

Statistical Monitoring of Nonlinear Product and Process Quality Profiles

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Abstract

In many quality control applications, use of a single (or several distinct) quality characteristic(s) is insufficient to characterize the quality of a produced item. In an increasing number of cases, a response curve (profile), is required. Such profiles can frequently be modeled using linear or nonlinear regression models. In recent research others have developed multivariate T^2 control charts and other methods for monitoring the coefficients in a simple linear regression model of a profile. However, little work has been done to address the monitoring of profiles that can be represented by a parametric nonlinear regression model. Here we extend the use of the T^2 control chart to monitor the coefficients resulting from a parametric nonlinear regression model fit to profile data. We give three general approaches to the formulation of the T^2 statistics and determination of the associated upper control limits for Phase I applications. We also consider the use of nonparametric regression methods and the use of metrics to measure deviations from a baseline profile. These approaches are illustrated using the vertical board density profile data presented in Walker and Wright[1].

KEY WORDS: Multivariate statistical process control; T^2 -chart; Vertical density profile; Nonlinear regression; Functional data; Minimum volume ellipsoid.

1. INTRODUCTION

In statistical process control (SPC) applications, manufactured items are sampled over time and quality characteristics are measured. Often a product's quality can be determined through measuring several characteristics at each sampling interval. Multivariate T^2 control charts and other methods have been developed for this scenario. See, for example, Fuchs and Kenett [2] and Mason and Young [3]. Increasingly, however, a sequence of measurements of one or more quality characteristics are taken across some continuum producing a curve or surface that represents the quality of the item. This curve or surface is referred to as a profile. Woodall, Spitzner, Montgomery, and Gupta [4] give an introductory overview of the emerging field of profile monitoring.

Profile data consist of a set of measurements with a response variable y and one or more explanatory variables $x_j, j = 1, \dots, k$, which are used to assess the quality of a manufactured item. For example, the density profile of a particleboard is measured on a vertical cross-section, which reveals patterns in board density across the depth of the board. Another example is the estimated dose-response curve of a manufactured drug. Once a batch of the drug is produced, several different doses of the drug are administered to subjects and the responses measured. The resultant dose-response curve summarizes the quality of the particular batch of the drug, indicating the maximal effective response, minimal effective response, and the rate in which the response changes between the two (see Williams, Birch, Woodall, and Ferry [5]). In these examples, a single measurement is insufficient to adequately assess quality. Instead, a relationship between two variables, referred to as the profile, should be monitored over time. Profile data is multivariate, but it is not appropriate to apply standard multivariate control chart methods since this leads to overparameterization. It is more efficient to model the structure of the data via regression techniques.

In Phase I analysis, we are concerned with distinguishing between in-control conditions and the presence of assignable causes so that in-control parameters may be estimated for further product or process monitoring in Phase II analysis. If out-of-control observations are included in the estimation of in-control parameters, then the subsequent monitoring procedure will be less effective. Therefore it is imperative in Phase I that abnormal profiles be identified and excluded from further analysis. Further, we seek to identify step or ramp shifts (if any) in the mean profile, so that in-control parameters may be estimated to reflect what would be expected from a stable process.

Profiles can take on several different functional forms, depending on the specific application. For many calibration problems, the profile can be represented by a simple linear regression model (see, e.g., Mahmoud and Woodall [6] and Gupta, Montgomery, and Woodall [7]). Kang and Albin [8] proposed two methods, including a multivariate T^2 control chart, to monitor such profiles. Specifically, we let the subscript i index each individual profile ($i = 1, \dots, m$) in the historical Phase I data. In the simple linear regression case, the i^{th} profile is modeled as

$$y_{ij} = \beta_{i0} + \beta_{i1}x_{ij} + \epsilon_{ij},$$

where y_{ij} is the j^{th} measurement ($j = 1, \dots, n$), ϵ_{ij} is the j^{th} random error, and x_{ij} is the j^{th} value of the explanatory variable corresponding to the i^{th} profile. It is assumed that the values of x_{ij} are the same for all i . This assumption is often reasonable since in many engineering applications product or process profiles are measured at fixed values of the explanatory variable at each sampling stage. Kang and Albin's [8] multivariate T^2 chart is used to monitor simultaneously the β_0 , the y -intercept, and β_1 , the slope. Kim, Mahmoud, and Woodall [9] proposed an alternative approach with better statistical properties such that individual control charts can be used for the y -intercept and slope independently.

In general we refer to any profile that can be modeled by the linear regression function

$$y_{ij} = \beta_{i0} + \beta_{i1}x_{ij1} + \beta_{i2}x_{ij2} + \cdots + \beta_{ik}x_{ijk} + \epsilon_{ij} \quad (1)$$

as a linear profile, where $x_{ijl}, l = 1, \dots, k$, are k predictor variables. The predictor variables can be the original variables themselves or any function of the variables. In matrix notation, we let $\mathbf{y}_i = [y_{i1}, y_{i2}, \dots, y_{in}]'$ be the vector of responses for profile i , $\boldsymbol{\beta}_i = [\beta_{i0}, \beta_{i1}, \dots, \beta_{ik}]'$ be the vector of parameters to be monitored, $\mathbf{x}'_{ij} = [1, x_{ij1}, x_{ij2}, \dots, x_{ijk}]$ be the vector of explanatory variables for item i , and $\boldsymbol{\epsilon}_i = [\epsilon_{i1}, \epsilon_{i2}, \dots, \epsilon_{in}]'$ be the corresponding vector of random errors. After collecting the \mathbf{x}'_{ij} vectors into an $n \times p$ matrix, where $p = k + 1$, as

$$\mathbf{X}_i = \begin{bmatrix} \mathbf{x}'_{i1} \\ \mathbf{x}'_{i2} \\ \vdots \\ \mathbf{x}'_{in} \end{bmatrix}.$$

model (1) can be written in matrix form as

$$\mathbf{y}_i = \mathbf{X}_i\boldsymbol{\beta}_i + \boldsymbol{\epsilon}_i, i = 1, \dots, m.$$

We assume that \mathbf{X}_i is the same for each profile and that the vectors $\boldsymbol{\epsilon}_i$ are independent and identically distributed (i.i.d.) multivariate normal random vectors with mean vector zero and covariance matrix $\sigma^2\mathbf{I}$. For an example of profile monitoring where the covariance matrix is allowed to take on a more general form, see Williams, et al. [5].

Jensen, Hui, and Ghare [10] proposed a control chart based on the F -distribution to monitor the $k + 1$ parameters (coefficients) from a multiple linear regression model for Phase II applications. Given the parameter vector estimator for item i , $\hat{\boldsymbol{\beta}}_i$, and the target parameter vector $\boldsymbol{\beta}_0$, one plots on their control chart the well-known F

statistic

$$F_i = (\hat{\boldsymbol{\beta}}_i - \boldsymbol{\beta}_0)' \mathbf{X}_i' \mathbf{X}_i (\hat{\boldsymbol{\beta}}_i - \boldsymbol{\beta}_0) / (k + 1) s_i^2$$

against i , where $s_i^2 = \sum_{i=1}^n (y_i - \hat{y})^2 / (n - p)$. A Phase I procedure for this general linear case has yet to be developed.

In many cases, however, profiles cannot be well-modeled by a linear regression function. Walker and Wright [1] proposed a nonparametric approach for comparing profiles using additive models. Such models do not have a specific functional form and have no model parameters to estimate, but rather one employs smoothing techniques such as kernel smoothing or spline smoothing to model a profile. Nonparametric regression techniques provide great flexibility in modeling the response. One disadvantage of nonparametric smoothing methods is that the subject-specific interpretation of the estimated nonparametric curve may be more difficult, and may not lead the user to discover as easily assignable causes that lead to an out-of-control signal. Ding, Zeng, and Zhou [11] proposed an alternative nonlinear profile monitoring method based on a two stage process of (1) data reduction from a high-dimensional space to a lower-dimensional subspace and (2) employing the control charts methods described in Sullivan [12].

