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Phase I Distribution-Free Analysis of Multivariate Data

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ABSTRACT

In this study, a new distribution-free Phase I control chart for retrospectively monitoring multivariate data is developed. The suggested approach, based on the multivariate signed ranks, can be applied to individual or subgrouped data for detection of location shifts with an arbitrary pattern (e.g., isolated, transitory, sustained, progressive, etc.). The procedure is complemented with a LASSO-based post-signal diagnostic method for identification of the shifted variables. A simulation study shows that the method compares favorably with parametric control charts when the process is normally distributed, and largely outperforms other multivariate nonparametric control charts when the process distribution is skewed or heavy-tailed. An R package can be found in the supplementary material.

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Change-point detection; Control charts; LASSO; Multivariate signed ranks; Nonparametric methods; Statistical process control

1. Introduction

Statistical process control (SPC) consists of ideas and methods that are useful for maintaining a process in a stable and, hopefully, satisfactory state. There are generally two phases in the application of these methods. In Phase I, a fixed-size sample of time-ordered data is analyzed to assess the process stability. Specifically, Phase I control charts are statistical and graphical tools used to understand the nature of process variation over time. Using the knowledge of the process gathered during the first phase, a sequential scheme is then designed for the prospective monitoring of the incoming data (Phase II).

Distribution-free techniques for Phase I analysis have received increasing attention in recent literature. Indeed, the ability of parametric Phase I control charts to correctly distinguish between in-control (IC) and out-of-control (OC) observations is connected to the correct specification of the IC probability model. However, during Phase I, little information on IC distribution is available to practitioners. When distributional assumptions underlying a parametric control chart are not satisfied, or cannot be tested, the performance and sensitivity of parametric Phase I methods deteriorate. For example, the real false alarm probability (FAP), that is, the probability of declaring a stable process unstable, may be substantially larger than the desired value. Thus, several researchers (see, e.g., Chakraborti, Human, and Graham 2009; Jones-Farmer et al. 2014; Capizzi 2015) recommend verifying the form of the underlying IC distribution only after process stability has been established using a suitable distribution-free control chart.

Several distribution-free methods have been suggested for analyzing Phase I univariate data (e.g., Zou et al. 2007; Jones-Farmer, Jordan, and Champ 2009; Jones-Farmer and Champ 2010; Graham, Human, and Chakraborti 2010; Capizzi and Masarotto 2013; Zou et al. 2014; Capizzi 2015). When the joint distribution of multiple quality characteristics is unknown,

some distribution-free control charts have also been proposed for Phase II monitoring (see, e.g., Liu 1995; Qiu and Hawkins 2001, 2003; Qiu 2008; Zou and Tsung 2011; Holland and Hawkins 2014; Li 2015; Chen, Zi, and Zou 2016; Liang, Xiang, and Pu 2016). These proposals can be properly modified for Phase I data. However, statistical methods for these two phases may benefit of being different because of practical and statistical peculiarities of prospective and retrospective monitoring (see Qiu 2013, p. 7). For example, the main aim of Phase II control charts consists in detecting a single change-point while Phase I data can be easily contaminated by multiple changepoints. Unfortunately, although some multivariate distributionfree methods have been proposed for Phase II, "very little published research has considered the issue of robust, distributionfree, or nonparametric multivariate control charts for use in Phase I" (Jones-Farmer et al. 2014, p. 276).

The current state-of-the-art approach consists of the two multivariate Shewhart-type control charts recently proposed by Bell, Jones-Farmer, and Billor (2014) and Cheng and Shiau (2015) for the detection of location shifts for subgrouped data from elliptical distributions. The two control charts are based on the ranks of the Mahalanobis depths and the spatial signs, respectively. However, concerning the practical applicability and efficiency of these proposals, we would point out that: (a) Both control charts require subgrouped observations, notwithstanding the collection of individual data is increasingly common in many applications. (b) These procedures are not completely distribution-free. Indeed, they require to test in Phase I, before establishing the stability of the process, the assumption that the IC process distribution is elliptical. (c) The ranks of the Mahalanobis depths only depend on the magnitude of the distances of the observed points from the center of the data cloud. On the contrary, the spatial signs only reflect the directions of the vectors connecting the observed points to the center. It seems

intuitively reasonable that a more efficient scheme could be based on both the distances and directions. (d) Shewhart-type control charts offer a very good performance against isolated shifts. However, since they do not explicitly use the time-order of the data, they are not efficient against other types of shifts (transitory, sustained, progressive, oscillatory, etc.) that are often encountered in Phase I data.

In an effort to overcome these drawbacks, we develop a new distribution-free Phase I control chart for both individual and subgrouped multivariate data. We avoid the need for any distributional assumption using a permutation approach (Pesarin 2001; Good 2005; Lehmann and Romano 2005). The new control chart is based on the multivariate signed ranks that optimally integrate the spatial signs and ranks of the Mahalanobis depths (Hallin and Paindaveine 2002, 2004, 2005). Following an idea developed in the univariate framework by Capizzi and Masarotto (2013), the chart combines different elementary control statistics designed for detecting the presence of one, two, or more, either isolated or step location shifts. As other types of shifts can be approximated using multiple step shifts, the proposed scheme offers good protection against a wide range of shift patterns. Furthermore, since in many practical situations shifts involve only a small number of variables, we complement the procedure with a LASSO-based method for identifying the variables that are likely to be responsible for an OC condition. An easy-to-use R package, available as supplementary material, allows practitioners to perform the proposed Phase I analysis.

Following Bell, Jones-Farmer, and Billor (2014) and Cheng and Shiau (2015), we consider the "standard framework" handled in multivariate statistical process monitoring. In particular, we assume that (i) the number of data points is larger than number of the variables, and (ii) the observation vectors are independent and identically distributed (iid) when the process is IC. Extensions to the high-dimensional and/or time-dependent framework will require further research. Some possible ideas are outlined in Section 5 (and also in Section S1 of the supplementary materials). Notwithstanding these limitations, we believe that the suggested method can be quite useful in many practical situations, and provide a viable and effective alternative to the procedures described by Bell, Jones-Farmer, and Billor (2014) and Cheng and Shiau (2015).

The article is organized as follows. In Section 2, we illustrate two practical applications of the proposed procedure. In Section 3, we describe the suggested Phase I control chart. In Section 4, we compare the new proposal with other methods. Concluding remarks are given in Section 5. Additional comments, performance evaluations, and examples are provided in the online supplementary material.

