

Charting Techniques for Dynamic Processes: Literature Review and Extensions

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Abstract: In modern manufacturing environments, both multivariate and dynamic natures have become increasingly important. Many multivariate and dynamic processes, such as processes with feedback control and with high-frequency automatic sampling, have raised new challenges to conventional statistical process control (SPC) and statistical quality control (SQC). For the efficient and effective monitoring of multivariate processes with dynamic (time-varying) shifts, some conventional SPC schemes have been extended and implemented. Meanwhile, new techniques have also been proposed to handle these challenges. This paper provides a literature review on the existing SPC techniques for multivariate and dynamic process monitoring. In addition, some novel alternatives based on the ideas of joint monitoring and adaptive control chart are proposed. Illustrative examples are used to demonstrate and compare these techniques, and practical guidelines to implement the dynamic process control and monitoring are provided accordingly.

Key words: Statistical Process Control, SPC, Dynamic Process, Multivariate Process.

Mathematical Subject Classification: 62P30

1 Introduction

In the modern business environment, quality is one of the decisive factors for the success and sustained development of an enterprise. In order to reduce the cost of poor quality, the root cause of quality problems must be identified. According to [1], “quality is inversely proportional to variability”. The author of [2] also defines quality as “the never-ending reduction of variation around a customer defined target in the absence of defects”. Therefore, the root cause of poor quality is large variability. Reducing process variations is the most important way of improving quality.

Variations in processes can be classified as either common cause variations or assignable cause variations. The former type refers to the natural variability that causes the processes to vary within an acceptable tolerance. The latter type, however, is caused by certain isolated, identifiable and removable reasons. Identifying the existence of such assignable causes and helping remove them are the fundamental function of Statistical Process Control (SPC).

No matter whether a sustained shift ([3], [4], [5] and [1]) or a deterministic drift happens ([6], [7], [8]) in a process, the behavior of observable variables may be very complex in a dynamic process. As [9] points out that a dynamic process, rather than responding to input changes immediately, undergoes a transitional

period before establishing a new process level. Furthermore, the dynamic behavior of a continuous process in the modern manufacturing environment has been strengthened by employing short-interval sampling plans ([10]).

Inertial systems are one type of application that exhibit dynamic natures. Depending on the degree of inertia, such systems respond slowly or quickly to sudden changes. More importantly, in the event of a constant shift in the process, the observed sequences usually demonstrate time-varying shift patterns. An example of shifts in inertial systems is shown in Figure 1. The process is subject to a sudden mean shift, while the observed output shows a slowly increasing trend. After the shift has happened, it takes around 50 steps for the output to reach a new level.

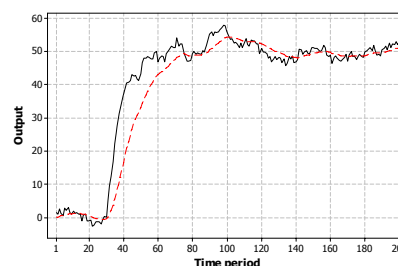


Figure 1. An example of time-varying shifts in inertial systems. Solid: observations; dashed: EWMA predictions.

To achieve a better control of quality, most processes are equipped with certain types of feedback controllers instead of being left alone ([11], [12], [13], [14]). If any deviation from the target is observed, the information will be fed into the controller to generate an optimal control action, which aims to compensate the deviation by changing the input variables. The trajectories of a feedback-controlled process are shown in Figure 2. The process is subject to a constant mean shift. However, the observed process output and control action exhibit strong oscillations.

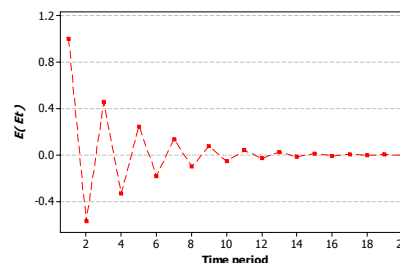


Figure 2. An example of time-varying shifts in feedback-controlled processes.