Often, however, scientific theory or subject-matter knowledge leads to a natural nonlinear function that well-describes the profiles. Hence, an alternative method is to model each profile by a nonlinear regression function. A *nonlinear profile* of an item can be modeled by the nonlinear regression model given generally by

$$y_{ij} = f(\mathbf{x}_{ij}, \boldsymbol{\beta}_i) + \epsilon_{ij}, \quad (2)$$

where \mathbf{x}_{ij} is a $k \times 1$ vector of regressors for the j^{th} observation of the i^{th} profile, ϵ_{ij} is the random error, $\boldsymbol{\beta}_i$ is a $p \times 1$ vector of parameters for profile i , and f is nonlinear in the parameters. The random errors ϵ_{ij} are assumed to be i.i.d. normal random variates with mean zero and variance σ^2 . In many applications, there is only

one regressor ($k = 1$), but there are multiple parameters to monitor ($p > 1$). An example of this form of the model is the 4-parameter logistic model, often used to model dose-response profiles of a drug, given by

$$y_{ij} = A_i + \frac{D_i - A_i}{1 + \left(\frac{x_{ij}}{C_i}\right)^{B_i}} + \epsilon_{ij}, \quad (3)$$

where y_{ij} is the measured response of the subject exposed to dose x_{ij} for batch i , $i = 1, \dots, m$, $j = 1, \dots, n$. In Equation (3), we have $k = 1$ and $p = 4$, giving four parameters to monitor, each parameter having a specific interpretation. For example, A_i is the upper asymptote parameter, D_i is the lower asymptote parameter, C_i is the ED_{50} parameter (the dose required to elicit a 50% response), and B_i is the rate parameter for the i^{th} batch. Another example is the “bathtub” function described in Section 3 where the density of particleboard is measured across the vertical profile. Note that for any given application, the specific form of the nonlinear function, f , in Equation (2) must be specified by the user.

In Section 2 of this paper we give a brief review of nonlinear regression. We introduce the multivariate T^2 statistic in the context of monitoring nonlinear profiles. We then introduce three formulations of the T^2 statistic and discuss the determination of the upper control limits for the corresponding charts. In addition, a control chart to monitor the variance σ^2 in the context of monitoring profile data is proposed. Finally, we discuss a nonparametric regression approach to monitoring the profiles. In Section 3 we illustrate the T^2 control charts and the nonparametric approaches using the vertical density profile data of Walker and Wright [1]. In Section 4 we discuss the effects that autocorrelation in the error terms may have on the analysis. Finally, in Section 5 we discuss potential alternative methods and give directions for future research topics in nonlinear profile monitoring.

2. METHODOLOGY

We begin a Phase I analysis with a baseline dataset consisting of m items sampled over time. For each item i we observe a response y_{ij} and a set of predictor variables \mathbf{x}_{ij} , $i = 1, \dots, m$, $j = 1, \dots, n$, resulting in the quality profile for item i , i.e., $(y_{i1}, \mathbf{x}_{i1}), (y_{i2}, \mathbf{x}_{i2}), \dots, (y_{in}, \mathbf{x}_{in})$. In this section we develop the methodology to analyze the profiles to gain understanding of the product or process in a Phase I setting.

2.1 Nonlinear Model Estimation

For simplicity of notation, we write the scalar model given in Equation (2) in matrix form by stacking the n observations within each profile as $\mathbf{y}_i = (y_{i1}, y_{i2}, \dots, y_{in})'$, $\mathbf{f}(\mathbf{X}_i, \boldsymbol{\beta}_i) = (f(\mathbf{x}_{i1}, \boldsymbol{\beta}_i), f(\mathbf{x}_{i2}, \boldsymbol{\beta}_i), \dots, f(\mathbf{x}_{in}, \boldsymbol{\beta}_i))'$, and $\boldsymbol{\epsilon}_i = (\epsilon_{i1}, \epsilon_{i2}, \dots, \epsilon_{in})'$. The vector form is then given by

$$\mathbf{y}_i = \mathbf{f}(\mathbf{X}_i, \boldsymbol{\beta}_i) + \boldsymbol{\epsilon}_i, \quad i = 1, \dots, m. \quad (4)$$

For the nonlinear regression model given in Equation (4), estimates of $\boldsymbol{\beta}_i$ for each sample must be obtained. This is usually accomplished by employing the Gauss-Newton procedure and iterating until convergence to obtain the maximum likelihood estimates. Upon convergence of the algorithm, the estimated covariance matrix of $\hat{\boldsymbol{\beta}}_i$ is the estimated Fisher information matrix. See Myers [13] or Schabenberger and Pierce [14] for a concise discussion of nonlinear regression model estimation. A more detailed treatment can be found in Gallant [15] and Seber and Wild [16].

Unlike linear regression, the small-sample distribution of parameter estimators in nonlinear regression is unobtainable, even if the errors ϵ_{ij} are assumed to be i.i.d. normal random variables. Instead, asymptotic results must be applied. Seber and Wild [16] give the asymptotic distribution of $\hat{\boldsymbol{\beta}}_i$ and the necessary assumptions and regularity conditions for the asymptotic distribution to be obtained.

2.2 Multivariate T^2 Control Chart

In order to develop the methodology to monitor nonlinear profiles, we first consider the general framework of the multivariate T^2 statistic. Given a sample of m independent observation vectors to be monitored, \mathbf{w}_i ($i = 1, \dots, m$), each of dimension p , the general form of the T^2 statistic in Phase I for observation i is

$$T_i^2 = (\mathbf{w}_i - \bar{\mathbf{w}})' \mathbf{S}^{-1} (\mathbf{w}_i - \bar{\mathbf{w}}), \quad (5)$$

where $\bar{\mathbf{w}} = \frac{1}{m} \sum_{j=1}^m \mathbf{w}_j$ and \mathbf{S} is some estimator of the variance-covariance matrix of \mathbf{w}_i (Mason and Young [3]). We then plot the T_i^2 statistics, $i = 1, \dots, m$, against i and out-of-control signals will be given for any T_i^2 value exceeding an upper control limit (UCL). For determining the statistical properties of the T^2 -chart it is usually assumed that each of the \mathbf{w}_i vectors follows a multivariate normal distribution with common mean vector $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$. This assumption is critical to finding the marginal distribution of T_i^2 , as discussed in Section 2.3.

In the nonlinear regression model given in Equation (2), $\boldsymbol{\beta}_i$ is a $p \times 1$ vector of parameters that determines the curve $f(\mathbf{X}_i, \boldsymbol{\beta}_i)$. We employ the the multivariate T^2 statistic to assess stability of the the p parameters simultaneously, i.e., to evaluate the assumption $\boldsymbol{\beta}_i = \boldsymbol{\beta}$, $i = 1, \dots, m$. We do not employ individual control charts for each of the p nonlinear regression parameters since this may give misleading results due to the built-in correlation structure of the parameter estimators in nonlinear regression.

Once $\hat{\boldsymbol{\beta}}_i$ is obtained from each sample in the baseline dataset, we calculate the average vector $\bar{\boldsymbol{\beta}}$ and some corresponding estimate of the covariance matrix, replace \mathbf{w}_i with $\hat{\boldsymbol{\beta}}_i$ and $\bar{\mathbf{w}}$ with $\bar{\boldsymbol{\beta}}$ in Equation (5) to obtain

$$T_i^2 = \left(\hat{\boldsymbol{\beta}}_i - \bar{\boldsymbol{\beta}} \right)' \mathbf{S}^{-1} \left(\hat{\boldsymbol{\beta}}_i - \bar{\boldsymbol{\beta}} \right).$$

A large value of T_i^2 indicates an unusual $\hat{\boldsymbol{\beta}}_i$, suggesting that the profile for item i

is out-of-control. In contrast to the traditional use of the T^2 statistic to monitor a multivariate quality characteristic vector, we employ the T^2 statistic to monitor the coefficient vectors of the nonlinear regression fit to each individual profile.