2. Examples

As a first example, we use the data given in Table 9.2 by Ryan (2011, p. 323). The sample comprises 20 subgroups, each with four observations, on two quality characteristics X_1 and X_2 . According to Ryan (2011), the 10th and 20th subgroups are OC. Figure 1(a) illustrates the application of the proposed Phase I analysis. The p-value, shown in the center above the graphics, can be used to assess the stability over time of the process location. In particular, the procedure gives an alarm and the process is declared unstable if the *p*-value is less than α , where α denotes an acceptable value for the false alarm probability. As previously mentioned, the validity of the p-value does not require any assumption on the IC distribution. In this example, the observed p-value (0.001) is so small that an alarm is given for all

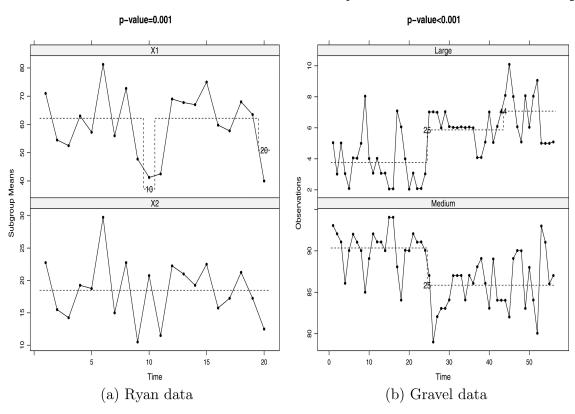


Figure 1. Phase 1 analysis of two datasets.

conventional levels of α , say 0.01, 0.05, and 0.1. Graphics can be used for diagnostic purposes. In particular, the solid lines in the two panels show the sample subgroup means of X_1 and X_2 , respectively, and the dashed lines an estimate of the possibly time-varying process means. In this case, the dashed lines correctly suggest that the subgroups 10 and 20 could have a different location. Figure 1(a) points to the OC subgroups but also provides additional information. Indeed, the constant dashed line in the second panel indicates no shift for X_2 and, hence, the procedure suggests that only X_1 is OC. In addition, the estimated mean of X_1 offers information on the direction and magnitude of the shifts. In particular, it suggests that, for both subgroups, the shift was toward lower values and that the process was more severely OC for subgroup 10 than for subgroup 20. In Section 4.3, we show that this diagnostic information is usually quite accurate.

In the second example, we consider a dataset consisting of 56 individual observations from a European gravel-producing plant, which have already been considered by Holmes and Mergen (1993) and Sullivan and Woodall (2000). There are two variables measuring the percentage of the particles (by weight) that are large or medium in size, respectively. Figure 1(b) shows the output of the proposed Phase I procedure. The small *p*-value points to an unstable process, and, in particular, Figure 1(b) suggests the presence of two step-shifts: the first, at time 25, due to an increase in the percentage of large particles and a simultaneous decrease in the percentage of medium particles; the second, at time 44, due to an increase of the percentage of large particles not involving the other variable.

3. Detecting Location Changes in Multivariate Data

3.1 Overview

Assume that a sample of m time-ordered subgroups of size n, collected on g variables, is available, and denote with $\mathbf{x}_{i,j}$ the g-dimensional vector containing the jth observation from the ith subgroup. Individual observations, that is, process data without subgrouping, can be accommodated by setting n=1. We also assume that (i) mn>g, that is, the number of the observed vectors is greater than the number of the variables; (ii) when the process is IC, $\mathbf{x}_{i,j}$ are iid with an unknown but common density function $p_0(\cdot)$; (iii) we are interested in the detection of location shifts, that is, when the process is OC, at least two subgroups have a different location.

As illustrated in the previous section, the proposed Phase I analysis provides a statistical test to verify if the process is incontrol or out-of-control and some graphical aids able to suggest times and types of the shifts and responsible variables. It can be divided into four distinct stages.

1. Preprocessing. During the first stage, using suitable location and scatter estimates, data are standardized and transformed to the corresponding multivariate signed ranks, in the following denoted by $\mathbf{u}_{i,j}$. This transformation has some optimal properties (see Hallin and Paindaveine 2002, 2004, 2005), and we have verified that it improves the performance when the process distribution is heavy-tailed and/or skewed, without substantially affecting the test procedure in other cases.

Essentially, the next three stages consist in fitting the following multivariate linear regression model

$$\mathbf{u}_{i,j} = \boldsymbol{\beta}_{\text{common}} + \sum_{\tau=2}^{m-1} \boldsymbol{\beta}_{\text{step},\tau} I(i \ge \tau) + \sum_{\tau=1}^{m} \boldsymbol{\beta}_{\text{isolated},r} I(i = \tau) + (\text{residual})_{i,j} \quad (1)$$

where the β 's are unknown g-dimensional vectors of parameters, and I(C) is equal to one if condition C is true, and to zero otherwise. Observe that (i) β_{common} represents the "stable" level of the signed ranks; (ii) $\beta_{\text{step},\tau}$ introduces a level change starting from time τ and affecting all the subsequent observations; (iii) $\beta_{\text{isolated},\tau}$ affects only the observations at time τ and, hence, it corresponds to an isolated outlier. In the framework of model (1), checking process stability is equivalent to test the null hypothesis

$$H_0$$
: all the $\beta_{step,.}$ and $\beta_{isolated,.}$ are zero.

Observe that in a "pure" distribution-free framework it is not possible to detect an isolated outlier when n = 1. Indeed, a single observation that is far from the others can be the consequence of an isolated shift. However, it can also be due to an extremely long-tailed IC distribution. Since discrimination between the two possibilities is not possible without further information on the shape of the IC distribution, only the presence of (multiple) step shifts is considered for individual observations. Note that model (1) is able to represent exactly any possible time-varying location patterns. Since m location vectors are represented using 2m-1 vectors of parameters, the model is clearly overparameterized. However, we expect the model to be sparse, that is, that most of the β 's are zero. Hence, following what have been done for Phase II monitoring by Zou and Qiu (2009); Capizzi and Masarotto (2011); Jiang, Wang, and Tsung (2012); Liang, Xiang, and Pu (2016), the next three stages are based on a variable-selection approach. Observe that the idea of using variable-selection methods for retrospectively detecting outliers and step changes is not new (see Harchaoui and Lévy-Leduc 2010; She and Owen 2011; Ciuperca 2014; Zou, Tseng, and Wang 2014, for some recent examples). However, we believe that our proposal is distinct from earlier works because (i) it addresses the multivariate Phase I framework; (ii) it tries to simultaneously detect multiple isolated and step changes; (iii) it emphasizes the testing phase (see below) and the control of the FAP.