The various dynamic shifts shown above have given rise to distinct challenges to SPC. The fact that time-varying shifts are more difficult to identify in a proc-

ess drives the need for advanced charting techniques. In this paper, we review the charting techniques for monitoring dynamic processes. The basic model for illustrating dynamic signals and the conventional treatments for process monitoring are presented in Section 2. In Section 3, some new extensions to this issue are introduced. Section 4 presents a simulation example to demonstrate the performance of the new extensions. Section 5 concludes this paper with future research topics.

2 Signal modeling and literature review

Any dynamic shift of a univariate process can be characterized by two pieces of information: fault signature f_t , which is a function of time that illustrates the fluctuation of the shift signal; and shift magnitude δ , which indicates the shift's size. Therefore, the output of a univariate process can be represented by the following model ([4], [5]):

$$x_t = a_t + \delta f_t, \quad (1)$$

where a_t is a series of white noises from which we want to detect signal f_t . The exact form of f_t depends on the process dynamics, the feedback control schemes being used, and the true disturbance models.

For a p -dimensional multivariate process, replacing the variables in Equation (1) by vectors leads to the following model:

$$\mathbf{x}_t = \mathbf{a}_t + \delta \mathbf{f}_t, \quad (2)$$

where \mathbf{x}_t , \mathbf{a}_t , and \mathbf{f}_t are vectors of observations, noises, and failure signatures, respectively. The control chart to be used in practice depends heavily on the dimensions of the processes, p , and the format of the failure signatures, \mathbf{f}_t .

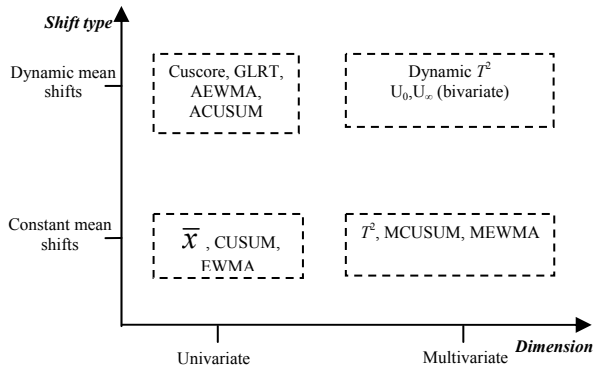


Figure 3. A classification of conventional SPC charts.

The area of SPC has seen substantial growth since the pioneering work of [15]. Early studies have focused on the monitoring of univariate processes with constant mean shifts ([15]). With the development of manufacturing and sensing technology, the monitoring of autocorrelated processes ([16], [17], [18], [19], [20]) [21]) and multivariate processes ([22], [23], [24], [25], [26]) has gradually drawn wide attention. This

trend is better summarized by Figure 3, within which popular SPC methods are also labeled.

2.1 Monitoring constant mean shifts

The lower-left block of Figure 3 assumes that the quality $f_t = 1$ holds in Equations (1). Under such a condition, the shift becomes a constant level shift of size δ . Several univariate control charts, such as \bar{x} chart, CUSUM chart and EWMA chart, are designed for this type of shifts.

If the process dimension exceeds one, multivariate control charts should be considered. Given the assumption that $\mathbf{f}_t = \mathbf{1}$ holds in Equation (2), the Hotelling T^2 chart, MCUSUM chart and MEWMA charts are suitable for such applications.

The Hotelling T^2 chart due to [22] has gained wide attention ever since its appearance. Recent discussions are given by [24], [27], [26] and [28]. The Hotelling T^2 chart takes the form:

$$T^2 = (\mathbf{x}_t - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}_t - \boldsymbol{\mu}) > h_H. \quad (3)$$

When the covariance matrix, $\boldsymbol{\Sigma}$, is known, the T^2 statistics follow a chi-square distribution with p degrees of freedom. If the covariance matrix is estimated from samples, the control limit is usually modified to gain a desired in-control ARL (see, e.g., [26], [1]).

