Chapter 1

Introduction

1.1 Control Charts

Control charts are known to be effective tools for monitoring the quality of processes and are applied in many industries. Data occur sequentially in time and often data are reduced to a statistic or two which represent the current state of the process. If the successively observed chart statistics are plotted within the upper and lower control limits (UCL and LCL), the process is deemed *stable* or *in control*. Chart statistics that are plotted outside of the control limits are signals that the process may be *out of control* and corrective action on the process may be needed.

1.2 Phase I vs. Phase II

Statistical process control (SPC) involves the use of control charts (both univariate and multivariate) in two phases. Phase I of the monitoring scheme consists of determining whether or not historical data indicate a stable (or in-control) process. Phase II consists of monitoring future observations using control limits calculated from Phase I to determine if the process continues to be in-control. In Phase I historical data, trends, step changes, outliers and other types of instability can have an adverse effect on the resulting Phase II control limits. So it becomes very important to discover the data points associated with these features prior to calculating the control limits. Control limits based on data coming from unstable (or out-of-control) processes can be inaccurate and reduce the effectiveness of the Phase II scheme. Both phases use control charts but the emphasis in Phase I is process understanding and data cleaning while the emphasis in Phase II is real time process monitoring.

1.3 Robust Estimation

Classical estimation methods for multivariate control charts will not yield appropriate control limits if there is instability in the data. Robust estimation methods have a distinct advantage over classical methods in that they are not unduly influenced by unusual data points. Consequently, they are much more effective in detecting such points and ensuring that the control limits are reasonable. The term *robustness* refers to methods that are insensitive to departures from one's assumptions, which in our case are independence and identically distributed normal data.

Some robust estimation methods such as the minimum volume ellipsoid (MVE) or the minimum covariance determinant (MCD) are well suited for detecting outliers because of their high breakdown points. The general idea of the breakdown point is "the smallest proportion of the observations which can render an estimator meaningless" (Hampel et al., 1986; Rousseeuw and Leroy, 1987). In other words, the breakdown point refers to the percentage of "bad" data that can be present before the estimator no longer is accurate for the “good” data. The “good” data simply refer to the data in the majority and the “bad” data refer to the data in the minority. It is desirable to accurately determine which data are bad (if any).

Because of the inherent difficulties in computation of robust estimation methods, many algorithms have been proposed to obtain them. In Chapter 3 we consider the subsampling algorithm to obtain the MVE estimators and the FAST-MCD algorithm to obtain the MCD estimators. Previous studies have not clearly determined which of these two estimation methods is best for multivariate control chart applications. The comprehensive simulation study in Chapter 3 gives guidance for when to use which estimators. Control limits are provided. High breakdown estimation methods based on the MVE and MCD can be applied to a wide variety of multivariate quality control data.

1.4 Profile Monitoring

Due to advances in technology, it is becoming much more common to obtain profiles (a series of data points forming a curve) at each time period that represents the quality state of a process. Profile monitoring consists of a series of data points or a curve (the “profile”) collected at regular time intervals. See Section 1.5 for examples of situations that yield profiles. It combines the idea of fitting regression models with the idea of separating common cause variability from special cause variability over time in quality control. A good introduction to the concept of profile monitoring, and examples of its application can be found in Woodall et al. (2004).

Croarkin and Varner (1982), Stover and Brill (1998), Kang and Albin (2000), Kim, Mahmoud, and Woodall (2003), Mahmoud and Woodall (2004), Wang and Tsung (2005), and

Gupta, Montgomery, and Woodall (2006) all considered monitoring of linear profiles. After fitting the linear profiles, Kang and Albin (2000) proposed a Phase II method to monitor the data with separate control charts for the slope and intercept. However, the statistics for separate charts are correlated and a better method proposed by Kim, Mahmoud, and Woodall (2003) proposed to first center the data. This centering produces more interpretable charts that have uncorrelated statistics with superior properties. Mahmoud and Woodall (2004) focused on Phase I applications and proposed a global F test based on a multiple regression model with indicator variables. They showed that their approach was superior to Phase I methods proposed by Stover and Brill (1998), Kang and Albin (2000) and Kim, Mahmoud, and Woodall (2003). Gupta, Montgomery, and Woodall (2006) evaluated Phase II performance and found the method of Kim, Mahmoud, and Woodall (2003) to be better than that of Croarkin and Varner (1982).

Williams, Woodall, and Birch (2003) gave a broad treatment of nonlinear profile monitoring where separate nonlinear regression models are fit to each profile. The nonlinear model may contain multiple regressors but often the number of parameters is larger than the number of regressors used. Williams, Woodall, and Birch (2003) proposed a Phase I method based on the T^2 statistic to detect outlying profiles. However, the performance of this method was not evaluated in terms of its probability of a signal. Their method does not guarantee a nominal false alarm rate because of the asymptotic properties of the maximum likelihood (ML) estimators of the nonlinear model. Williams et al. (2006a) gave an application of nonlinear profile monitoring to dose-response data.