2. Screening. During the second stage, we use the popular forward search (FS) algorithm to select, between the 2m-2 parameter vectors $\boldsymbol{\beta}_{\text{step.}}$ and $\boldsymbol{\beta}_{\text{isolated.}}$, K < m vectors, which can be viewed as "promising" shifts suggested by the data. Here, K denotes the maximum number of shifts we want to search for. When no a priori information is available, we suggest using K =

 $\min(50, \text{ integer closest to } \sqrt{m}), \text{ which offers good per-}$ formances in a variety of OC scenarios (see also Ing and

We choose the FS algorithm since (i) it is simple, fast, and well-known to practitioners; (ii) it offers a very good screening performance, that is, FS can identify all the relevant predictors, together with few irrelevant ones, even if the predictor dimension is larger than the sample size (see Wang 2009; Ing and Lai 2011); (iii) as shown by Capizzi and Masarotto (2015), Phase II FSbased control charts are competitive with schemes based on other variable-selection approaches like LASSO, LAR,

- 3. Testing. During the second stage, K elementary test statistics are computed for detecting the presence of 1, \dots , K either isolated or step shifts. Then, in the third stage, these statistics are aggregated and a single p-value is computed.
- 4. Post-signal diagnostic. The FS algorithm tends to select the relevant predictors together with some unneeded shifts. Hence, following a suggestion by Wang (2009), when the hypothesis of a stable process is rejected, we prune the model using the adaptive LASSO algorithm (Zou 2006) and the information criterion proposed by Chen and Chen (2008). During this stage, the g variables enter into the model independently, that is, we use the adaptive LASSO also for identifying the subset of variables involved in each shift.

3.2 Stage 1: Data Standardization and Computation of the **Multivariate Signed Ranks**

This stage consists of the following two steps.

- 1. Compute suitable estimates of the multivariate location vector and dispersion (scatter) matrix. Since an investigation of the properties of our Phase I method, based on different estimates of location and scatter, is beyond the aim of this article, we here consider only the following estimates:
 - · Location. We use the transformation-retransformation spatial median (see Oja and Randles 2004; Oja 2010) of the subgroup means, that is,

$$\ell = \mathbf{S}^{1/2}$$
 (spatial median of $\mathbf{S}^{-1/2}\overline{\mathbf{x}}_1, \dots, \mathbf{S}^{-1/2}\overline{\mathbf{x}}_m$),

where

$$\bar{\mathbf{x}}_i = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_{i,j} \tag{2}$$

and $S^{1/2}$ is any square-root of the scatter matrix Sgiven by Equation (3), that is, $S^{1/2}$ is a $g \times g$ matrix, so that $S = S^{1/2}(S^{1/2})'$. This location estimate is extremely robust, and can be computed using the fast and simple algorithm given by Oja (2010, p. 71).

• Dispersion. The estimate is different in the case of individual (n = 1) or subgrouped data (n > 1). In

particular, we use

$$\mathbf{S} = \begin{cases} \frac{1}{2(m-1)} \sum_{i=2}^{m} (\mathbf{x}_{i,1} - \mathbf{x}_{i-1,1}) (\mathbf{x}_{i,1} - \mathbf{x}_{i-1,1})' & \text{if } n = 1; \\ \frac{1}{m(n-1)} \sum_{i=1}^{m} \sum_{j=1}^{n} (\mathbf{x}_{i,j} - \overline{\mathbf{x}}_{i}) (\mathbf{x}_{i,j} - \overline{\mathbf{x}}_{i})' & \text{if } n > 1. \end{cases}$$

Both estimators have been studied in the SPC literature. See Williams et al. (2007) and Paynabar, Qiu, and Zou (2015) for individual data, and Montgomery (2009), Ryan (2011), and Qiu (2013) for subgrouped data. In particular, note that S tends to be resistant against location shifts. In the following, we will assume that **S** is nonsingular. Otherwise, the monitoring can be restricted to a set of linearly independent variables.

2. Using ℓ and S, standardize the observed data obtaining $\mathbf{z}_{i,j} = \mathbf{S}^{-1/2}(\mathbf{x}_{i,j} - \boldsymbol{\ell})$ and then compute the multivariate signed ranks of the standardized data as

$$\mathbf{u}_{i,j} = \begin{cases} \mathbf{0} & \text{if } \mathbf{z}_{i,j} = \mathbf{0}; \\ \sqrt{F_{\chi_g^2}^{-1} \left(\frac{r_{i,j}}{1+mn}\right)} & \\ \frac{1}{||\mathbf{z}_{i,j}||} \mathbf{z}_{i,j} & \text{if } \mathbf{z}_{i,j} \neq \mathbf{0}, \end{cases}$$
(4)

where $||\mathbf{v}|| = \sqrt{\mathbf{v}'\mathbf{v}}$ denotes the Euclidean norm of \mathbf{v} , $r_{i,j}$ is the rank of $||\mathbf{z}_{i,j}||$ among $||\mathbf{z}_{1,1}||, \ldots, ||\mathbf{z}_{m.n}||$, and $F_{\chi_z^2}(\cdot)$ is the cumulative function of a χ^2 random variable with g degrees of freedom. Observe that the multivariate signed ranks, are g-dimensional vectors with the same directions as z's. However, they are scaled so that the norms ||u||'s are those expected for a Gaussian IC process.

3.3 Stage 2: Screening and Computation of the **Elementary Tests Statistics**

In this stage, a model with an increasing number of parameters (either isolated or step shifts) is fitted to the signed ranks using an FS algorithm. In particular, the fitted values at the kth step are $\hat{\mathbf{u}}_i^{(k)} = \widehat{\boldsymbol{\beta}}_0^{(k)} + \widehat{\boldsymbol{\beta}}_1^{(k)} \xi_i^{(1)} + \dots + \widehat{\boldsymbol{\beta}}_k^{(k)} \xi_i^{(k)} \quad (i = 1, \dots, m)$ where $\widehat{\boldsymbol{\beta}}_r^{(k)}$, $r = 0, \dots, k$, are g-dimensional vectors of parameters and $\xi_i^{(k)}$ is a scalar sequence corresponding either to an isolated or a step shift, that is, $\xi_i^{(k)} = I(i = \tau^{(k)})$ or $\xi_i^{(k)} = I(i \ge \tau^{(k)})$, for some $\tau^{(k)}$. The type (isolated or step) and time $(\tau^{(k)})$ of the shift $\xi_i^{(k)}$ introduced at step k as well as the parameters $\widehat{\boldsymbol{\beta}}_r^{(k)}$, $r = 1, \dots, k$, are determined by minimizing the residual sum of squares $\sum_{i=1}^{m} \sum_{j=1}^{n} ||\mathbf{u}_{i,j} - \hat{\mathbf{u}}_{i}^{(k)}||^2$ conditionally to the shifts (type and time) identified during the previous k-1 steps. After every step, we compute the explained variance

$$T_k = n \sum_{i=1}^m ||\hat{\mathbf{u}}_i^{(k)}||^2 - mn||\overline{\overline{\mathbf{u}}}||^2,$$



where $\overline{\overline{\mathbf{u}}} = \sum_{i=1}^{m} \sum_{j=1}^{n} \mathbf{u}_{i,j} / mn$. Since we are dealing with a linear model, the FS implementation is straightforward. In particular, in our R package, we use a Gram-Schmidt approach that is optimized by the exclusive presence of dummy regressors in the model.

