

Machine Learning Approaches for Statistical Process Control

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Abstract: Machine learning approaches are widely used in different applications, including the ones involving statistical process control (SPC). In a traditional SPC problem (e.g., online monitoring of a production line), a small set of in-control (IC) process observations is routinely collected before online process monitoring for estimating certain parameters of the IC process distribution. This dataset, however, does not contain any out-of-control (OC) process observations. Thus, supervised machine learning methods would be inappropriate to use in such cases since they require a training dataset that contains both IC and OC process observations. To overcome this difficulty, some machine learning methodologies specific for SPC have been developed based on one-class classifications, artificial contrast, real-time contrast, transparent sequential learning, and more. This article provides an overview on these methods. Copyright © 2017 John Wiley & Sons, Ltd.

1. Introduction

Machine learning methods are widely used in practice these days. Their basic idea is to approximate a real-world problem by a computer algorithm after learning the data structure of the problem from a training dataset (Aggarwal, 2018; Hastie et al., 2001). In recent years, a number of machine learning methods have also been developed specifically for statistical process control (SPC). This paper gives an overview on these methods.

SPC charts are originally developed for monitoring production lines in the manufacturing industry for quality control purposes (Qiu, 2014). Monitoring of a production line can be divided into two phases. When the production line is first installed, we usually let it to produce a small batch of products, and then an SPC chart is used to check whether the observed quality variables measured from the products meet the designed requirements. If the answer is negative, then the production line needs to be adjusted and then another small batch of products is produced. This control-and-adjustment process continues until the production line is determined to be in-control (IC). This phase of process monitoring is called Phase I SPC in the literature. After Phase I SPC, the production line should be IC, and it is usually required to produce a small batch of products to generate an IC data of the quality variables. From the IC data, the IC process distribution or some of its parameters can be estimated for the next phase of process monitoring, called Phase

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II SPC, during which the production line keeps producing products that are sampled regularly, the observed quality variables collected from the sampled products are monitored by a control chart simultaneously, and the production stops once a shift in the process distribution is detected by the control chart. If there is no further specification, this paper focuses on Phase II SPC (i.e., online process monitoring). For discussions about Phase I SPC, see papers such as Capizzi and Masarotto (2013), Jones-Farmer et al. (2013), and the references cited therein.

Traditional SPC charts, including the Shewhart (Shewhart, 1931), cumulative sum (CUSUM) (Page, 1954), exponentially weighted moving average (EWMA) (Roberts, 1959), and change-point detection (CPD) (Hawkins et al., 2003) charts are developed based on the assumptions that IC process observations at different time points are independent and identically distributed with a parametric (e.g., normal) IC distribution. Besides production lines, SPC charts have been used widely for monitoring data streams in applications such as environment monitoring and disease surveillance, and the assumptions mentioned above are rarely valid in these applications (Yang and Qiu, 2020; Zhang et al., 2015b). In the SPC literature, it has been well demonstrated that traditional SPC charts would be unreliable to use in cases when their model assumptions are violated (Qiu and Hawkins, 2001; Qiu and Xiang, 2014). So, many more flexible SPC charts have been developed in recent years for cases when process observations are serially correlated (Apley and Tsung, 2002; Capizzi and Masarotto, 2008; Qiu et al., 2020), the IC process distribution changes over time (Qiu and Xiang, 2014, 2015; Qiu and You, 2022; Qiu, 2024), and/or the IC process distribution cannot be described well by a pre-specified parametric distribution family (Chakraborti and Graham, 2019; Qiu, 2018).