There are several choices for the estimator \mathbf{S} . Here we discuss the effects of three choices and later discuss under what conditions, if any, each should be used.

The first choice we consider for \mathbf{S} is the *sample covariance* matrix, given by

$$\mathbf{S}_C = \frac{1}{m-1} \sum_{i=1}^m (\hat{\boldsymbol{\beta}}_i - \bar{\boldsymbol{\beta}}) (\hat{\boldsymbol{\beta}}_i - \bar{\boldsymbol{\beta}})'$$

Consequently, the T_i^2 statistics take on the form

$$T_{C,i}^2 = (\hat{\boldsymbol{\beta}}_i - \bar{\boldsymbol{\beta}})' \mathbf{S}_C^{-1} (\hat{\boldsymbol{\beta}}_i - \bar{\boldsymbol{\beta}}). \quad (6)$$

Use of the T_C^2 values was mentioned by Brill [17] in the context of monitoring nonlinear profiles of a chemical product. The advantage of this statistic is that it is very well understood and widely used. However, as was shown by Sullivan and Woodall [18] and Vargas [19], a T^2 statistic based on \mathbf{S}_C is ineffective in detecting sustained shifts in the mean vector during the Phase I period. In fact, it was shown that as the step shift size increased, the power to detect the shift actually decreased.

An alternative choice of \mathbf{S} is one based on *successive differences*, proposed originally by Hawkins and Merriam [20] and later by Holmes and Mergen [21]. To obtain the estimator, we define $\hat{\mathbf{v}}_i = \hat{\boldsymbol{\beta}}_{i+1} - \hat{\boldsymbol{\beta}}_i$ for $i = 1, \dots, m-1$ and stack the transpose of these $m-1$ difference vectors into the matrix $\hat{\mathbf{V}}$ as

$$\hat{\mathbf{V}} = \begin{bmatrix} \hat{\mathbf{v}}_1' \\ \hat{\mathbf{v}}_2' \\ \vdots \\ \hat{\mathbf{v}}_{m-1}' \end{bmatrix}.$$

The estimator of the variance-covariance matrix is

$$\mathbf{S}_D = \frac{\hat{\mathbf{V}}' \hat{\mathbf{V}}}{2(m-1)}.$$

Sullivan and Woodall [18] showed that \mathbf{S}_D is an unbiased estimator of the true covariance matrix if the process is stable in Phase I. The resulting T_i^2 statistics are given by

$$T_{D,i}^2 = \left(\hat{\boldsymbol{\beta}}_i - \bar{\boldsymbol{\beta}} \right)' \mathbf{S}_D^{-1} \left(\hat{\boldsymbol{\beta}}_i - \bar{\boldsymbol{\beta}} \right). \quad (7)$$

Sullivan and Woodall [18] and Vargas [19] showed that a T^2 chart based on values of $T_{D,i}^2$ was effective in detecting both a step and ramp shift in the mean vector during Phase I. Sullivan and Woodall [18] also showed that the T_D^2 values are invariant to a full-rank linear transformation on the observations.

Our third choice for \mathbf{S} is a robust estimator of the variance-covariance matrix known as the minimum volume ellipsoid (MVE) estimator, first proposed by Rousseeuw [22] and studied in profile monitoring for Phase I analysis by Jensen, Birch, and Woodall [23]. In our application of the MVE method, we find outlier-robust estimates for both the in-control parameter vector and the variance-covariance matrix based on finding the ellipsoid with the smallest volume that contains at least half of the $\hat{\boldsymbol{\beta}}_i$ vectors, $i = 1, \dots, m$. The MVE estimator of $\boldsymbol{\beta}$ is the mean vector of the smallest ellipsoid, and the estimator of the variance-covariance matrix is the sample covariance matrix of the observations within the smallest ellipsoid multiplied by a constant to make the estimator unbiased for multivariate normal data. In a simulation study, Vargas [19] studied the power properties of several different choices of \mathbf{S} in the context of the T^2 statistic given in Equation (5) and found that the T^2 statistic based on the MVE estimators of $\boldsymbol{\beta}$ and the variance-covariance matrix was very powerful in detecting multivariate outliers. We denote the MVE estimators of $\boldsymbol{\beta}$ and the covariance matrix by $\hat{\boldsymbol{\beta}}_{MVE}$ and \mathbf{S}_{MVE} , respectively. Hence, the fourth choice of T^2 is

$$T_{MVE,i}^2 = \left(\hat{\boldsymbol{\beta}}_i - \hat{\boldsymbol{\beta}}_{MVE} \right)' \mathbf{S}_{MVE}^{-1} \left(\hat{\boldsymbol{\beta}}_i - \hat{\boldsymbol{\beta}}_{MVE} \right), \quad i = 1, \dots, m. \quad (8)$$

2.3 Control Limits

The distribution of the T_i^2 statistics for monitoring nonlinear profiles is more complex than in the linear profile case. Recall that the distribution of the parameter estimators in nonlinear regression is difficult to obtain for small sample sizes. Instead we employ the asymptotic distribution (as $n \rightarrow \infty$) of $\hat{\beta}_i$, $i = 1, \dots, m$. Hence, in order to determine the marginal distribution of T_i^2 in this case, we assume that the sample size, n , from each item in the baseline data set is of sufficient size such that the distributions of $\hat{\beta}_i$, $i = 1, \dots, m$ are approximately multivariate normal. The subsequent upper control limits (UCLs) for the multivariate T^2 control charts are determined based on this normality assumption.

In order to control the overall probability of a false alarm, based on some appropriate UCL, the joint distribution of the T_i^2 values is required. However, these values are correlated since $\bar{\beta}$ and \mathbf{S} are used in all T_i^2 statistics ($i = 1, \dots, m$), thus making the joint distribution of the T_i^2 values difficult to obtain. As an alternative, Mahmoud and Woodall [6] suggested using an approximate joint distribution assuming that the T_i^2 statistics are independent. We let α be the probability of a false alarm for any individual T_i^2 statistic. Then the approximate overall probability of a false alarm for a sample of m items is given by $\alpha_{overall} = 1 - (1 - \alpha)^m$. Thus, for a given overall probability of a false alarm, we use $\alpha = 1 - (1 - \alpha_{overall})^{1/m}$ in the calculation of UCLs. In their simulation study, Mahmoud and Woodall [6] found that this approximation used to determine the UCLs performed well.

As noted in Tracy, Young, and Mason [24], Gnanadesikan and Kettenring [25] proved that for a stable process the marginal distribution of $T_{C,i}^2$ is proportional to a beta distribution, i.e.,

$$T_{C,i}^2 \frac{m}{(m-1)^2} \sim B\left(\frac{p}{2}, \frac{m-p-1}{2}\right).$$

A formal proof can be found in Chou, Mason, and Young [26]. Note that it is assumed

that the distribution of $\hat{\beta}_i$ is approximately normal. Therefore, an approximate UCL is

$$UCL_C = \frac{(m-1)^2}{m} B_{1-\alpha, p/2, (m-p-1)/2} \quad (9)$$

where $B_{1-\alpha, p/2, (m-p-1)/2}$ is the $1 - \alpha$ quantile of a beta distribution with shape parameters $p/2$ and $(m-p-1)/2$.

The marginal distribution of the $T_{D,i}^2$ statistic is unknown. However, Williams, Woodall, Birch, and Sullivan [27] gave an approximate distribution based on the chi-squared distribution for large sample sizes and an approximate distribution based on the beta distribution for small sample sizes. For large sample sizes, defined by $m > p^2 + 3p$, the UCL is given by

$$UCL_D = \chi^2(1 - \alpha, p).$$

For small sample sizes, defined by $m \leq p^2 + 3p$ and $p < 10$, the UCL is a vector given by

$$\mathbf{UCL}_D = (UCL_1, UCL_2, \dots, UCL_m), \quad (10)$$

where

$$UCL_i = MV(m, i)BETA_{1-\alpha, \beta(m, p, i), \gamma(m, p, i)}, \quad i = 1, \dots, m,$$

and $\beta(m, p, i)$ and $\gamma(m, p, i)$ are functions of m , p , and i that define the two shape parameters for the beta distribution. The specific forms of $\beta(m, p, i)$ and $\gamma(m, p, i)$ given by Williams, et al. [27], are included in the Appendix.