3.4 Stage 3: Testing

Following the approach proposed for Phase II monitoring by Zou and Qiu (2009) and Capizzi and Masarotto (2011), the idea consists of aggregating the K elementary statistics T_k in the overall test statistic

$$W_{\text{OBS}} = \max_{k=1,\dots,K} \frac{T_k - E_0(T_k)}{\sqrt{\text{var}_0(T_k)}}$$

and then computing the p-value as p-value = $Prob_0(W > V)$ $W_{\rm OBS}$). Here, W denotes the random variable underlying $W_{\rm OBS}$, and Prob₀, E₀ and var₀ are computed under the IC hypothesis.

The direct application of this idea is unfeasible, since the IC probability distribution of T_1, \ldots, T_K depends on $p_0(\cdot)$, the IC density function of the Phase I data. However, we can use a permutation approach (Pesarin 2001; Good 2005; Lehmann and Romano 2005). In particular, organize the Phase I multivariate observations in the matrix $Y = (\mathbf{x}_{1,1}, \dots, \mathbf{x}_{1,n}, \mathbf{x}_{2,1}, \dots, \mathbf{x}_{2,n}, \dots, \mathbf{x}_{m,1}, \dots, \mathbf{x}_{m,n}),$ and let P_Y be the set of all the matrices obtainable by permuting the columns of Y. If we assume that, when the process is IC, the observations are iid, the IC density of Y, that is, $\prod_{i=1}^{m} \prod_{j=1}^{n} p_0(\mathbf{x}_{i,j})$, is constant over $\mathbf{P}_{\mathbf{Y}}$. Hence, the IC conditional distribution of Y given Py does not depend on the unknown density function $p_0(\cdot)$.

The results suggest to compute the p-value conditionally to P_{y} . However, the exact computation of the conditional *p*-value is possible only if m and n are very small, say $m \cdot n < 10$. Therefore, we suggest proceeding as follows:

- (a) Compute the statistics T_1, \ldots, T_K for L randomly generated (column) permutations of Y. Let $T_{l,k}^{\star}$ be the value of the kth statistic obtained in the lth replication, l = $1, \ldots, L, k = 1, \ldots, K.$
- (b) Compute the *p*-value as

$$p\text{-value} = \frac{1}{L} \sum_{l=1}^{L} I\left(\max_{k=1,\dots,K} \frac{T_{l,k}^{\star} - a_k}{b_k} > \max_{k=1,\dots,K} \frac{T_k - a_k}{b_k}\right),$$

where
$$a_k = \sum_{l=1}^{L} T_{l,k}^{\star}/L$$
 and $b_k^2 = \sum_{l=1}^{L} (T_{l,k}^{\star} - a_k)^2/(L-1)$.

We found that using L = 1000 Monte Carlo replications provides sufficient accuracy. An alternative approach based on the assumption that the IC distribution is elliptical is discussed in the supplementary material.

3.5 Stage 4: Post-Signal Diagnostic

In this subsection, we discuss how the process mean can be estimated. When *p*-value $\geq \alpha$, with α equal to a desired FAP, the hypothesis that the process is IC is accepted. Therefore, the common mean of each subgroup can be estimated by the overall

sample mean

$$\overline{\overline{x}} = \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} \mathbf{x}_{i,j}.$$
 (5)

On the contrary, when *p*-value $< \alpha$, the test suggests that the process location is not stable. Hence, it is important, for diagnostic purposes, to identify the times of the location changes as well as the involved variables. With this aim in mind, substitute, in the model obtained at the last step of the FS outlined in Section 3.3, the parameter vectors $\boldsymbol{\beta}_k$ with $\mathbf{S}^{-1/2}\boldsymbol{\delta}_k, k = 0, \dots, K$, obtaining the regression model

$$\mathbf{u}_{i,j} = \mathbf{S}^{-1/2} \boldsymbol{\delta}_0 + \mathbf{S}^{-1/2} \boldsymbol{\delta}_1 \boldsymbol{\xi}_i^{(1)} + \dots + \mathbf{S}^{-1/2} \boldsymbol{\delta}_K \boldsymbol{\xi}_i^{(K)} + (\text{residual})_{i,j}.$$
(6)

In Equation (6), δ_0 is the intercept term while $\delta_1, \ldots, \delta_K$ represent the directions of the potential location shifts in the observed data. Indeed, since $\mathbf{u}_{i,j} \propto \mathbf{S}^{-1/2}(\mathbf{x}_{i,j} - \boldsymbol{\ell})$, a shift of $\boldsymbol{\delta}$ in $\mathbf{x}_{i,j}$ results in a shift with direction $\mathbf{S}^{-1/2}\boldsymbol{\delta}$ in the corresponding signed rank $\mathbf{u}_{i,j}$ (see Figure 2). An estimate of these parameters can be obtained by minimizing the sum of squares

$$s^{2}(\boldsymbol{\delta}_{0},\ldots,\boldsymbol{\delta}_{K}) = \sum_{i=1}^{m} \sum_{j=1}^{n} ||\mathbf{u}_{i,j} - \mathbf{S}^{-1/2}\boldsymbol{\delta}_{0} - \sum_{k=1}^{K} \mathbf{S}^{-1/2}\boldsymbol{\delta}_{k}\boldsymbol{\xi}_{i}^{(K)}||^{2}.$$

However, we expect that part, if not most, of the elements of δ_1 , ..., δ_K are zeros since (i) K can be larger than the true number of change-points, and (ii) only a subset of the variables can be involved in a shift. Therefore, we suggest fitting model (6) using the adaptive LASSO method, that is, to estimate $\delta_0, \ldots, \delta_K$ minimizing the penalized sum of squares

$$s^{2}(\boldsymbol{\delta}_{0},\ldots,\boldsymbol{\delta}_{K}) + \lambda \sum_{k=1}^{K} \sum_{h=1}^{g} \left| \frac{\delta_{k,h}}{\hat{\delta}_{k,h}^{ls}} \right|, \tag{7}$$

where $\delta_{k,h}$ is the *h*th element of δ_k and $\delta_{k,h}^{ls}$ is its estimate obtained using the unpenalized least-square method. See Zou (2006) for the definition and motivation of the adaptive LASSO; Tibshirani (1996) for the definition of the original, nonadaptive LASSO; and Zou, Jiang, and Tsung (2011) for an application of a similar idea in Phase II post-signal diagnosis.