However, the Hotelling T^2 chart considers only the most recent observations and is a Shewhart-type control chart. It gives a satisfactory performance for larger shifts, but suffers from poor sensitivity to small shifts. Therefore, the multivariate version of EWMA and CUSUM charts, the multivariate EWMA (MEWMA) chart and the multivariate CUSUM (MCUSUM) chart respectively, have been developed in parallel ([29], [30], [31]).

For processes with high dimensions, dimension reduction techniques are usually adopted to improve charting performance. One of the solutions is to reduce the dimension by utilizing principle component analysis (PCA) ([32], [33], [34], [35]). The basic idea of PCA monitoring is to find efficient principle components (PCs), which are the linear combinations of the original variables, and monitor these PCs instead of the original ones. The number of principle components to be monitored is usually less than that of the process variables.

Recently, [13] proposed to monitor dynamic processes with dynamic PCA. Instead of using fixed principle components, [13] proposed to conduct PCA online, which is more suitable for time-varying shifts. The application of dynamic PCA is also found in [36] and [37].

All the above control charts assume the process is subject to a constant shift. If this assumption is violated, as [6] and [38] demonstrate, an increased number of false alarms will be seen. In the following section, we will introduce some conventional charts that are designed for dynamic shift detection.

2.2 Monitoring dynamic mean shifts

One of the natural solutions to dynamic process monitoring is applying conventional control charts. As excessive false alarms are usually seen due to process dynamics, the control limits of these charts are usually adjusted beforehand.

In the univariate scenario, the practice of detecting dynamic shifts using EWMA charts ([19]) and CUSUM charts ([39], [20]) can be found. Since both types of charts are designed for detecting sustained shifts with known magnitudes, the optimal design of these charts requires the shift magnitude, δ , be known in advance. Therefore, the resulting performance is usually not satisfactory as a single shift magnitude is insufficient to represent a dynamic shift pattern ([40]).

To adapt for time-varying shifts, [41] proposed an adaptive EWMA control chart. The smoothing parameter of the EWMA chart is modified step by step based on the most recent observations. However, the design of the adaptive EWMA chart needs to solve a complex optimization problem, which is beyond the scope of most practitioners. Similar extension of the CUSUM chart is given by [42]. The adaptive CUSUM chart due to [42] updates the reference parameter in the conventional CUSUM chart and tries to capture the true shift magnitudes. The ARL performance of the adaptive CUSUM chart has recently been studied by [43].

As a control chart specific designed for monitoring time-varying shifts in univariate processes, the Cuscore chart was developed from Fisher's efficient score ([44]), and it was later studied by [40, 45-49]. Given the dynamic signals, f_t , the stopping time of a one-sided Cuscore chart is ([48]):

$$T_{SO} = \inf \left\{ t \geq 1 : \max_{1 \leq k \leq t} \left[\sum_{i=t-k+1}^t r_i \left(x_i - \frac{r_i}{2} \right) \right] > h_{Cuscore} \right\}, \quad (4)$$

where $\{r_i = \delta f_i\}$ is the reference signature. It is easy to learn from (4) that in order to set up a Cuscore chart, the shift pattern and magnitude must be known in the design phase.

The GLRT chart is another chart that is designed for detecting dynamic shift patterns in a univariate process ([50]). [4] developed the GLRT chart for monitoring autocorrelated processes and found that the performance of GLRT is superior to either CUSUM or a Shewhart chart on the residuals for various models. However, the implementation of the GLRT chart requires the shift pattern information, f_t , to be known prior to design. The magnitude of the shift, μ , is replaced by its maximum likelihood estimator. The downside of this procedure is its demand for intensive computation since it cannot be expressed in a recursive form. One method suggested by [4] is to apply a sliding window with a fixed size to reduce the computational demand. The shift magnitude is therefore estimated from the observations covered by the sliding window.

Lately, the RFCuscore chart proposed by [40] has suggested a simple solution to detecting dynamic shifts in univariate processes. Compared with the aforementioned two charts, the RFCuscore chart has further released the requirement for prior information about the process. In the RFCuscore chart, the absolute value of the latest observation, $|x_t|$, is treated as an estimation of the current shift. The resulting chart can be implemented in a recursive form like the conventional CUSUM and Cuscore charts. However, the estimation of dynamic shifts using $|x_t|$ is easily contaminated by process noises. [40] summarized that RFCuscore and Cuscore are better than the GLRT in detecting small mean changes, and RFCuscore is quicker than Cuscore when the mean change is large.