Besides the control charts discussed above, a number of SPC charts based on machine learning approaches (e.g., random forest) have been developed in the literature (Megahed and Jones-Farmer, 2013; Qiu, 2020; Weese et al., 2010; Zhang et al., 2015a). An attractive feature of such methods is their flexibility since they usually do not require restrictive model assumptions explicitly when constructing their decision rules. However, supervised machine learning approaches (e.g., artificial neural networks and support vector machines) can hardly be applied to a traditional SPC problem (e.g., online monitoring of a production line) directly, since they require a training dataset that contains both IC and out-of-control (OC) process observations, while the IC data collected before online process monitoring in SPC can be used as a training dataset but it contains IC process observations only as discussed earlier. To overcome this difficulty, a number of novel ideas have been suggested to construct SPC charts based on machine learning approaches, including the one-class classification (OCC) (Sun and Tsung, 2003), artificial contrast (Tuv and Runger, 2003), real-time contrast (Deng et al., 2012), and transparent sequential learning (Qiu and Xie, 2022) methods. These methods and some of their modifications will be introduced in the next several sections. More specifically, Section 2 introduces some SPC charts based on OCC and support vector machines. Section 3 discusses the ideas of artificial contrast and real-time contrast and how they can be used for online process monitoring. The control chart based on transparent sequential learning for monitoring processes with correlated data is described in Section 4, along with its generalized version for monitoring dynamic processes with correlated data. Section 5 concludes the article with several remarks.

2. Process Monitoring by One-Class-Classification

Because the IC data collected before online process monitoring in a traditional SPC problem do not contain any OC process observations, supervised machine learning approaches cannot be used directly. In the literature, several SPC methods based on one-class OCC algorithms have been developed, which are described briefly in this section.

Let $\mathbf{X} = (X_1, X_2, \dots, X_p)'$ be a vector of p quality variables and $\mathcal{X} = \{\mathbf{X}_{-m+1}, \mathbf{X}_{-m+2}, \dots, \mathbf{X}_0\}$ be the IC data collected before online process monitoring. Sun and Tsung (2003) suggested a support vector data description (SVDD) for \mathcal{X} based on the support vector machine (SVM) algorithm (Vapnik, 1995), and then used it for online process monitoring. The basic idea of this approach is that a hypersphere boundary with the shortest radius is first computed

for \mathcal{X} using SVDD, and then a future process observation is claimed to be IC if it is located within the hypersphere boundary and OC otherwise. Details of this method are given below.

Let \mathbf{O} be the center of the hypersphere boundary, and R be its radius. Then, \mathbf{O} and R can be computed by using the following Lagrange function:

$$L(\mathbf{O}, R, \alpha_1, \dots, \alpha_m) = R^2 - \sum_{i=1}^m \alpha_i [R^2 - \langle (\mathbf{X}_{-m+i} - \mathbf{O}), (\mathbf{X}_{-m+i} - \mathbf{O}) \rangle], \quad (1)$$

where $\{\alpha_i \geq 0, i = 1, 2, \dots, m\}$ are the Lagrange multipliers satisfying the condition that $\sum_{i=1}^m \alpha_i = 1$, and $\langle \mathbf{a}, \mathbf{b} \rangle$ denotes the inner product of the vectors \mathbf{a} and \mathbf{b} . From (1), it can be checked that

$$\mathbf{O} = \sum_{i=1}^m \alpha_i \mathbf{X}_{-m+i},$$

and $\{\alpha_i\}$ are the solution of the following maximization problem:

$$\max_{\alpha_i \geq 0, \sum_{i=1}^m \alpha_i = 1} \sum_{i=1}^m \alpha_i \langle \mathbf{X}_{-m+i}, \mathbf{X}_{-m+i} \rangle - \sum_{i,j=1}^m \alpha_i \alpha_j \langle \mathbf{X}_{-m+i}, \mathbf{X}_{-m+j} \rangle. \quad (2)$$

In (1) and (2), the inner product $\langle \mathbf{a}, \mathbf{b} \rangle$ can be defined by the following Gaussian kernel or other alternative kernels:

$$\langle \mathbf{a}, \mathbf{b} \rangle = \exp\left(\frac{\|\mathbf{a} - \mathbf{b}\|^2}{h}\right),$$

where $\|\cdot\|$ denotes the Euclidean norm, and $h > 0$ is a bandwidth constant. After \mathbf{O} and $\{\alpha_i \geq 0, i = 1, 2, \dots, m\}$ are computed, R can be computed by $R^2 = \langle (\mathbf{X}_{-m+i^*} - \mathbf{O}), (\mathbf{X}_{-m+i^*} - \mathbf{O}) \rangle$, where α_{i^*} is one of the non-zero elements of $\{\alpha_i \geq 0, i = 1, 2, \dots, m\}$. Then, the process under monitoring can be claimed to be OC at time n if the process observation \mathbf{X}_n is located outside the hypersphere boundary, i.e.,

$$\langle (\mathbf{X}_n - \mathbf{O}), (\mathbf{X}_n - \mathbf{O}) \rangle > R^2, \quad \text{for } n \geq 1. \quad (3)$$