In (7), λ is a positive tuning parameter. The unpenalized least-square estimate is obtained when $\lambda = 0$. As λ increases, the estimates are progressively shrunk toward zero, with some (or many) of the parameters becoming exactly zero. The LARS algorithm developed by Efron et al. (2004) can be used to compute the estimates for every $\lambda \geq 0$, with a computational cost equal to that necessary to compute the unpenalized least-square estimate. In selecting λ , we obtain good results using the extended BIC criterion proposed by Chen and Chen (2008):

$$\begin{split} \text{EBIC}_{\gamma}(\lambda) &= \textit{mng} \log \left(\frac{s^2(\hat{\pmb{\delta}}_0(\lambda), \dots, \hat{\pmb{\delta}}_K(\lambda))}{\textit{mng}} \right) \\ &+ \nu(\lambda) \log(\textit{mng}) + 2\gamma \log \binom{2\textit{gm} - \textit{g}}{\nu(\lambda)}, \end{split}$$

where $\hat{\delta}_k(\lambda)$ denotes the estimate of δ_k obtained by minimizing (7), and $\nu(\lambda)$ is the number of nonzero elements in

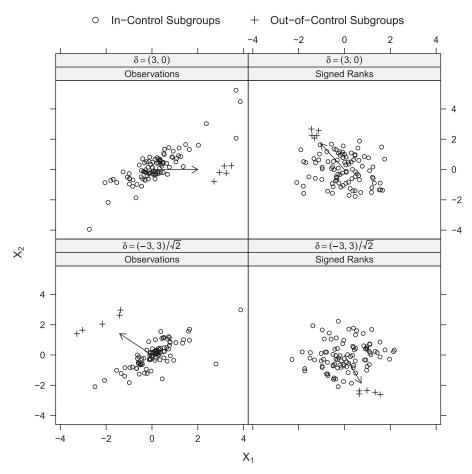


Figure 2. Two simulated datasets (m = 20, n = 5) and their signed ranks. The IC data have been simulated from a bivariate Student's t distribution with 3 degrees of freedom, so that $E(X_1) = E(X_2) = 0$, V var(V var

 $\hat{\delta}_0(\lambda),\ldots,\hat{\delta}_K(\lambda)$. Observe that 2gm-g is the dimension of the searched parameter space. Indeed, in addition to δ_0 , we have 2m-2 possible choices for $\xi_i^{(k)}$, each introducing g parameters in the model. As illustrated in Section 4.3 and in the supplementary material, γ can be used to balance the probability to detect real changes with that of signaling false changes. Typical values are $\gamma=0$, corresponding to the standard BIC criterion, and $\gamma=0.5$ or $\gamma=1$, which offer better protection against false signals.

Notwithstanding that all computation has been performed using the signed ranks, it seems reasonable to present the results to users on the scale of the original, untransformed observations (see, e.g., Figure 1). Therefore, the last step of our procedure consists of refitting the model selected using the adaptive LASSO to the x's. Numerical details are discussed in the supplementary material.

4. Simulation Study

4.1 Study Design

In this section, we summarize the results of an extensive simulation study. In particular, in Section 4.2, we compare the IC and OC alarm probabilities of the Phase I control charts described in Table 1. Then, in Section 4.3, we study the performance of the post-signal diagnostic method based on the adaptive LASSO.

Additional performance results are presented in the supplementary material. All the presented performance measures have been estimated using 10,000 Monte Carlo replications.

The multivariate distributions considered in the study are presented in Table 2. Observe that Normal and Student belong to the family of the multivariate elliptical distributions, Student having heavier tails than Normal. In contrast, Gamma and Poisson are not elliptical. In particular, Poisson is a discrete distribution introduced to show that the suggested method also attains the desired FAP when the distribution is not continuous.

For studying the OC performance of the considered Phase I methods, we assume that the observations are generated by $\mathbf{x}_{i,j} = \delta \xi_i + \epsilon_{i,j}$, where δ is a g-dimensional vector giving the direction and size of the shift, ξ_i a scalar sequence describing the dynamic pattern and $\epsilon_{i,j}$ are iid drawn from the distributions described in Table 2. The considered patterns, which represent some of the real patterns encountered in Phase I, are summarized in Table 3. Observe that the onset and duration of the shifts are stochastic. Indeed, in a real application, they are unknown and vary from case to case.

4.2 In-Control and Out-of-Control Alarm Probabilities

In this section, we compare the proposed test procedure with that of other Phase I control charts. As performance metrics, we use the FAP, that is, the probability of declaring unstable an IC

Table 1. Six parametric and nonparametric Phase I control charts (CL = control limit).

Chart	Description and references	Applicability		
MPhase1	The procedure described in this article ($K = (\text{integer closest to } \sqrt{m}), L = 1000, I \text{min} = 5).$	Individual ^(*) and subgrouped observations from <i>any</i> distribution.		
T ²	The Hotelling's T^2 chart that signals if, for some i , $n(\overline{\mathbf{x}}_i - \overline{\overline{\mathbf{x}}})'\mathbf{S}^{-1}(\overline{\mathbf{x}}_i - \overline{\overline{\mathbf{x}}}) > CL$ (Montgomery 2009; Ryan 2011; Qiu 2013). See (2), (5), and (3) for the definition of $\overline{\mathbf{x}}_i$, $\overline{\overline{\mathbf{x}}}$, and \mathbf{S} . We also consider the version with $\overline{\overline{\mathbf{x}}}$ and \mathbf{S} replaced by the minimum covariance determinant (MCD) estimates.	Individual and subgrouped normally distributed observations.		
GLR	The scheme signals if GLR = $\max_{\tau=2,,m} \mathbf{r}_{\tau}>$ CL where $ \mathbf{r}_{\tau} $ is the likelihood ratio test statistic for verifying, assuming a normal distribution, that the mean of $\mathbf{x}_{i,j}$, $i<\tau$, is equal to the mean of $\mathbf{x}_{i,j}$, $i\geq\tau$ (Zamba and Hawkins 2006; Chen and Gupta 2011; Qiu 2013).	Individual ^(**) and subgrouped <i>normally</i> distributed observations.		
LLC	The procedure, proposed by Lung-Yut-Fong, Lévy-Leduc, and Cappé (2011), is a GLR-type control chart based on component-wise ranks.	Individual $^{(*)}$ observations from any distribution.		
Depth Ranks	The scheme, proposed by Bell, Jones-Farmer, and Billor (2014), signals if, for some i , $\sum_{j=1}^{n}(nm+1-MDR_{i,j})/n>CL \text{ where }MDR_{i,j} \text{ denote the ranks of the Mahalanobis depth }1/[1+(\mathbf{x}_{i,j}-\boldsymbol{\ell}_{BACON})'\mathbf{S}^{-1}(\mathbf{x}_{i,j}-\boldsymbol{\ell}_{BACON})]. \text{ Here, } \boldsymbol{\ell}_{BACON} \text{ is the center of the data cloud computed using the BACON algorithm (Billor, Hadi, and Velleman 2000) and \mathbf{S} the scatter estimate given in Equation (3).$	Subgrouped observations from <i>elliptical</i> distributions.		
Spatial Signs	The scheme, proposed by Cheng and Shiau (2015), signals if, for some i , $n \sum_{j=1}^n \mathbf{v}_{i,j}/n ^2 > CL \text{ where } \mathbf{v}_{i,j} = \mathbf{S}_{HR}^{-1/2}(\mathbf{x}_{i,j} - \boldsymbol{\ell}_{HR})/ \mathbf{S}_{HR}^{-1/2}(\mathbf{x}_{i,j} - \boldsymbol{\ell}_{HR} . \text{ Here, } \boldsymbol{\ell}_{HR} \text{ and } \mathbf{S}_{HR} \text{ denote the Hettmansperger–Randles location and scatter estimates, respectively (Hettmansperger and Randles 2002).}$	Subgrouped observations from <i>elliptical</i> distributions.		