Similar to the extension of CUSUM and EWMA charts to monitor univariate processes with dynamic shifts, the T^2 chart, MCUSUM and MEWMA chart can be implemented by ignoring the dynamics in process shifts.

In an endeavor to monitor feedback-controlled processes, [51] proposed a U_0 chart and a U_∞ chart. As time-varying shifts are exhibited in feedback controlled processes, the author identified two snapshots of the dynamic shifts, \mathbf{f}_0 and \mathbf{f}_∞ , which are believed to be important to fault detection. The quantity \mathbf{f}_0 is the direction of the process shift in the transient stage and \mathbf{f}_∞ is the shift direction when the process enters its steady state. The U_0 chart and U_∞ chart, which are given by:

$$U_0 = \mathbf{f}_0 \boldsymbol{\Sigma}^{-1} \mathbf{x}_t, \quad (5)$$

and

$$U_\infty = \mathbf{f}_\infty \boldsymbol{\Sigma}^{-1} \mathbf{x}_t, \quad (6)$$

respectively, are optimized for detecting the two specific shifts. However, as the real shift direction keeps changing, none of the charts is uniformly better than others.

To improve the efficiency of a directionally variant chart with unknown shifts, [52] proposed to use both directionally variant and invariant charts simultaneously. In their example, the vector, \mathbf{V}_t , contains the largest ten principle components of a forging machine. Directionally variant charts are designed to detect pre-known process faults and a directionally invariant chart is used to detect unknown and general process faults. However, the establishment of the directionally variant charts requires the assumption that some pre-known faults are more frequently encountered than others, this information may still be difficult to obtain in practice. Furthermore, the assumed shifts, once they occur, should be a constant over time. Otherwise, the usefulness of the directionally variant charts will be degraded.

In order to improve the performance in detecting dynamic shifts in multivariate processes, [53] proposed an autoregressive (AR) chart. By collecting L successive historical observations, the AR-chart first forms a L -dimensional vector,

$\mathbf{X}_t = [x_t, x_{t-1}, \dots, x_{t-L+1}]^T$, then monitors the vector by Hotelling's T^2 chart. The work was further extended by [5] to a dynamic T^2 chart to monitor feedback-controlled processes. The idea of using lagged observations for monitoring was also addressed by [54].

3 New extensions

One noticeable phenomenon that differentiates a univariate process from a multivariate process is the observable failure patterns, which define the way in which process variables behave when a failure occurs. As there is only one response variable in a univariate process, its shift pattern is usually simple. In a multivariate process, however, the pattern is much more complicated. Each process fault could lead to a different number and combination of variables to deviate. For example, in the aforementioned DRIE process, a shift in etching/deposition ratio would lead to deviations in trench profiles, but not uniformity; while a shift in gas pressure has an impact on uniformity but not trench profiles. Furthermore, an increase in platen power can result in an increase in both etching rate and selectivity. Obviously, different physical failures are reflected by different quality characteristics. If a failure is known to have happened in the gas flow, the wafer's uniformity should be checked more carefully than other variables. Therefore, monitoring and putting emphasis on the appropriate variables will improve charting performance.

Depending on the sensitivity to a specific shift, a control chart can be classified as either a directionally variant or a directionally invariant chart. A control chart that is designed to detect shifts along a particular direction is a directionally variant chart. For example, in order to gain fast detection of platen power shifts in the DRIE process, a chart that monitors a weighted sum of all variables but puts more weight on the etching rate and the selectivity is more sensitive than a chart that treats all variables equally. However, this chart is undoubtedly insensitive to gas pressure shifts, as the charting variables are not influenced by gas pressure. Generally, a directionally variant is usually favored in detecting known shifts. While if an unexpected shift in other directions indeed occurs, the chart will perform worse than a general chart. Likewise, a control chart that has no prior assumption of shift direction and is designed for general process failures is called a directionally invariant chart ([26]). A directionally invariant chart has good performance in detecting general failures with large shift magnitudes but not a specific failure of interest.