There are a few modified versions of the SVDD chart (3) in the literature. For instance, to save computing time in defining the decision rule (3) using the entire IC dataset \mathcal{X} , Sukchotrat et al. (2010) suggested using the k nearest neighbors in \mathcal{X} of the process observation \mathbf{X}_n to generate a decision rule at the current time n . In addition, the related chart using the decision rule (3) is a Shewhart chart since it makes its decision using the observation \mathbf{X}_n only. To reduce the variability of the charting statistic, He et al. (2003) suggested using the average distance between the center \mathbf{O} of the hypersphere boundary and the process observations in a moving window of \mathbf{X}_n to make a decision at n . From the above discussion, the SVDD chart (3) and its modified versions do not accommodate serial data correlation and other data structure explicitly in their construction. Thus, the IC dataset \mathcal{X} needs to be very large in order for them to have a reliable IC performance. To address this issue, Xie and Qiu (2022) suggested a modification for them to have a more effective performance when monitoring processes with serially correlated data, and Xie and Qiu (2023a) suggested another modification for them to have a reliable IC performance when monitoring dynamic processes whose IC distributions could change over time.

3. Process Monitoring by Artificial Contrasts

To address the issue that the IC data collected before online process monitoring usually do not contain any OC process observations and thus a supervised machine learning approach cannot be used directly, Tuv and Runger (2003)

suggested generating some artificial OC process observations (or, artificial contrasts (ACs)) from an off-target (e.g., uniform) distribution. Then, the combination of the IC data and these artificial OC process observations can be used as a training dataset for a supervised machine learning approach (e.g., SVM and random forest (RF)) to generate a decision rule for online process monitoring.

The AC method discussed above is essentially a Shewhart chart since its decision at time n depends on the observation \mathbf{X}_n only once its decision rule is developed. In the SPC literature, it has been well demonstrated that Shewhart charts would not be effective for detecting persistent and small shifts in the process distribution (cf., Qiu, 2014, Section 4.1). To overcome this limitation, Hu and Runger (2010) suggested using the following EWMA chart. Let f_0 and f_1 be the probability density functions of the IC and OC process distributions, respectively, which can be estimated from the training data. Then, the EWMA charting statistic is defined to be

$$E_{AC,n} = \lambda \left[\log \left(\frac{f_1(\mathbf{X}_n)}{f_0(\mathbf{X}_n)} \right) - \tilde{\mu}_0 \right] / \tilde{\sigma} + (1 - \lambda)E_{AC,n-1}, \quad \text{for } n \geq 1, \quad (4)$$

where $E_{AC,0} = 0$, $\tilde{\mu}_0$ and $\tilde{\sigma}$ are the IC mean and IC standard deviation of $\log(f_1(\mathbf{X}_n)/f_0(\mathbf{X}_n))$ that can be estimated from the IC data, and $\lambda \in (0, 1]$ is a weighting parameter. The chart gives a signal at time n when

$$E_{AC,n} > \rho \sqrt{\frac{\lambda}{2 - \lambda}}, \quad (5)$$

where $\rho > 0$ is a constant chosen to achieve a pre-specified value of the IC average run length, denoted as ARL_0 . Note that the quality $\log(f_1(\mathbf{X}_n)/f_0(\mathbf{X}_n))$ in (4) is a log likelihood ratio. Thus, the EWMA chart (4)-(5) is constructed based on the likelihood ratio statistic.