NOTES: (**) MPhase1 and LLC are not effective against isolated shifts in individual observations (see Section 3.1). (**) GLR has a low power against isolated shifts in individual observations.

Table 2. Four multivariate distributions.

Distribution	Definition	Properties							
Elliptical distributions									
Normal	$\mathbf{x}_{i,j} \sim N_g(0, \mathbf{\Sigma}).$	(i) The univariate marginal distributions are normal; (ii) ${\sf E}({\bf x}_{i,j})={\bf 0}$ and ${\sf var}({\bf x}_{i,j})={\bf \Sigma}.$							
Student	$\mathbf{x}_{i,j} = \widetilde{\mathbf{x}}_{i,j} / \sqrt{w_{i,j}^2/3} \text{ with } \widetilde{\mathbf{x}}_{i,j,r} \sim N_g(0, \mathbf{\Sigma}) \text{ and } w_{i,j}^2 \sim \chi_3^2.$	(i) The univariate marginal distributions are Student's t with three degrees of freedom; (ii) $E(\mathbf{x}_{i,j}) = 0$ and $\mathrm{var}(\mathbf{x}_{i,j}) = 2\Sigma$.							
	Nonelliptical distrib	utions							
Gamma	$\mathbf{x}_{\mathbf{i},\mathbf{j}} = \operatorname{diag} \sum_{r=1}^4 \widetilde{\mathbf{x}}_{i,j,r} \widetilde{\mathbf{x}}_{i,j,r}' / 2$ where $\widetilde{\mathbf{x}}_{i,j,r} \sim \mathcal{N}_g(0, \mathbf{\Sigma})$ and $\operatorname{diag}(\mathbf{A})$ is the vector of the diagonal entries of matrix \mathbf{A} (see Stoumbous and Sullivan 2002).	(i) The univariate marginal distributions are gamma with shape parameter equal to two; (ii) $E(\mathbf{x}_{i,j}) = 2 \text{diag}(\Sigma)$ and $\text{var}(\mathbf{x}_{i,j}) = 2\Sigma^{(2)}$, where $\Sigma^{(2)}$ is the matrix obtained by squaring the individual entries of the matrix Σ .							
Poisson	$\mathbf{x}_{i,j} = (r_{i,j,0} + r_{i,j,1}, \dots, r_{i,j,0} + r_{i,j,g})'$ where $r_{i,j,r}$ are iid. Poisson random variables with mean θ if $r = 0$ and $1 - \theta$ otherwise ($0 \le \theta \le 1$).	(i) The univariate marginal distributions are Poisson with mean one; (ii) The correlation between two elements of $\mathbf{x}_{i,j}$ is θ .							

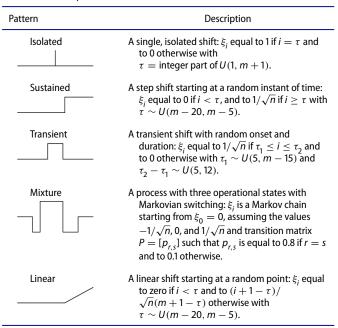
process (first type error), and the detection power, that is, the probability to signal as OC an unstable process. All the considered Phase I methods, with the only exception of *LLC*, are invariant with respect to affine transformations. Hence, if the distribution is elliptical, (i) the IC performance does not depend on $E(\mathbf{x}_{i,j})$ and $\text{var}(\mathbf{x}_{i,j})$; (ii) the OC alarm probabilities depend only on the noncentrality parameter $\sqrt{\delta' \text{var}^{-1}(\mathbf{x}_{i,j}) \delta}$. This is not exactly true for nonelliptical distributions, and, in general, for the LLC chart. However, for all the considered cases, we observe comparable results using different shift directions and covariance matrices. Hence, we will assume that (i) only the first variable shifts, that is, only the first element of δ is different from zero; and (ii) $\text{var}(\mathbf{x}_{i,j})$ is a matrix with all diagonal elements equal to one and off-diagonal elements equal to 0.6.

Figure 3 shows the real FAPs attained by the proposed method for the IC distributions given in Table 2 when an FAP = 0.05 is desired. Since we obtain comparable results for different numbers of variables, only the case of five variables (g = 5) is considered in Figure 3. The figure clearly shows that the suggested Phase I method attains the desired FAP for each sample size and all the considered multivariate distributions.

Figure 3 also presents the real FAPs of two versions of the T^2 control charts based on (i) the classical location and scatter estimates $\overline{\overline{\mathbf{x}}}$ and \mathbf{S} , and (ii) the highly robust MCD estimators. The results illustrate the disadvantages of using a Phase I control chart whose distributional assumptions are not satisfied. In particular, observe that the T^2 schemes can be used only under their design condition, that is, if the IC distribution is normal. Indeed, in many nonnormal cases considered in the simulation, the real FAPs are unacceptably higher, sometimes even close to one, than the nominal value. It is also interesting to observe that using a robust estimators like MCD can even worsen the problem.

Figures 4 and 5 compare the OC performance of the suggested method with those of its competitors in the case of normally distributed data. Since we obtain similar results using different numbers of subgroups (or individual observations), only the results obtained for m=50 are reported. Observe that our proposal offers basically the same protection as the Hotelling's T^2 control chart against isolated shifts in subgrouped data, but better protection against the other patterns (both for individual and subgrouped data). The opposite happens with GLR: our

Table 3. Five shift patterns^(*).