In this section, we propose an adaptive T^2 chart to monitor multivariate processes. The basic idea is to make use of the predictability of a shift. First, a forecasting algorithm is utilized to estimate shift directions. Then, the adaptive T^2 chart, which is a directionally variant chart, will adjust its reference vector and maximize its detection power for the predicted shift.

Let \mathbf{x}_t be a vector of observations sampled from a multivariate process at step t . The vector follows a p -dimensional normal distribution with mean $\boldsymbol{\mu}$ and variance $\boldsymbol{\Sigma}$, $\mathbf{x}_t \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Without loss of generality, we assume $\boldsymbol{\mu} = \mathbf{0}$ when the process is in-control. In the event of any physical failure, the mean of the process shifts to a new position, \mathbf{d}_t . The statistic, \mathbf{d}_t , is a time-varying statistic that reflects the dynamic shifts of the process. The following hypothesis illustrates the concern of the process status:

$$\begin{cases} H_0 : \boldsymbol{\mu} = \mathbf{0} \\ H_1 : \boldsymbol{\mu} = \mathbf{d}_t \end{cases}, \quad (7)$$

The log-likelihood ratio of the previous hypothesis is a powerful statistic for testing whether the process is in-control. Therefore, we construct a control chart based on the log-likelihood ratio:

$$T_{AT2}^2 = \mathbf{d}_t^T \boldsymbol{\Sigma}^{-1} \mathbf{x}_t - \frac{1}{2} \mathbf{d}_t^T \boldsymbol{\Sigma}^{-1} \mathbf{d}_t > h_{AT2}. \quad (8)$$

We define the above procedures an adaptive T^2 (AT2) chart. The new charting statistic subscribes the shifts of interest by a time stamp. By continuously updating \mathbf{d}_t , the chart adjusts itself at each step to maximize its detection power for shift \mathbf{d}_t . The resulting performance is expected to be optimized.

A close examination of (8) reveals that the prior knowledge, \mathbf{d}_t , plays an essential role in determining the performance of the chart. However, in industrial practices, the occurrence of physical failures is rarely known in advance. The only way to obtain information about \mathbf{d}_t is to use forecasting algorithms.

In general, a forecasting algorithm is either model-based or model-free. A model-based algorithm involves fitting an ARMA(p, q) model to the dataset for each stream first, then obtaining the one-step-ahead estimations based on the model and treating them as the true values ([55], [53]). However, the performance of model-based forecasting depends heavily on the accuracy of the time series model. Poor estimates of model parameters will lead to poor forecasting accuracy. A model-free method does not require an explicit fitting of any specific models. As suggested by [56], the EWMA statistic is, in many cases, a good approximation of time series models. [9] successfully utilized an EWMA-base method in intensity forecasting in a plastic product manufacturing station. In addition, the EWMA procedure has a simple form and good interpretability. Therefore, EWMA forecasting will be utilized in this chapter for mean shift estimation.

In the EWMA forecasting procedure, the recursive updating of \mathbf{d}_t is achieved by calculating the weighted average of the latest observation and the previous estimation:

$$\mathbf{d}_t = \lambda \mathbf{x}_t + (1 - \lambda) \mathbf{d}_{t-1}, \quad (9)$$

where λ is a smoothing parameter. The above modeling procedure is analogous to the multivariate EWMA

procedure for monitoring multivariate applications (see [26] and the references therein).

The smoothing parameter in (9), which satisfies $0 \leq \lambda \leq 1$, determines the spread of weights over the most recent and historical observations. A large λ gives a higher emphasis to the most recent observation. Therefore, changes in the process would be captured quickly. However, the resulting predicted series may be easily contaminated by noises. Conversely, a small λ makes the EWMA forecasting robust to process noises but insensitive to real process shifts. The impact of λ on the performance of the adaptive T^2 chart will be analyzed in later sections.