The exact marginal distribution of $T_{MVE,i}^2$ is also unknown and intractable. Hence, in order to find the UCL for $T_{MVE,i}^2$ we used simulation.

2.4 Monitoring the Variance

In addition to checking the stability of each profile in the baseline dataset, it is important to check the stability of the variability about each profile. This is analogous to monitoring the process variance in the standard univariate case. In the

case of monitoring profiles, we seek to monitor the variability about each profile, or the within-profile variability. Our measure of within-profile variability is the mean squared error (MSE) defined as $MSE_i = \sum_{j=1}^n (y_{ij} - \hat{y}_{ij})^2 / (n - p)$, where \hat{y}_{ij} is the predicted value of y_{ij} based on the nonlinear regression model in Equation (2). Wludyka and Nelson[28] recommended a method to monitor variances based on an analysis-of-means-type test utilizing $S_i^2 = MSE_i$. In their paper, S_i^2 is plotted against i with associated lower- and upper-control limits equal to $(L_{\alpha, m, n-p})m\bar{S}^2$ and $(U_{\alpha, m, n-p})m\bar{S}^2$, respectively, where L and U are critical values given in their paper and \bar{S}^2 is the average of the S_i^2 values, $i = 1, \dots, m$. For large n , their approximate upper and lower control limits are $\bar{S}^2 \pm h_{\alpha, m, \infty}\hat{\sigma}$ where h is a critical value given in Nelson[29] and $\hat{\sigma} = \bar{S}^2 \sqrt{2(m-1)/m(n-p)}$. The S_i^2 statistics are plotted on a separate control chart to monitor the variance of the error terms and lack of fit simultaneously with a T^2 control chart for the nonlinear regression parameters. We recommend use of this method when within-profile error terms are independent.

2.5 Nonparametric Approach

When a parametric form of a profile would be overly complex, nonparametric procedures may be more appropriate. These include fitting each profile via some smoothing method, such as local polynomial regression, spline smoothing, or wavelets. Walker and Wright[1] give a spline-fitting approach to the vertical density profile (VDP) of particleboard, which we use as an illustration in Section 3. However, these authors discussed using splines to assess variation, not to monitor profiles in a Phase I analysis to check for process stability. Winistorfer, Young, and Walker[30] illustrated the use of splines to model the VDP of oriented strandboard generated from a 3^2 factorial design with 3 replicates. However, their spline-fitting method is used in the context of comparing profiles among differing experimental conditions, not monitoring

profiles in a Phase I or Phase II analysis.

For the case of a single explanatory variable, we denote the nonparametric fit of profile i by \dot{y}_{ij} , for the corresponding value of the explanatory variable equal to x_j , $j = 1, \dots, n$. The general nonparametric approach to monitoring profiles in Phase I analysis is to establish a “baseline” curve with which to compare all other curves. A natural choice of baseline profile is the average estimated profile across all m profiles, denoted by $\tilde{y}_j = \sum_{i=1}^m \dot{y}_{ij}/m$, $j = 1, \dots, n$. Once a baseline curve is found, some appropriate distance metric can be used to measure how “different” each individual curve is from the baseline. Researchers at Boeing [31] proposed the following three metrics:

1. $M_{i1} = \text{sign}(\max_j |\dot{y}_{ij} - \tilde{y}_{ij}|)$
2. $M_{i2} = \sum_{j=1}^n |\dot{y}_{ij} - \tilde{y}_{ij}|$
3. $M_{i3} = \sum_{j=1}^n |\dot{y}_{ij} - \tilde{y}_{ij}|/m$.

The three metrics, M_{i1} , M_{i2} , and M_{i3} , are referred to as the maximum deviation, sum of absolute deviations, and the mean absolute deviation, respectively. Further, it may be of interest to compute the absolute value of M_{i1} , which obviously reflects the magnitude of the dissimilarity between \dot{y}_{ij} and \tilde{y}_{ij} disregarding the direction of dissimilarity. We denote this metric by M_{i4} . Other metrics are proposed in Gardner, *et. al.*[32], who note that metrics can be defined to detect changes in profiles resulting from particular known process faults. One of these metrics is the sum of squared differences between each estimated profile and the average profile, denoted $M_{i5} = \sum_{j=1}^n (\dot{y}_{ij} - \tilde{y}_{ij})^2$. For a given metric, one plots the metric value for profile i against i ($i = 1, \dots, m$) and checks for unusual observations. Researchers at Boeing [31] suggested using a standard univariate I -chart on the metrics to establish control limits. The method of smoothing splines with several dissimilarity metrics is

illustrated in Section 3.

3. EXAMPLE

In this example to illustrate the application of the various approaches we use the vertical density profile data from Walker and Wright [1], available at the website <http://filebox.vt.edu/users/bwoodall/VDP%20nonlinear%20profile%20data.txt>. In the manufacture of particleboard, the density properties of the finished boards are quality characteristics that are monitored through time. It is well known that the density (in pounds per ft³) near the core of a particleboard is much less than the density at the top and bottom faces of a board (see Young, Winistorfer, and Wang [33]). The standard sampling procedure calls for a laser-aided density measuring device to scan fixed vertical depths of a board and record the density at each depth. Since the depths are fixed for each board, we denote the depth x_{ij} by simply x_j . Density measurements for this dataset were taken at depths of $x_j = (0.002)j$ inches, $j = 0, 1, 2, \dots, 313$. Correspondingly, a sequence of ordered pairs, $(x_j, y_{ij}), j = 1, \dots, n$, results for board i and forms a *vertical density profile* (VDP) of the board. A baseline sample of twenty-four particleboards was measured in this way, and the twenty-four profiles are illustrated in Figure 1.

[Insert Figure 1 about here.]

Young, Winistorfer, and Wang [33] introduced a statistical method to monitor VDP data. With their method, one summarizes the density measurements into three average density measurements: one near the core and one near each face. The three averages are the quality characteristics that are subsequently monitored using a standard multivariate T^2 control chart. With this method one basically summarizes each nonlinear profile into only three numbers with a corresponding loss of information.

An alternative approach without such a considerable loss of information is to model the profiles themselves parametrically. The nonlinear function we use to model profile i is a “bathtub” function given by

$$f(x_{ij}, \boldsymbol{\beta}) = \begin{cases} a_1(x_{ij} - c)^{b_1} + d & x_j > c \\ a_2(-x_{ij} + c)^{b_2} + d & x_j \leq c \end{cases} \quad i = 1, \dots, m; j = 1, \dots, n, \quad (11)$$

where $\boldsymbol{\beta} = (a_1, a_2, b_1, b_2, c, d)$. One advantage of this nonlinear model is the interpretability of the model parameters. For example, a_1 , a_2 , b_1 , and b_2 determine the “flatness”, c is the center, and d is the bottom, or the “level” of the curve. Differing values of a_1 and a_2 or different values of b_1 and b_2 allow for an asymmetric curve about the center c . Figure 2 contains the “bathtub” function fit to board 1 from the VDP data.

[Insert Figure 2 about here.]

The profile of board 1 is well-modeled by this parametric fit ($R^2 > 0.9999$). For each of the twenty-four boards in the baseline sample we fit the nonlinear model in Equation (11), and calculated the T_C^2 , T_D^2 , and T_{MVE}^2 statistics of Equations (6), (7), and (8), respectively. based on the $\hat{\boldsymbol{\beta}}_i$ values. Parameter estimates for each of the twenty-four boards and the corresponding T^2 statistics are given in Table 1. We plot the six parameter estimates for each of the twenty-four boards in Figure 3.