Note: * $U(f_1, f_2)$ denotes a uniform random variable between f_1 and f_2 .

method outperforms this chart in the case of isolated shifts, and globally offers at least a comparable performance for the other patterns. Hence, the suggested procedure can be considered a reasonable alternative to the two normal-based control charts $(T^2 \text{ and GLR})$ offering a satisfactory performance for a wide range of shift patterns, even when the distribution is actually

Regarding the comparison with the nonparametric competitors:

• Figure 4 shows that the suggested Phase I method performs considerably better than the two schemes that are based on the Mahalanobis depth ranks and the spatial signs, in the case of subgrouped normally distributed data. We obtain similar results with nonnormal distributions. For example, Figure 6 displays the alarm probabilities in the case of a multivariate Student's t distribution. In this case, the chart based on the depth ranks is never competitive with our scheme, while the chart based on the spatial signs is competitive only in detecting isolated shift when g is equal to 5 or 10, but is substantially inferior in all the other scenarios. Therefore, when compared to these recently proposed Shewhart-type control charts, our procedure not only has a wider applicability (it can also be used for individual observations and/or nonelliptical distributions) but also offers considerably better protection in the situation (subgrouped data from an elliptical distribution) for which the control charts based on the depth ranks and spatial signs have been originally designed.

In the case of individual normally distributed data, Figure 5 shows that our method outperforms the LLC procedure (Lung-Yut-Fong, Lévy-Leduc, and Cappé 2011), based on the component-wise ranks. Similar results have been obtained when the distribution is not normal (see the supplementary material).

4.3 Efficiency of the Post-Signal Procedure

To illustrate the performance of the post-signal diagnostic method described in Section 3.5, we consider observations $\mathbf{x}_{i,j} = (x_{i,j,1}, \dots, x_{i,j,g})'$ generated by the model $x_{i,j,r} = \mu_{i,r} + 1$ $\epsilon_{i,j,r}$, where $\mu_{i,r}$ denotes the mean at time i of the rth variable and $\epsilon_{i,j} = (\epsilon_{i,j,1}, \dots, \epsilon_{i,j,g})'$ are iid *g*-variate Student's *t* random variables with three degrees of freedom, such that $E(\epsilon_{i,i,r}) = 0$, $var(\epsilon_{i,j,r}) = 1$, and $cor(\epsilon_{i,j,r}, \epsilon_{i,j,h}) = 0.6$. We also assume that

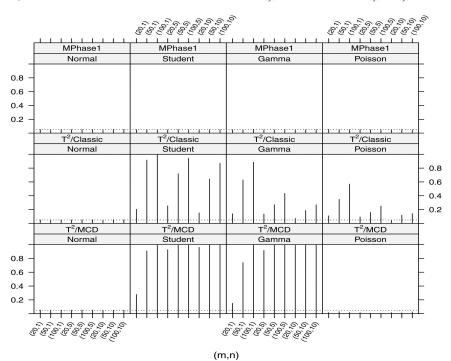


Figure 3. Attained false alarm probability for different distributions, different number of subgroups (m), and different subgroup sizes (n) when the number of variables (q) is five. The nominal false alarm probability $\alpha = 0.05$ is shown by the dotted lines.

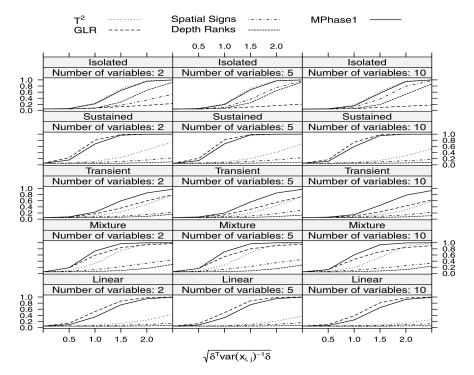


Figure 4. Out-of-control alarm probability of Phase I control charts for subgrouped normal observations (m = 50, n = 5).

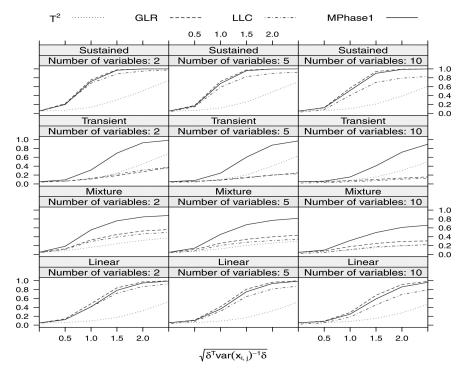


Figure 5. Out-of-control alarm probability of Phase I control charts for individual normal observations (m = 50, n = 1).

the Phase I sample is given by m = 50 subgroups, each with n = 5 observations, and that the number of variables g is either 5 or 10. The following two scenarios for $\mu_{i,r}$ are considered:

A.
$$\mu_{i,r} = \begin{cases} \delta & \text{if } i = 11 \text{ and } r = 1\\ \frac{\delta}{\sqrt{5}} & \text{if } i \ge 31 \text{ and } r = 2\\ -\frac{\delta}{\sqrt{5}} & \text{if } i \ge 31 \text{ and } r = 3\\ 0 & \text{otherwise} \end{cases}$$

$$\text{B. } \mu_{i,r} = \begin{cases} \frac{\delta}{\sqrt{5}} & \text{if } 1 \leq i \leq 10 \text{ or } 21 \leq i \leq 30 \\ \sqrt{5} & \text{or } 41 \leq i \leq 50 \\ \text{and } r = 1 \text{ or } r = 2 \end{cases}$$
$$-\frac{\delta}{\sqrt{5}} & \text{if } 11 \leq i \leq 20 \text{ or } 31 \leq i \leq 40 \text{ .}$$
$$-\frac{\delta}{\sqrt{5}} & \text{and } r = 1 \text{ or } r = 2 \\ \delta & \text{otherwise} \end{cases}$$

In the first case, the process experiences an isolated shift in the first variable and a simultaneous step shift in the second and

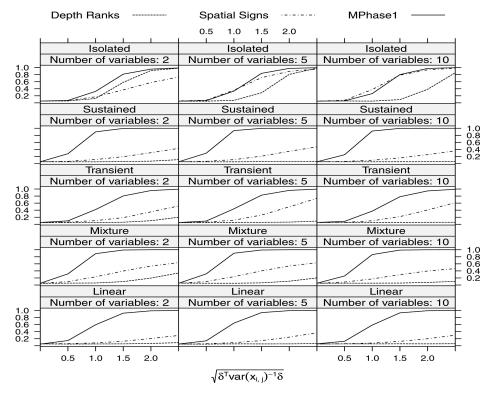


Figure 6. Out-of-control alarm probability of Phase I control charts for subgrouped Student's t observations (3 degrees of freedom, m = 50, n = 5).

third variables. This means that the total number of true mean shifts to detect is three. For the second scenario, the means of the first two variables alternate between two values; the third and fourth variables experience an isolated shift. The total number of true mean shifts to detect is 10 (four step shifts for each of the first two variables; one isolated shift for the third and fourth variables).

