{k-1} + 1, \ldots, r_k \ (= T),
\end{align}
$$

(15)

where $K$ indicates the number of changes in the process variance until the chart signals. Also, $\tau^{(k)}=(\tau_0, \ldots, \tau_{k-1})$ and $\sigma^{(2k)}=(\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2)$ express change points and process variances in some out-of-control condition after $\tau_0 + 1$. Note that $K$, $\tau^{(k)}=(\tau_0, \ldots, \tau_{k-1})$, and $\sigma^{(2k)}=(\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2)$ are unknown and those should be estimated from the observations.

For the statistical model in eq.(15), a log-likelihood function is given as follows:

$$\ell_{\hat{\tau},\hat{\sigma}}(\sigma^{(2k)}) = \sum_{k=0}^{K} \sum_{i=0}^{\tau_k} \log f_{\hat{\sigma}_i^2}(\hat{\sigma}_i^2; \sigma_i^2)$$

$$= \frac{(n-1)T}{2} \log \left( \frac{n-1}{2} \right) - T \log \Gamma \left( \frac{n-1}{2} \right)$$

$$+ \sum_{k=0}^{K} \frac{(n-1)(\tau_k - \tau_{k-1})}{2} \log \sigma_k^2$$

$$+ \left( \frac{n-1}{2} - 1 \right) \sum_{i=1}^{n} \log \hat{\sigma}_i^2 - \sum_{k=0}^{K} \sum_{i=\tau_k+1}^{\tau_{k+1}} \frac{(n-1)s_i^2}{2\sigma_k^2}.
$$

(16)

where $\tau_{-1} = 0$.

For a given $\tau^{(k)}$, we have the following equation about the MLEs $\hat{\sigma}^{(2k)}=(\hat{\sigma}_0^2, \hat{\sigma}_1^2, \ldots, \hat{\sigma}_k^2)$ for $\sigma^{(2k)}=(\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2)$ by differentiating $\ell_{\hat{\tau},\hat{\sigma}}(\sigma^{(2k)})$ partially with respect to $\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2$.

$$\hat{\sigma}_i^2 = \frac{1}{r_k - r_{k-1} + 1} \sum_{i=r_k}^{r_k+1} s_i^2.
$$

(17)

Further, by inserting $\hat{\sigma}_i^2$ in eq.(17) into $\ell_{\hat{\tau},\hat{\sigma}}(\sigma^{(2k)})$ in eq.(16), we obtain the following maximum log-likelihood $\ell_{\hat{\tau},\hat{\sigma}}(\hat{\sigma}^{(2k)})$ for a given $\tau^{(k)}$:

$$\ell_{\hat{\tau},\hat{\sigma}}(\hat{\sigma}^{(2k)}) = \sum_{k=0}^{K} \sum_{i=0}^{\tau_k} \log f_{\hat{\sigma}_i^2}(\hat{\sigma}_i^2; \sigma_i^2)$$

$$= \frac{(n-1)T}{2} \log \left( \frac{n-1}{2} \right) - T \log \Gamma \left( \frac{n-1}{2} \right)$$

$$- \frac{(n-1)T}{2} \log \sigma_0^2 - \sum_{k=0}^{K} \sum_{i=1}^{\tau_k} \frac{(n-1)s_i^2}{2\sigma_k^2}$$

$$+ \left( \frac{n-1}{2} - 1 \right) \sum_{i=1}^{n} \log \hat{\sigma}_i^2
$$

Note that $\tau_{-1} = 0$.
\[
\hat{t}^{(K)} = \arg \min_{k} \hat{AIC}(K). \tag{24}
\]

The most appropriate \( K \) is obtained from eq.(24), and then, \( \hat{\sigma}^{2(k)} \) and \( \hat{\sigma}^{2(\hat{K})} \) are given as eqs.(19) and (17), respectively.

4. NUMERICAL EXAMPLES

In this section, we show some numerical examples. In this case, we compare our proposal with the methods in the traditional researches explained in this paper, that is, Samuel et al. (1998b) and Noorossana and Heydari (2009).