The idea of these previous methods is to model the linear or nonlinear profiles using some parametric method and then monitor the estimated parameters over time to determine if the profile changes. Our approach builds on this basic idea. Because the parameter estimators in our case may be correlated, it is convenient to monitor them using a multivariate control method such as one based on the T^2 statistic.

The previous work on nonlinear profile monitoring has assumed that the measurements within a profile are independent of each other. This is often an unrealistic assumption in practice for many types of data. For example, profiles may exhibit spatial correlation if they represent measurements of the physical dimensions of an objects. The may exhibit serial correlation if the observations within a profile are collected over time. Therefore, we propose the use of mixed models to monitor the profiles in order to account for the correlation structure within profiles and show using simulation situations when the mixed model approach is preferable. We will focus here on Phase I control chart applications.

1.5 Profile Monitoring Examples

Due to advances in technology, it is now much easier and much more common to obtain large amounts of data. This data explosion has created many different situations where profile monitoring could be applied. We briefly discuss some of the potential applications of profile monitoring. Linear profiles appear to be more common for calibration applications.

For example, Mahmoud and Woodall (2004) used profile monitoring for linear calibration where measurements of compound concentration are obtained by analytical chemistry methods. The obtained curves can be modeled by a linear relationship to ensure that measurement equipment is properly calibrated.

Sahni, Aastveit, and Naes (2005) discussed an example of profile monitoring in food production. They consider the manufacture of mayonnaise and measure the viscosity of the product over time, thus obtaining growth profiles that can be compared to each other to determine the consistency of the product as it ages.

Staudhammer et al. (2005) presented an example where the response of interest is the measured thickness of cut boards in lumber manufacturing. Automated data gathering equipment is able to obtain thousands of thickness measurements for a particular board and the resulting profile exhibits many spikes and trends. They noted that there many other related applications in lumber manufacturing.

Wang and Tsung (2005) considered a data scenario where a visual image of a liquid crystal display of electronic equipment is described by the color intensity of the pixels that make up the image. They summarized the large amount of data with a Q-Q plot and monitored the resulting linear profiles with univariate charts. A defect in the display will result in a non-normal distribution of data points which can be detected by some nonlinear profile among the linear (normal) profiles.

Williams, Woodall, and Birch (2003) considered nonlinear profiles and discussed the particleboard data presented in Walker and Wright (2002). Here the density of a piece of particleboard is measured at equally spaced locations from the top to the bottom of the board. The resulting profile is nonlinear because the density is higher at the edges of the board than in the middle. Nonetheless, it is desirable to determine how similar the boards are to each other and determine if any of them are different from each other.

Williams et al. (2006a) considered the nonlinear profiles of a dose-response curve from a bioassay measuring the impact of a dosage of herbicide on plant growth. A standard bioassay on compounds with known properties is performed each week to ensure consistency of the plants used in other bioassays on compounds with unknown properties. It is desirable that the plants react similarly to the compounds to ensure that comparisons of the compounds will be valid.

Zhou, Sun, and Shi (2006) considered much more complicated profiles that represented the forging cycle of a stamping process. Instead of using a linear or nonlinear model, they used wavelet transforms as an approximation of the profile, then monitored the wavelet coefficients to determine if any of the forging cycles are different from each other.

Woodall et al. (2004) discussed other examples. In all of these described examples, the goal is to determine whether or not the profiles are similar to each other or whether or not they are changing over time.

1.6 Outline of Dissertation

The outline of this dissertation is as follows. In Chapter 2, we review concepts in multivariate data and multivariate quality control methods with primary focus on the T^2 statistic. Chapter 3 covers the first part of our research on high breakdown estimation methods in multivariate quality control that are effective when outliers are present. We also present the results of a simulation study to determine when these methods are preferred.

Profile monitoring is the focus of the rest of the dissertation. Chapter 4 reviews the linear mixed model which we propose as an alternative model to the classical linear model for monitoring linear profiles. It also contains a review of methods proposed in the literature for detecting influential points and outliers in the linear mixed model. The results of extensive simulation studies to evaluate the effectiveness of the linear mixed model approach and an example of the application of the linear mixed model to the calibration data of Mestek, Pavlik, and Suchánek (1994) are shown in Chapter 5. Chapter 6 contains a review of the nonlinear and nonlinear mixed models and their properties and Chapter 7 contains the simulation studies done to evaluate the effectiveness of both the nonlinear and nonlinear mixed model approaches and our proposed method that combines both approaches. In Chapter 7 we also apply the nonlinear mixed model to the dose-response data of Williams et al. (2006a) and to the particle board data of Wright and Walker (2002). Finally, in Chapter 8 we present a summary of our conclusions and discuss open research questions.