Table 4 shows averages (and standard deviations) of the numbers of true and false shifts detected by the diagnostic method based on the adaptive LASSO. Results are shown for δ equal to 1 or 2, and for γ , the tuning parameter of the information criterion $EBIC_{\gamma}(\lambda)$, equal to 0, 0.5, and 1. We consider a step shift

as approximately detected (third and fourth columns of Table 4) if the procedure signals a step shift in the involved variables and $|(\text{signaled time}) - (\text{true onset})| \le 5$, that is, for scenario A, the step shift in the second variable is considered exactly detected if it is signaled at i = 31, and approximately detected if signaled at $26 \le i \le 36$. Table 4 also shows the average number of false shifts detected when the process is IC, that is, when $\delta = 0$.

The suggested approach shows a satisfactory performance since it consistently detects almost all the medium/large shifts ($\delta=2$), and most of the small/medium shifts ($\delta=1$) even, when $\gamma=0.5$ and $\gamma=1$, maintaining an acceptable number of false detections. Observe that the number of false detections

Table 4. Averages, and, in parentheses, standard deviations, of the number of true or false shifts detected by the post-signal diagnostic method based on the adaptive LASSO ($\alpha = 0.05$).

	Number of true detections									
	Exact		Approximated		Number of false detections					
	$\delta = 1$	$\delta = 2$	$\delta = 1$	$\delta = 2$	$\delta = 0$	$\delta = 1$	$\delta = 2$			
	Scenario A / Number of variables: 5 / Number of true shifts: 3									
$\gamma = 0$	2.39 (0.87)	2.98 (0.17)	2.64 (0.62)	2.99 (0.09)	0.17 (1.25)	2.15 (2.58)	2.10 (2.72)			
$\gamma = 0.5$	2.12 (0.89)	2.97 (0.22)	2.37 (0.68)	2.98 (0.17)	0.06 (0.47)	0.53 (1.42)	0.52 (1.24)			
$\dot{\gamma}=1$	1.84 (0.77)	2.95 (0.30)	2.07 (0.63)	2.97 (0.26)	0.05 (0.27)	0.20 (0.74)	0.20 (0.74)			
		Scenario A / Number of variables: 10 / Number of true shifts: 3								
$\gamma = 0$	2.33 (0.88)	2.99 (0.17)	2.60 (0.64)	3.00 (0.10)	0.17 (1.04)	2.34 (2.08)	2.11 (2.07)			
$\gamma = 0.5$	2.12 (0.90)	2.98 (0.22)	2.36 (0.71)	2.99 (0.16)	0.06 (0.48)	0.51 (1.27)	0.45 (1.21)			
$\gamma = 1$	1.84 (0.82)	2.96 (0.30)	2.08 (0.70)	2.97 (0.25)	0.05 (0.30)	0.18 (0.75)	0.14 (0.77)			
		Scenario B / Number of variables: 5 / Number of true shifts: 10								
$\gamma = 0$	7.39 (2.49)	9.68 (0.82)	9.02 (2.27)	9.98 (0.31)	0.16 (1.14)	1.85 (2.19)	1.41 (1.32)			
$\gamma = 0.5$	6.31 (3.07)	9.66 (0.88)	7.70 (3.32)	9.97 (0.37)	0.06 (0.46)	0.63 (0.67)	0.66 (0.54)			
$\gamma = 1$	4.09 (2.00)	9.62 (0.98)	4.88 (2.16)	9.92 (0.64)	0.05 (0.28)	0.12 (0.12)	0.28 (0.24)			
		Scenario B / Number of variables: 10 / Number of true shifts: 10								
$\gamma = 0$	7.05 (2.54)	9.70 (0.77)	8.79 (2.43)	9.99 (0.23)	0.17 (1.64)	2.19 (2.17)	1.32 (1.85)			
$\gamma = 0.5$	5.98 (2.95)	9.68 (0.81)	7.35 (3.20)	9.97 (0.35)	0.06 (0.58)	0.67 (1.01)	0.54 (1.23)			
$\gamma = 1$	3.77 (1.65)	9.64 (0.94)	4.56 (1.77)	9.93 (0.57)	0.05 (0.32)	0.12 (0.43)	0.24 (0.85)			



does not essentially depend on either the number of true shifts or the number of variables. As expected, increasing γ results in a decrease of the number of false detections, but also in a reduced ability to detect small/medium shifts. Therefore, γ should be chosen balancing the importance of detecting small/medium shifts with the cost of investigating a larger number of false shifts. In general, our results show that $\gamma = 0.5$ provides a reasonable compromise. Alternatively, when there is an alarm, it is possible to repeat the post-signal procedure with different values of γ . A practitioner can be highly confident about the shifts signaled by $EBIC_1(\lambda)$, while additional shifts selected by $EBIC_{0.5}(\lambda)$ and, above all, $EBIC_0(\lambda)$ should be investigated more carefully.

5. Conclusions

We have suggested a new distribution-free approach for Phase I analysis of multivariate data, which shows wide applicability, and offers a satisfactory performance in a broad class of OC scenarios. The suggested method combines a statistical test, based on the multivariate signed ranks, for verifying the hypothesis that the location of the process is stable, with a LASSO-based post-signal diagnostic procedure for identifying the timing of the shifts and the involved variables. The application of the suggested Phase I procedure is straightforward using the R package available in the supplementary material.

Given the good results, it seems worthwhile to investigate the extension of the proposed approach to the monitoring of the dispersion and dependence structure of multivariate observations. A natural possibility consists of combining the ideas developed in this article with the test based on the multivariate signed ranks for the homogeneity of scatter, as studied by Hallin and Paindaveine (2008). It also seems interesting to consider the extension to high-dimensional data, that is, to situations in which either $g \approx nm$ or g > mn. In these cases, it is not possible to estimate the entire covariance matrix. However, a procedure similar to our proposal can be based on suitable tests for high-dimensional data (see, for some examples, Chen and Qin 2010; Ro et al. 2015; Feng, Zou, and Wang 2016). Further, it seems interesting to investigate the use of alternative estimates of the multivariate location and scatter parameters. In addition, as discussed in remarks C and D in Section S1 of the supplementary material, it seems worthwhile to explore the possibility of handling autocorrelated data using some bootstrap for time series techniques and the substitution of the two-stage model identification approach based on the FS and LASSO algorithms with alternative variable selection algorithms.

Supplementary Materials

mphase1-supplementary.pdf: Additional simulation results and computational details.

mphase1-example.pdf: A vignette illustrating the use of the R package.

mphase1-package.zip: An R package implementing the Phase I method described in the article. The archive includes the source package, a version compiled for MS Windows and the manual.

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