There is an obvious limitation of the charts using ACs that the off-target distribution used for generating the artificial OC process observations may not represent the actual OC process distribution well. To overcome this limitation, Deng et al. (2012) suggested the so-called real-time contrast (RTC) idea, by which the process observations $\{\mathbf{X}_{n-w+1}, \mathbf{X}_{n-w+2}, \dots, \mathbf{X}_n\}$ in the moving window of \mathbf{X}_n at the current observation time n were regarded as OC data and combined with the IC data to form a training dataset for a supervised machine learning algorithm (e.g., RF) to generate a classification rule, where w is the window size. Then, the classification error in the training data by the classification rule could be used as a charting statistic for making a decision about the process status at time n . The motivation of this method is that process observations in the moving window of \mathbf{X}_n should be more similar to the OC process observations, compared to the artificial OC process observations used in the AC methods, especially in cases when a shift has occurred by the time n . However, there could be some observations in the window that are actually IC, which would compromise the effectiveness of the RTC method.

4. Process Monitoring by Transparent Sequential Learning

A machine learning approach often works as a "black box" in the sense that the structure of the observed data is usually not described properly and thus it is difficult to interpret its learning mechanism and the statistical properties of its decision rule. In addition, its performance depends heavily on how well a training dataset represents the population in concern. These features are shared by the control charts discussed in the previous two sections that are constructed based on machine learning algorithms. To overcome these limitations, Qiu and Xie (2022) suggested a general learning framework, called transparent sequential learning (TSL), for online process monitoring, which is described below.

The TSL-based control chart developed in Qiu and Xie (2022) can be used for monitoring a multivariate process $\{\mathbf{X}_n = (X_{n1}, X_{n2}, \dots, X_{np})', n \geq 1\}$ when an initial IC dataset $\mathcal{X}^{(0)} = \{\mathbf{X}_{-m+1}, \mathbf{X}_{-m+2}, \dots, \mathbf{X}_0\}$ is available before

online process monitoring. The process observations are allowed to be serially correlated, and the serial correlation is assumed to be stationary and short-ranged, in the sense that i) $\boldsymbol{\gamma}(s) = \text{Cov}(\mathbf{X}_n, \mathbf{X}_{n-s})$, for $n \geq -m + 1$ and $s \geq 0$, does not depend on n , and ii) $\boldsymbol{\gamma}(s) = 0$ when $s \geq b_{max}$, where b_{max} denotes the time range of serial correlation. These assumptions should be reasonable in applications like production line monitoring in the manufacturing industry. Then, for process monitoring, the IC process characteristics to learn from the IC data are well defined, which include the IC mean $\boldsymbol{\mu}_0$ and the IC covariance matrices $\{\boldsymbol{\gamma}(s), 0 \leq s \leq b_{max}\}$. These quantities catch the major features of the IC process distribution.

The TSL procedure and the related online process monitoring scheme can be described by the diagram in Figure 1. First, the IC parameters $\boldsymbol{\mu}_0$ and $\{\boldsymbol{\gamma}(s), 0 \leq s \leq b_{max}\}$ are estimated by moment estimation from the initial IC data $\mathcal{X}^{(0)}$ collected before online process monitoring. Second, at the current time n during online process monitoring, after the process observation \mathbf{X}_n is collected, it needs to be decorrelated with all previous observations first using the Cholesky decomposition of the estimated IC covariance matrices. Third, a control chart is applied to the decorrelated data at time n . If a shift is detected by the chart, then a signal is given. Otherwise, \mathbf{X}_n is combine with the IC data $\mathcal{X}^{(n-1)}$ at the previous time $n - 1$ to form a new IC data $\mathcal{X}^{(n)}$, i.e., $\mathcal{X}^{(n)} = \{\mathcal{X}^{(n-1)}, \mathbf{X}_n\}$. Fourth, estimates of the IC parameters need to be updated using the updated IC data $\mathcal{X}^{(n)}$, and the process monitoring proceeds to the next time point $n + 1$.