The philosophy of the adaptive T^2 procedure can be illustrated by a radar example. The Hotelling T^2 chart performs like a global-wised radar that tries to scan the full horizon for any abnormal signals, as shown in Figure 4 (a). The conventional directionally variant chart concentrates on only one part of the circle and performs like a specific radar, as shown in Figure 4 (b). However, the adaptive T^2 chart performs like a smart tracking radar. As shown in Figure 4 (c), it starts from a specific direction, and keeps tracking the most likely suspect by changing its beaming direction.

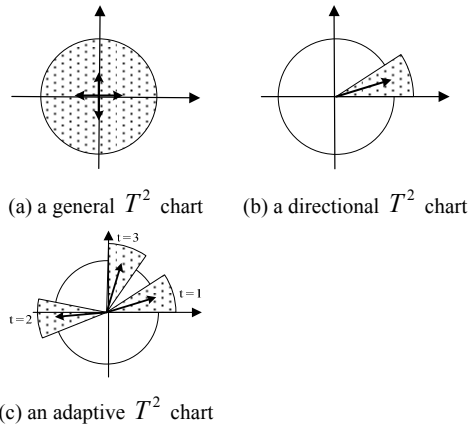


Figure 4. The philosophy of different control charts.

It is also interesting to consider two extreme cases of the adaptive T^2 chart. If the smoothing parameter is chosen as $\lambda = 1$, the equality $\mathbf{d}_t = \mathbf{x}_t$ always holds, and the predicted sequence becomes identical to the observed sequence. The adaptive T^2 procedure in Equation (8) would reduce to

$$T_{AT2}^2 = \mathbf{x}_t^T \Sigma^{-1} \mathbf{x}_t / 2, \quad (10)$$

which is equivalent to the Hotelling T^2 chart. If, instead, $\lambda = 0$, it results in $\mathbf{d}_t = \mathbf{d}_{t-1} = \dots = \mathbf{d}_0$. The predicted shift direction remains constant as the initial value. The adaptive procedure would reduce to

$$T^2 = \mathbf{d}_0^T \Sigma^{-1} \mathbf{x}_t - \mathbf{d}_0^T \Sigma^{-1} \mathbf{d}_0 / 2, \quad (11)$$

which is equivalent to a directionally variant T^2 chart that is designed for a single specific shift, \mathbf{d}_0 . In general, the adaptive T^2 chart takes the value $0 < \lambda < 1$; it is then expected to maintain the advantages of both directionally variant and invariant charts, and give good overall charting performance.

According to [31], the ARL performance of an MEWMA chart depends on the process mean, $\boldsymbol{\mu}$, and covariance matrix, Σ , only through the value of the following noncentrality parameter (NCP)

$$c = \boldsymbol{\mu}^T \Sigma^{-1} \boldsymbol{\mu}. \quad (12)$$

It can be proved that the ARL performance the adaptive T^2 chart depends on the mean vector and covariance matrix only through the NCP. This leads to a much easier design guideline for the AT2 chart.

Figure 5 shows the optimal smoothing parameter for different design parameters. As is seen, the optimal λ increases with noncentrality parameter. Practitioners can choose the optimal settings based on this figure easily. More results are given in [57].

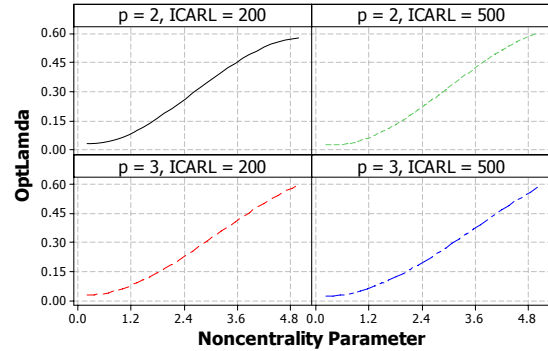


Figure 5. Optimal smoothing parameters.

