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Research paper

Optimal false alarm controlled support vector data description for multivariate process monitoring

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ABSTRACT

One-class classification plays a key role in the detection of outliers and abnormalities. Recently, several attempts have been made to extend the application of one-class classification techniques to statistical process control problems, where many of these one-class classification-based approaches have used a support vector data description algorithm. The monitoring statistics for a support vector data description-based control chart are sufficiently defined. However, the control limits are not obvious because the procedure used to derive the control limit does not include a method for controlling the false alarm rate (i.e., Type I error rate), which clearly limits its use in process monitoring. In this study, we propose a new multivariate control chart based on a technique for optimal false alarm-controlled support vector data description, which minimizes the radius of a spherically shaped boundary so that it includes the normal data that are equal to an assigned constant value. By modifying this constant value, users can precisely control the proportion of abnormal data determined by the spherically shaped boundary, which equals the expected Type I error rate. We demonstrated the usefulness of the proposed charts in experiments with simulated data and real process data based on a thin film transistor–liquid crystal display.

1. Introduction

Statistical process control (SPC) is one of the most widely used methods for quality control [1]. The basic objective of SPC is the rapid detection of any abnormal changes in a process that could lead to quality deterioration and the production of defective units [2,3]. An important technique in SPC involves employing a control chart to monitor a process over time to maintain a normal state. This monitoring process relies on statistics such as the average, range, standard deviation, moving average, proportion, and sample counts. Another component of a control chart is the control limit, which is generally calculated based on the probability distribution of the monitoring statistic. The control limit is used to determine whether the process is normal. If the monitoring statistic exceeds (or falls below) the control limit, a process abnormality is detected so an alarm can be issued. In general, control charts are constructed in two phases, where Phase I analysis separates the normal observations from the historical data and uses them to calculate the control limits, and these limits are then used in Phase II analysis to monitor the process [4].

Hotelling proposed a multivariate control chart to address the limitations of univariate controls in the multivariate settings encountered in many modern systems [5]. Hotelling's T^2 chart (T^2 chart) is one of the most popular multivariate control charts for efficiently monitoring multivariate processes [6,7]. The monitoring statistic for a T^2 chart is:

$$T^2 = (x - \bar{x})^T \Sigma^{-1} (x - \bar{x}), \quad (1)$$

where $\bar{x}$ is a sample mean vector and Σ is a sample covariance matrix estimated from Phase I data. The T^2 statistic is a scaled distance between the sample mean and an observation where the degree of scaling is determined by a covariance matrix. When an observation vector x follows the multivariate normal distribution, the T^2 statistic follows an F distribution [8]. Hence, the control limit of a T^2 chart is determined as the $1-a$ quantile of the F distribution to achieve the desired Type I error rate α. Studies have shown that if the underlying distribution is multivariate normal, the T^2 charts can optimally control the Type I and Type II error rates [9]. T^2 charts are effective in traditional manufacturing processes that generate normally distributed independent data, but these charts are incapable of processing the large streams of complex high-dimensional data that are found frequently in modern systems [10].

Modified T^2 charts have been developed to address these shortcomings by incorporating variable selection techniques such as a forward-selection algorithm or a least absolute shrinkage and

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selection operator [11,12]. However, when the process data do not follow a multivariate normal distribution, T^2 charts perform poorly at controlling the Type I and Type II error rates [4,13–15], where this occurs frequently in modern manufacturing systems [16]. Numerous data-driven control charts have been proposed to overcome the limitations posed by this distribution assumption [2,17,18,19,20–23] but no consensus has been reached on the best control chart for nonnormally distributed processes.

Recently, some studies have investigated the use of one-class classification methods as an alternative to traditional control chart techniques. Tuerhong et al. [21] proposed a hybrid novelty score-based control chart that uses monitoring statistics calculated based on the distance to local observations as well as the distance to the convex hull constructed by its neighbors. Tuerhong and Kim [15] compared eight novelty scores in terms of their control chart performance (e.g., average run length; ARL). Sukchotrat et al. [2] proposed k-nearest neighbor-based control charts, and Gani and Limam [24] presented k-means-based control charts, where these studies used modified versions of the k-nearest neighbor and k-means algorithms for one-class classification to derive the degree of abnormality for control charts. Among the various one-class classification-based approaches, the support vector data description (SVDD) algorithm proposed by Tax and Duin [25] has been used widely [26]. Sun and Tsung [27] proposed a kernel distance-based chart (K chart) where the monitoring statistics are the distances between the sample points and the center of a boundary, and the radius of the boundary determines the control limits. Sun and Tsung [27] showed that K charts outperformed the T^2 charts when the data distribution departed from normality. Kumar et al. [28] proposed a robust K chart based on the normalized monitoring statistics obtained from a robust support vector algorithm, which makes the decision boundary less sensitive to noisy observations. Cho et al. [29] proposed using the SVDD algorithm for monitoring a microrobotic system and detecting abnormal calibration conditions. Moreover, an improved design of SVDD-based charts using kernel principal component analysis (PCA) was proposed by Huang and Yan [22], where they successfully employed the SVDD algorithm to formulate control chart problems, but these charts still had limitations because the control limit for managing the rate of false alarms was unclear.