[Insert Table 1 about here.]

[Insert Figure 3 about here.]

The control limits for the T_C^2 , T_D^2 statistics are calculated from Equations 9 and 10, respectively. We simulated the UCL for the T_{MVE}^2 statistic to achieve an overall probability of a signal equal to 0.05 for $m = 24$ boards. In our simulation, we sampled from a multivariate normal distribution of dimension six, mean vector zero, and

variance-covariance matrix I , since the in-control performance of the methods does not depend on the assumed in-control parameter vector or the variance-covariance matrix. We repeated our simulation 200,000 times, giving a standard error for the estimated control limits less than 0.0005. The UCL values are 14.72 and 65.37, for the T_C^2 and T_{MVE}^2 control charts, respectively, and the control limit vector for the T_D^2 control chart is given in Table 1.

In Phase I analysis, we are interested in identifying “outlying” or out-of-control boards or a shift in the process which might affect the estimation of in-control parameters. We compared the four T^2 control charts for assessing process stability and identifying outlying profiles. In Figure 4 we illustrate all four T^2 control charts for the VDP data.

[Insert Figure 4 about here.]

Both the T_C^2 and the T_D^2 control charts indicate that board 15 has the only out-of-control profile, although the profile for board 18 is borderline. Note that the T_D^2 statistic accentuates the same outlying observations of the T_C^2 chart, but has a larger UCL. As discussed in Sullivan and Woodall [18], the T_C^2 control chart has greater power to detect isolated outlying observations than the T_D^2 control chart based on the successive differences variance-covariance matrix estimator, however the T_D^2 chart is better for detecting a sustained shift in the mean vector. For this dataset, there is no apparent sustained shift in the regression parameter vector.

The T_{MVE}^2 control chart based on the minimum variance ellipsoid estimator indicates that boards 4, 9, 15, 18, and 24 have outlying profiles. The most pronounced outlier is board 15, which both the T_C^2 and T_D^2 charts also indicated as the most severe outlier. As shown by Vargas[19], the T_{MVE}^2 control chart is very powerful in detecting multivariate outliers. Investigating the table of parameter estimates for these boards, given in Table 1, it seems reasonable that the boards 15 and 18 are outliers, with

boards 4, 9, and 24 worthy of further investigation.

As discussed in Section 2.5, an alternative approach to modeling the profiles with a parametric curve is to employ nonparametric smoothing techniques to model the profiles. Walker and Wright[1] employed spline smoothing with 16 degrees of freedom to model the twenty-four boards of the VDP data. We replicated their spline fits to each profile. After obtaining the spline fits to each profile, $\hat{y}_{ij}, i = 1, \dots, m; j = 1, \dots, n$, the average spline, \tilde{y}_j , is calculated. For example, the spline fit to board 1 and the average spline are illustrated in Figure 5.

[Insert Figure 5 about here.]

The spline fit with 16 degrees of freedom provides a concise summary of the shape of the profile from board 1. The average spline fit is systematically lower than the spline fit to board 1. In order to determine which boards are in-control we calculated dissimilarity metrics as given in Section 2.5. Since the metrics M_{i2} and M_{i3} differ only by a constant, it is not helpful to consider both metrics simultaneously. Instead we calculate the metrics M_{i1} , M_{i3} , M_{i4} , and M_{i5} , and then employ an I -chart based on the moving range to establish control limits, as suggested by researchers at Boeing[31]. We plot each metric versus i with associated control limits to obtain control charts. The four charts are given in Figure 6.

[Insert Figure 6 about here.]

The charts based on metrics M_{i1} and M_{i4} both give the same conclusion, that all the profiles of the boards are in-control. This is not surprising since M_{i4} is the absolute value of M_{i1} , but both are given for illustrative purposes. The most extreme value of the metrics came from board 14, with values of $M_{14,1} = -5.79$ and $M_{14,4} = 5.79$. This value represents the maximum (absolute) deviation of the spline fit to board 14 from the average spline fit.

Similarly, the charts based on metrics M_{i3} and M_{i5} both give the same conclusion, that the profile for board 6 is out-of-control. Referring to Figure 1, board 6 is the one with the profile that is consistently lower than all other boards. The next most extreme value of the two metrics is that of board 3, although it does not give an out-of-control signal. Again, referring to Figure 1, board 3 is the one with the profile that is consistently higher than all the other boards. It is apparent that these two metrics measure how *consistently* different each profile is from the average profile across the depth values, whereas metrics M_{i1} and M_{i4} measure the greatest extent to which a profile is from the average at any particular depth value. It is important to note that the results for the control charts on the metrics (Figure 6) do not show the same results as the control charts based on the regression estimators in Figure 4. If the profile can be adequately represented by a parametric model, then this, in general, will lead to more effective charts.

In addition to monitoring the regression parameter vectors of the profiles in a Phase I analysis, we should monitor the variation about the profiles to check for stability. As mentioned in Section 2.4, we recommend using the methods of Wludyka and Nelson [28] to monitor the variance σ^2 . Use of their method is appropriate when the error terms within a profile are independent. In our VDP example, however, the within-profile density measurements are spatially correlated. A more appropriate control chart in this case to monitor the process variance σ^2 is a topic for further research.

4. AUTOCORRELATION

Engineering applications that give rise to nonlinear profile data may lead to autocorrelated error terms. A common source of autocorrelated errors is the spatial or serial manner in which data are collected. The VDP data, for example, is spatially

correlated because the density measurements are taken at close intervals along the vertical depth of the particleboard. On the other hand, some nonlinear profiles may have independent error terms. One example of this is typical dose-response data where several doses of a particular drug are administered to different subjects and their responses are measured. The subsequent error terms in the nonlinear dose-response curve are typically assumed to be independent.

When the error terms are autocorrelated due to either serial, spatial or any other effects, the correlation structure should be taken into account in the analysis. Failure to do so might yield misleading results in some cases, particularly with the control chart to monitor σ^2 . In our example, given in Section 3, we estimated parameters of a nonlinear regression model for each board. For our nonlinear model we assumed that the errors ϵ_{ij} are i.i.d. For the VDP data, it may be reasonable to assume that the ϵ_{ij} are correlated. If this is the case, perhaps an alternative approach would be to employ either nonlinear mixed model methods or generalized estimating equations (GEE) methodology. Both methods can be used to estimate the mean function, or profile, while accounting for autocorrelation in the error structure. In the presence of an autocorrelated error term, Jensen and Birch [34] show that profile analysis based on a nonlinear mixed model offers an improved control chart performance over a nonlinear profile analysis assuming an independent error term. A more detailed treatment of these methods can be found in Schabenberger and Pierce [14] and Hardin and Hilbe [35]. In the context of analyzing nonlinear profiles for Phase I applications, this approach is a topic that requires further investigation.

5. DISCUSSION

In Phase I, we are interested in identifying outlying observations as well as identifying step or ramp shifts in the mean vector over time. As shown by Vargas [19], the

robust variance-covariance matrix and mean vector estimators employed in the T_{MVE}^2 statistic are very powerful in detecting multivariate outliers, but are not powerful in detecting a step shift. However, the opposite is true of the T_D^2 statistic. As shown by Sullivan and Woodall[18], the T_D^2 chart is powerful in detecting a step shift, but not powerful in detecting multivariate outliers. One possible alternative is to employ both the T_D^2 and T_{MVE}^2 charts simultaneously, the former chart sensitive to step shifts and the latter sensitive to outliers. However, in examining both charts simultaneously, one must be cautious of inflating the false alarm probability. This approach is also a topic for further research.

We have not given a detailed treatment of the nonparametric approaches to monitoring profiles discussed in Section 2.5. Rather, we have only described some methods that have been proposed and then illustrated their use with the VDP data. Some issues that need to be addressed, for example, are the best nonparametric estimation technique for a given scenario, the best metrics to apply, the strengths and weaknesses of each metric, and the distributional properties of the metrics in order to establish valid control limits.