4 Performance study

To better understand the performance of the adaptive T^2 chart, we apply the chart to a multivariate process with sustained shifts and investigate its performance. Without loss of generality, we assume a bivariate process, $\mathbf{x} = [x_1, x_2]^T$, that has the following covariance structure:

$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

That is, no correlation exists between the two variables. Furthermore, we assume the mean of the process is zero when it is in-control. If \mathbf{x} has a general covariance matrix, the transformed variable $\Sigma^{-1/2} \mathbf{x}$ has a zero mean and an identity covariance structure when the process is in-control, and a mean of $\Sigma^{-1/2} \boldsymbol{\mu}$ and an identity covariance structure when the process is out-of-control ([58]). As the general Hotelling T^2 chart (denoted as GT2) is a popular scheme for monitoring multivariate processes with general failures, we will compare it with the adaptive T^2 chart in terms of their ARL performance. For fair comparison, the in-control ARL of both charts are forced to be roughly 200. Each ARL value is obtained by running at least 10,000 replicates via Monte Carlo simulations.

Two shift patterns, which correspond to two different types of physical failures, are considered in the simulation: shifts in x_1 , and shifts in both variables. The noncentrality parameter, c , changes from zero to

three to cover both small and large shifts. Simulation results are shown in Figure 6.

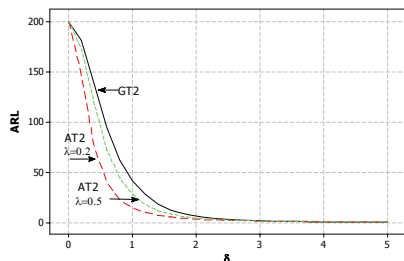


Figure 6. Performance comparison between GT2 and AT2 charts.

As is seen from Figure 6 that when the smoothing parameter, λ , takes the values 0.2, the AT2 chart outperforms the GT2 chart for all shifts less than 2.4. This range contains both small and moderate shifts. The performance of the AT2 chart deteriorates only when the shift magnitude becomes large. This obviously shows the power of the AT2 chart in detecting small process shifts. For small shifts, the EWMA prediction can easily capture the shift trend by smoothing historical observations. Therefore, the AT2 chart is powerful in detecting such shifts. When the shift magnitude is large, due to the averaging effect of the EWMA equation, the prediction sequence is slowed down. Therefore, the AT2 chart is slightly inferior to the GT2 chart.

Furthermore, the performance of the AT2 chart in detecting large shifts can be improved by adjusting the smoothing parameter, λ . When $\lambda=0.5$ is utilized, the AT2 chart performs better than or close to the GT2 chart for both small and large shifts. However, increasing the smoothing parameter makes the predictions less accurate when the shift size is small. Therefore, although the performance of the AT2 chart for small shifts with $\lambda=0.5$ is superior to that of the GT2 chart, it is inferior to the AT2 chart when $\lambda=0.2$ is utilized.

5 Conclusions

Both univariate and multivariate dynamic processes are widely seen in industrial practices. However, the charting techniques designed for monitoring time-varying shifts usually rely on certain assumptions and conditions. In this paper, we illustrate the development trend of SPC, and provide a literature review of the charting techniques for detecting time-varying shifts. The advantageous and limitations of these methods are identified. The results can serve as a guideline for practitioners to choose specific charts for practical applications.

An adaptive T^2 chart has been proposed as an extension to conventional methods. The purpose of the adaptive T^2 chart is to handle dynamic shift patterns in multivariate processes. The newly proposed chart features monitoring a directionally variant statistic and updating its reference vector repeatedly via exponentially weighted moving average (EWMA) forecasting. Therefore, its detection power is maximized

at each step with respect to the predicted shifts. It is shown that the average run length (ARL) performance of the adaptive T^2 chart depends on the process mean and covariance matrix only through the value of the noncentrality parameter of the charting statistic. In addition, the adaptive T^2 chart is flexible in design; its smoothing parameter can be tuned so that its performance over a desired shift range can be improved.

The current implementation of the adaptive T^2 chart is carried out based on EWMA-based or oscillated-EWMA-based forecasting methods. We believe that the EWMA forecasting is not a method that can be globally utilized. More advanced and accurate methods are required to further improve the performance of the adaptive T^2 chart.

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