A numerical example is shown using a series of statistics \( s_i \) in Figure 1. The model parameters are as follows: \( n = 10, \mu_0 = 100.0, \sigma_0^2 = 1.50^2 \). Then, a series of statistics \( s_i \) in Figure 1 are obtained by computer simulation under the condition that \( K = 2 \), \( \tau_0 = 15, \tau_1 = 25, \sigma_0^2 = 2.00^2, \sigma_1^2 = 2.50^2 \). Note that the condition of the process changes twice and the process mean maintains the in-control condition. Further, the parallel lines in Figure 1 express control limits. Hence, this \( s \) chart signals at 32th sampling.

Figures 2, 3, and 4 indicate outputs obtained by applying the methods in Samuel et al. (1998b), Noorossana and Heydari (2009), and our proposal. Note that the changes in process variance illustrate the lines going through any plotted points in the respective charts. The detail of outputs is explained as below.

From Figure 2, the method of Samuel et al. (1998b) has reported that the change point is estimated at \( \hat{t} = 27 \) and the process variance after the process change is estimated at \( \hat{\sigma}_1^2 = 2.72^2 \). As long as we see Figure 2, the estimators of \( \tau \) and \( \sigma_1^2 \) are not thought to be appropriate. We think that this is the reason why the single change point in the statistical model is considered, and then the estimator \( \hat{\sigma}_1^2 \) in Eq.(5) is given as the departure from the ideal process mean \( \mu_0 \).

From Figure 3, the method of Noorossana and Heydari (2009) has reported that the change point is estimated at \( \hat{t} = 17 \) and the magnitude of changes in the process variance after the process change is estimated at \( \hat{\beta} = 0.289 \) per unit time. As long as we see Figure 3, the change in the process variance after the process change is not grasped very well. This will be the reason why the kind of changes after the change point is specified as a linear trend, and then the departure from the ideal process mean \( \mu_0 \) is also considered on estimating \( \hat{\beta} \) associated with the process variance in this method.

Further, our proposal is confirmed through Figure 4. Our proposal has reported that the number of process changes is \( \hat{K} = 2 \), the change points are estimated at
As noted above, the process variance is assumed to be changed twice in a series of statistics $s_i$ for the numerical example. Hence, our proposal will be functioning well in the numerical example. On contrary, the method of Samuel et al. (1998b) or Noorossana and Heydari (2009) may be functioning well when the process variance is assumed to be changed according to a single change-point model or a linear trend model. It is simply that the respective situations are suitable for each method. However, it has been found through the above simulation that the method of Samuel et al. (1998b) or Noorossana and Heydari (2009) cannot be functioning well in the case that the situation that the situation of the observations is not suitable for respective methods. On one hand, our proposal has the possibility of covering extensive conditions as a multiple change-points model in the change of process variance in comparison with the methods in Samuel et al. (1998b) and Noorossana and Heydari (2009). Therefore, our proposal will be effective in practical usage.

5. CONCLUDING REMARKS

In this paper, we have considered a multiple change-points model with respect to a change of process variance. In the traditional researches, it has been assumed that a process mean always maintain the in-control condition until a chart signals. The estimation of a change point in process variance should be considered separately from a change of a process mean. Then, this paper has the assumption that the process mean does not always maintain the in-control condition until a chart signals. For the purpose of considering the assumption, the statistical model and likelihood function are constructed using the chi-square distribution expressing the probability distribution of unbiased estimator of process variance. Then, we have formulated the dynamic programming in order to maximize the maximum log-likelihood in multiple change points. Further, a theoretical method for estimating the number of
change points has been proposed using AIC. Lastly, the usefulness of our proposal has been shown through a numerical example.

In this paper, we have shown how to practice our proposed method when the chart signals. On one hand, our proposed method can be applied at any time. That is, it is possible to practice our proposed method with charting observations together at real time. In this case, it is possible to trace the state transition on time series of process variances by using our method. In this case, it is noted that application software to practice our method at real time needs to be developed. This will be a future work.

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