The field of profile monitoring using control charts has potential to extend statistical process control to a wide variety of engineering and pharmaceutical applications. With the increasing ease and efficiency in which processes and products can be measured, there is a need for statistical methodology to be developed which can accommodate the growing needs of industry. We have encountered a number of engineering applications in which a response curve is needed to assess quality. In some cases, the shape of the response curve can be well-represented by a parametric nonlinear regression function. In this paper we have developed control chart methodology to monitor such nonlinear profiles for Phase I applications. When a profile cannot be easily described by a parametric function, nonparametric methods may be applied.

APPENDIX

The function for $\beta(m, p, i)$ is

$$\beta(m, p, i) = I_{\{i=1, m\}} \left(\frac{p}{2} - \frac{1}{a_{11}(m - b_{11})} \right) + I_{\{i=2, \dots, m-1\}} (a_{12}p + b_{12}),$$

and the function for $\gamma(m, p, i)$ is given by

$$\gamma(m, p, i) = I_{\{i=1, m\}} a_{21} + I_{\{i=2, \dots, m-1\}} \left[a_{22} \left(i - \frac{m+1}{2} \right)^2 + b_{22} \right],$$

where

$$\begin{aligned} I_{\{i=1, m\}} &= \begin{cases} 1 & \text{if } i = 1 \text{ or } i = m \\ 0 & \text{otherwise} \end{cases} \\ I_{\{i=2, \dots, m-1\}} &= \begin{cases} 1 & \text{if } 2 \leq i \leq m-1 \\ 0 & \text{otherwise} \end{cases} \\ a_{11} &= 6.356e^{-0.825p} + 0.06 \\ b_{11} &= 0.5564p + 0.9723 \\ a_{12} &= 0.54 - 0.25e^{-0.25(m-15)} \\ b_{12} &= -0.085 + 0.2e^{-0.2(m-22)} \\ a_{21} &= (-0.5m + 2)p + \frac{1}{3}(m + 3)(m - 5) \\ a_{22} &= 0.99 + 0.38e^{0.38(p-13.5)} - \frac{1}{0.25e^{-0.25(p-10)} \left(m - 11 + \frac{(p-7)^2}{3} \right)} \\ b_{22} &= (0.07e^{-0.07(m-42)} - 1.95)p + 0.0833m^2 \end{aligned}$$

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Table 1: Estimated Parameter Values and T^2 Statistics for the VDP Data

Board	\hat{a}_1	\hat{a}_2	\hat{b}_1	\hat{b}_2	\hat{c}	\hat{d}	T_C^2	T_D^2	T_{MVE}^2	UCL_D
1	6560	3259	5.63	4.40	45.98	0.29	2.65	1.91	6.00	27.88
2	470	291	3.01	2.74	42.08	0.32	7.56	5.27	6.97	22.29
3	1812	2871	3.99	5.02	47.66	0.34	5.83	7.17	8.64	22.27
4	6171	15009	4.25	7.39	46.63	0.39	12.21	17.28	1131.81	22.24
5	4963	2251	5.14	4.20	43.43	0.30	1.65	2.27	2.88	22.21
6	4556	3758	5.28	4.72	40.13	0.30	8.49	13.03	9.83	22.17
7	5542	3815	5.25	5.00	44.15	0.31	2.15	3.49	3.58	22.12
8	3664	2979	4.89	4.41	44.06	0.30	0.79	0.97	2.69	22.07
9	28041	8872	7.58	4.95	43.22	0.26	4.62	7.10	385.03	22.01
10	1640	1207	4.17	3.39	41.84	0.28	4.30	5.05	4.61	21.95
11	3492	1031	5.82	3.17	46.06	0.25	8.66	8.95	10.00	21.91
12	915	750	3.45	3.52	44.37	0.32	1.80	1.99	2.22	21.88
13	989	1392	3.58	4.05	45.47	0.32	3.42	4.42	5.18	21.88
14	1474	620	4.82	3.29	42.52	0.27	3.28	4.50	7.04	21.91
15	129068	5420	12.40	3.33	45.90	0.15	21.45	22.18	17018.91	21.95
16	10166	3822	5.83	4.86	44.19	0.30	3.83	5.60	12.93	22.01
17	1483	603	4.07	3.26	44.83	0.30	2.30	2.53	2.36	22.07
18	31156	31069	7.70	5.94	46.46	0.27	14.55	19.75	8221.00	22.12
19	418	198	3.22	2.67	42.84	0.30	4.58	3.90	5.16	22.17
20	3207	4741	4.88	5.02	44.45	0.30	5.34	5.59	34.00	22.21
21	672	773	3.37	3.37	44.46	0.31	2.64	3.42	2.79	22.24
22	3520	1807	5.10	4.01	45.52	0.29	1.71	1.37	1.73	22.27
23	1979	845	4.24	3.66	45.53	0.32	4.45	4.85	7.38	22.29
24	6095	26778	5.41	6.67	44.46	0.31	9.75	10.55	6676.21	27.88