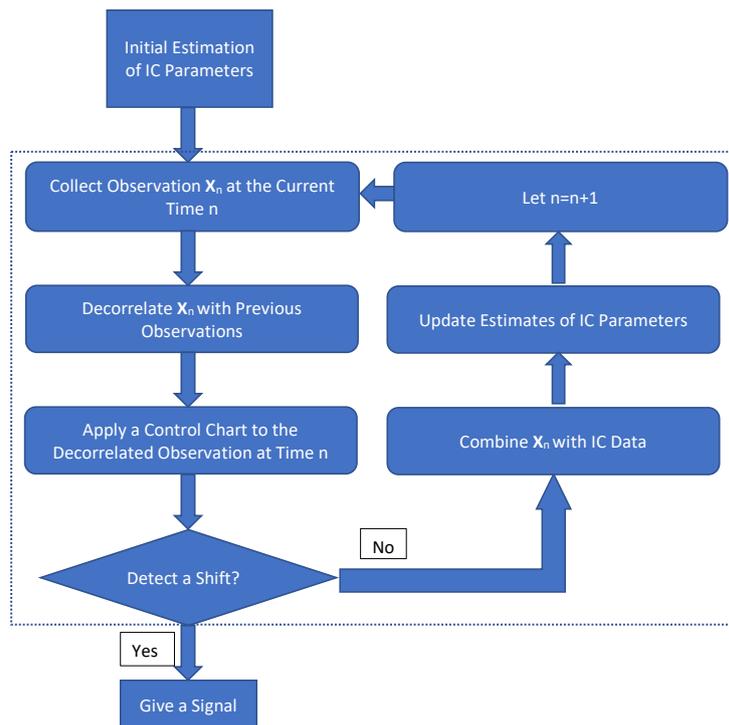


Figure 1. Diagram of the TSL procedure (highlighted by the dotted rectangle) and the related online process monitoring scheme.

From the above description, the TSL learning procedure suggested in Qiu and Xie (2022) is transparent in the sense that its learning objectives (i.e., the IC parameters $\boldsymbol{\mu}_0$ and $\{\boldsymbol{\gamma}(s), 0 \leq s \leq b_{max}\}$) are well defined and statistical properties of its learned objectives can be derived under some regularity conditions. It is sequential in the sense that the IC data keep being expanded and the estimates of the IC parameters keep being updated during online process

monitoring. The TSL-based online process monitoring scheme can accommodate serial data correlation when the autocorrelation is stationary and short-ranged. It does not require a pre-specified parametric expression to describe the IC process distribution if a nonparametric control chart is used for monitoring the decorrelated data.

There are a few generalizations of the TSL-based online process monitoring scheme discussed above. Xie and Qiu (2023b) generalized the monitoring scheme in two major aspects. First, the new method can monitor dynamic processes whose IC distributions could change over time. Second, the serial data correlation is not required to be stationary, although it is still assumed to be short-ranged. Xie et al. (2023) suggested a generalization for monitoring high-dimensional dynamic processes based on sequential principal component analysis. Xie and Qiu (2023c) suggested a general data transformation procedure for robust online process monitoring using parametric control charts. These generalizations and/or modifications greatly broaden the applications of the TSL-based online process monitoring scheme.

5. Concluding Remarks

In the previous several sections, we have discussed several types of machine learning approaches developed recently for online process monitoring. The methods discussed in Section 2 are obtained by modifying the regular SVM approach, which is a supervised machine learning algorithm, for one-class classification. The methods discussed in Section 3 are developed by generating artificial OC process observations, either from an off-target distribution or from a window of the current observation time, so that a supervised machine learning algorithm (e.g., RF) can be used for creating a decision rule. These two types of methods are both adapted from the existing machine learning algorithms that cannot take into account specific data structures (e.g., serial data correlation and time-varying IC process distribution) explicitly in their method construction. Thus, they may not be effective for monitoring processes with complex data structure (Xie and Qiu, 2022, 2023a). The TSL-based methods discussed in Section 4 can be regarded as generalizations of the self-starting process monitoring schemes in the SPC literature (Hawkins, 1987). While traditional self-starting monitoring schemes are constructed based on the assumptions that IC process observations are independent and identically distributed with a parametric IC distribution, the TSL-based monitoring schemes have avoided these model assumptions.

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