In the present study, we propose a multivariate control chart based on optimal false alarms controlled by the SVDD algorithm. The data description algorithm minimizes the radius of a spherically shaped boundary so it includes the normal data that are equal to an assigned constant value. By adjusting this constant value, users can precisely control the proportion of Phase I normal data delimited by the boundary, which allows the proportion of abnormal observations to match exactly with the expected Type I error rate in a Phase I process. The control chart monitors the distances between observations and the center of the decision boundary as monitoring statistics. The radius of the decision boundary determines the control limit of the control chart. The control chart can monitor a nonlinear and multimodal manufacturing process because the data description method using the kernel function can describe data with a flexible decision boundary.

The remainder of this paper is organized as follows. In Section 2, we describe the original SVDD-based control chart and its limitations. In Section 3, we explain the proposed control chart based on the optimal false alarm controlled by the SVDD algorithm. In Section 4, we present the results obtained when simulation data were used to demonstrate the effectiveness of the proposed optimal false alarm controlled by the SVDD-based control chart. In Section 5, we describe a case study where an actual thin film transistor–liquid crystal display (TFT–LCD) process was used to demonstrate the applicability of the proposed method. Finally, in Section 6, we give our conclusions and suggestions for future research.

Table 1
List of notations used in this study.

Term	Definition
D	Data set
a	Center of hypersphere
R	Radius of hypersphere
N	Number of data points in D
N_s	Number of support vectors in D
p	Number of features in D
i	Index of data point $i = 1, 2, \ldots, N$
j	Index of data point $j = 1, 2, \ldots, N$
k	Index of data point $k = 1, 2, \ldots, N$
x_i	i th observation in D
ξ_i	i th slack variable for SVDD
f	SVDD parameter for controlling the proportion of abnormal points
α	OSVDD parameter for controlling the proportion of abnormal points
C	Regularization parameter for SVDD ($C = 1/f{\cdot}N$)
e	vector with ones in all components
y	Dual decision variable
K	Kernel function
φ	Kernel mapping function
Q	Kernel mapping matrix
S	Width of the radial basis function
M	Big M: a large constant value
ε	A small constant value
μ	Mean vector
Σ	Covariance matrix
I	Identity matrix
B	Set of observations involved in an optimized decision boundary

2. SVDD

In this section, we describe the previously proposed data description method called SVDD for constructing a flexible decision boundary to detect abnormal points. Table 1 shows the notations used in this study.

SVDD is an extension of support vector machines for solving one-class classification problems [25]. SVDD produces a closed boundary around data D, which is called a hypersphere. A hypersphere is characterized by center a and radius R, which is the distance from a to the boundary. Let $x_i = [x_{i1}, x_{i2}, \ldots, x_{ip}]^T$, for $i = 1, 2, \ldots, N$ be a sequence of p-variate training observations. The aim of the SVDD is to find an optimal hypersphere with a minimum volume while maximizing the training observations captured by this hypersphere. To achieve this goal, the SVDD algorithm solves the following optimization problem:

$$\underset{a,R,\xi}{Minimize} R^2 + C\sum_{i=1}^{N}\xi_i, \tag{2}$$

$$Subject\ to \|x_i - a\|^2 \le R^2 + \xi_i,\ i = 1, 2, \ldots, N, \tag{3}$$

where $\xi_i \ge 0$ is the slack variable that allows x_i to be outside the hypersphere and $C(>0)$ is a regularization parameter that balances a tradeoff between the volume of the hypersphere and the errors allowed. We can avoid an overfitted hypersphere by allowing errors. Tax and Duin [25] proposed determining the best C by controlling f, which is the proportion of data points outside the decision boundary:

$$C = \frac{1}{fN}, \tag{4}$$

where N is the number of observations.