Figure 1: Vertical Density Profile (VDP) of 24 Particleboards

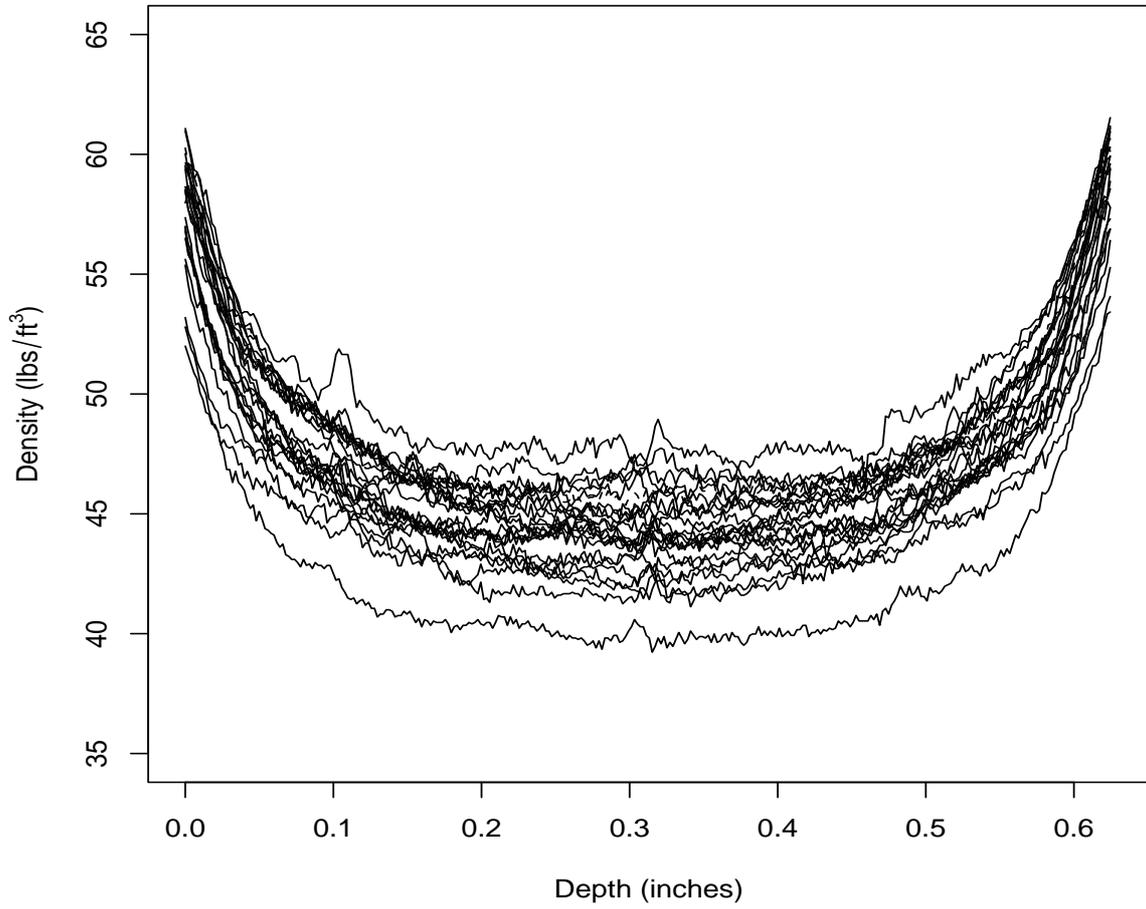


Figure 2: "Bathtub" Function Fit to Board 1

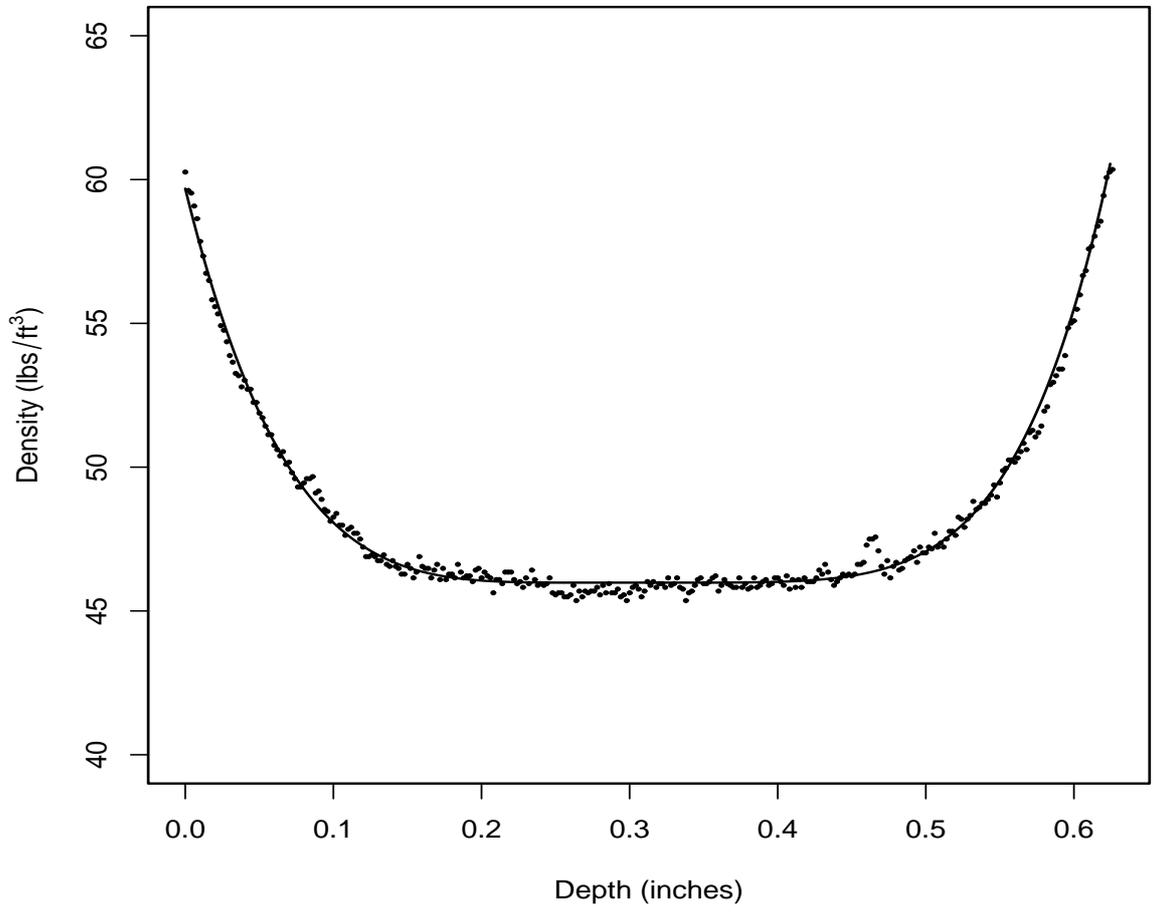


Figure 3: Nonlinear Regression Parameter Estimates a_1 , a_2 , b_1 , b_2 , c , and d by Board for the VDP Data

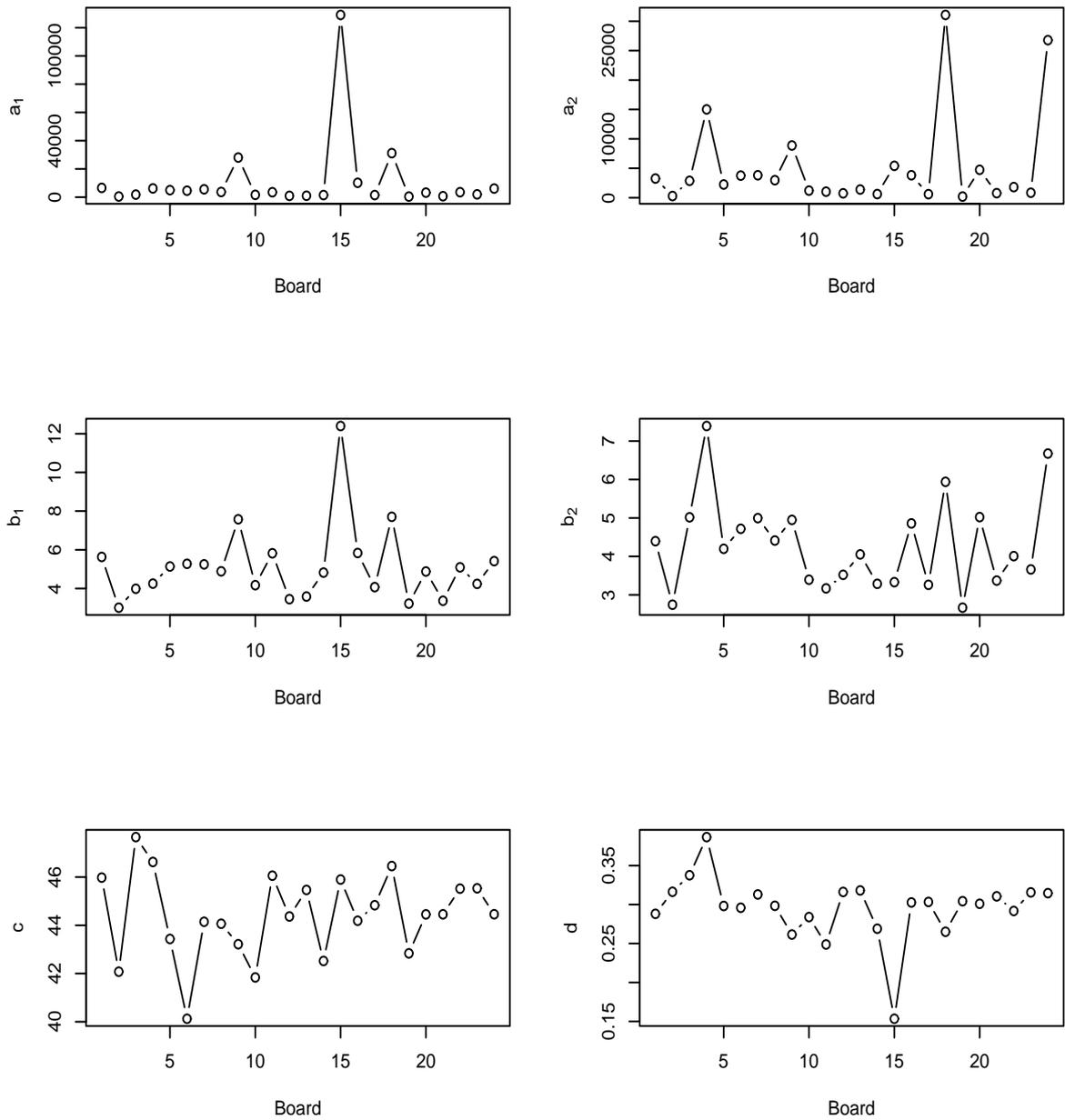


Figure 4: The T^2 Control Charts for the VDP Data. (a) The T_C^2 control chart based on the sample covariance matrix, (b) T_D^2 control chart based on the successive differences estimator, and (c) T_{MVE}^2 control chart based on the minimum volume ellipsoid.

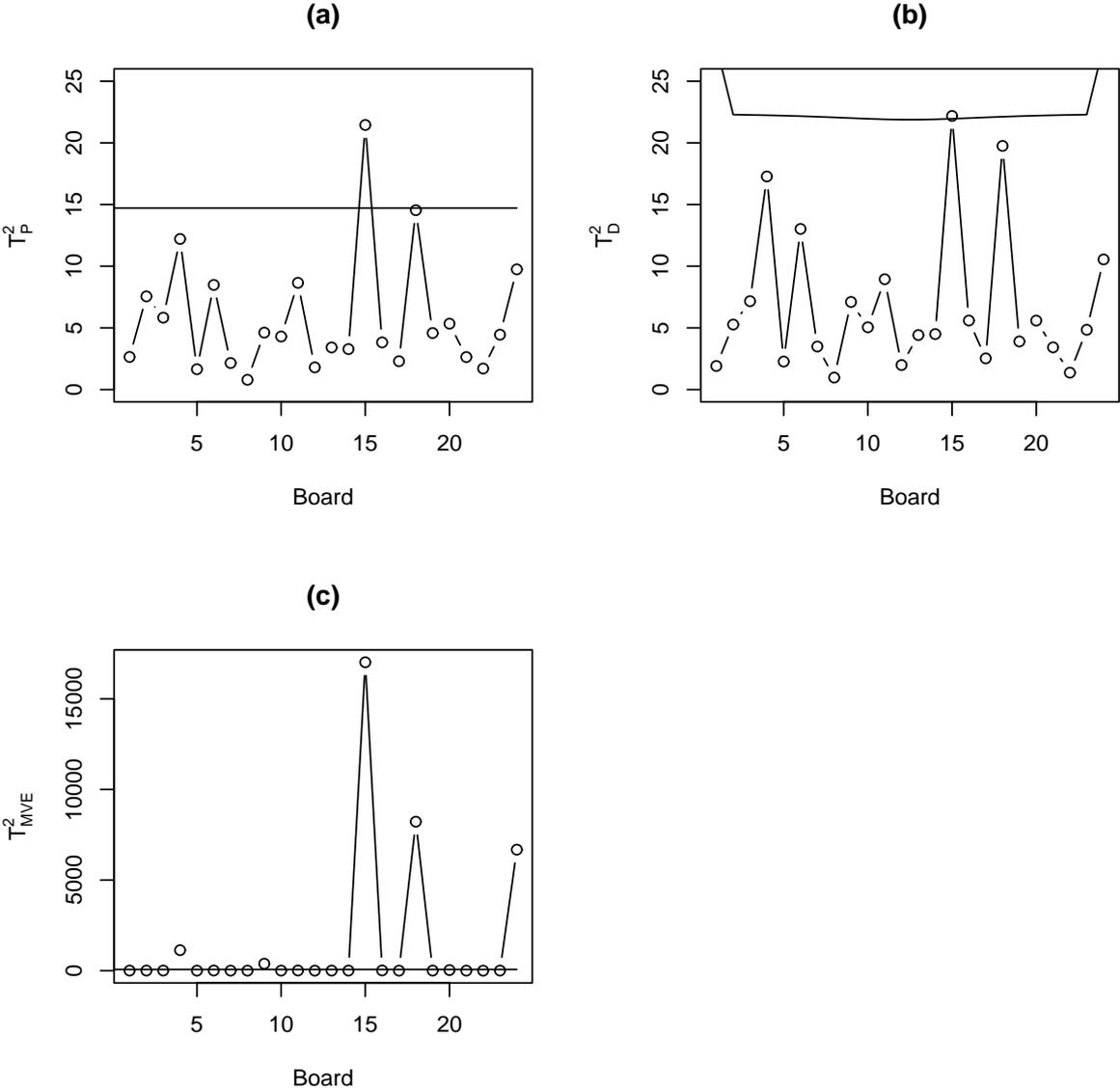


Figure 5: Spline Fit of Board 1 (Above) and Average Spline (Below) for the VDP Data

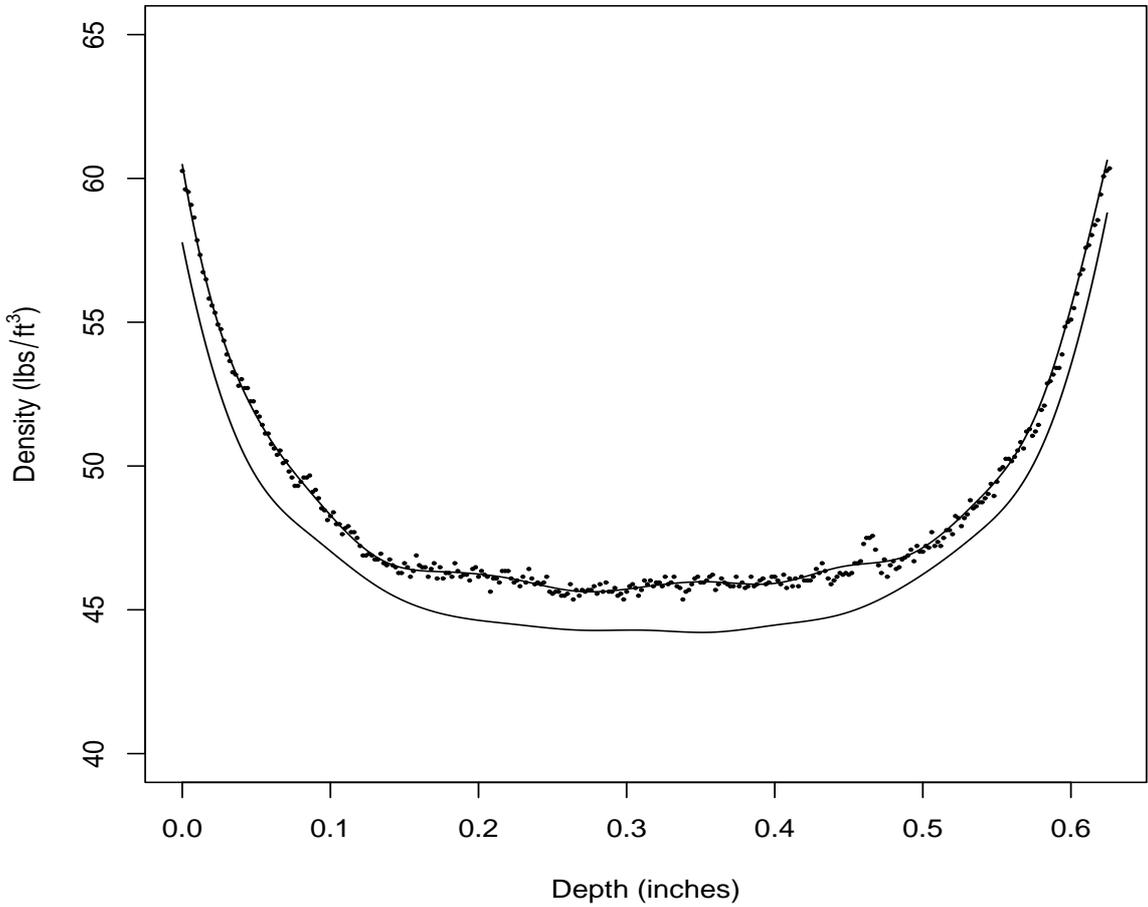


Figure 6: Control Charts on Metrics: (a) M_{i1} , the Maximum Deviation, (b) M_{i3} , the Maximum Absolute Deviation, (c) M_{i4} , the Sum of Squared Differences, and (d) M_{i5} , the Mean Absolute Deviation for the VDP Data

