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Signal Detection Based on Independent Components in Multivariate Statistical Quality Control

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Abstract

Multivariate statistical process control (MSPC) is one of the fastest developing and the most important issue in statistical process control (SPC). One of the aims of the MSPC approaches is the detection of the variable(s) which causes any signal in the process. In this paper, we presented a multivariate statistical process monitoring tool based on independent component analysis (ICA), which can detect signal variable(s) more useful and uncomplicated than the conventional methods. The proposed monitoring method utilizes a univariate statistical process control (USPC) chart based on ICA for signal identification. The basic idea of our approach is to improve the monitoring performance by detecting the source(s) of signal(s). The simulation results clearly show that the proposed IC-USPC method is more practical and feasible alternative to the other methods available in the literature.

Keywords: Process monitoring; Multivariate statistical process control; Independent component analysis; Signal source detection; Signal identification
JEL Codes: C22.

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1. Introduction

There may be many situations that require the monitoring or control of two or more quality characteristics simultaneously. Process monitoring problems involving two or more variables are generally known as Multivariate Statistical Process Control (MSPC). MSPC methods have been widely used in process control to detect signal(s) of a process. However, the functionality of the performances of these methods is limited due to some assumptions that independency of variables and that normality of variables. For example, they can not provide any information about the variable(s) causing these signals.
Nowadays, in industry, there are many situations in which the simultaneous monitoring or control, of two or more related quality – process characteristics is necessary. Process monitoring problems in which several related variables are of interest are collectively known as MSPC.
There are various extensions of MSPC in the literature. Some of those, multiway PCA-PLS for monitoring batch process (Wold et al., 1987), multiblock PCA-PLS for monitoring very large processes (MacGregor et al., 1994), dynamic PCA for including process dynamics in a PCA model (Ku et al., 1995), multiscale PCA based on wavelet analysis for monitoring signals at several different frequency ranges (Bakshi, 1998), model-based PCA for integrating a process model with PCA (Rotem et al., 2000), moving PCA that monitors change in directions of principal components (Kano et al., 2002). Also, Kosanovich and Piovoso (1997) suggest that the observed data can be de-noised by filters to improve the performance of process monitoring, and Chen et al. (2003) presented a new MSPC method based on blind source analysis and wavelet transform.
As Jackson (1991) states that, any multivariate quality control procedure should fulfill four conditions:

(i) The single answer to the question ‘Is the process in control?’
(ii) Specification of an overall Type I error
(iii) The relationship among the variables must be taken into account
(iv) Procedures should be available to answer the question ‘If the process is out of control, what is the problem?’

The last question has proven to be an interesting issue for many researchers. For example, Alt (1985) developed an elliptical control region. However, this approach can be applied to only two quality characteristics. The best well-known technique in this subject is the MYT Decomposition proposed by Mason, Tracy, and Young (1997). MYT decomposition separates a T^2 value into two orthogonal components. One of them is called an *unconditional component*, which is used to control whether an individual variable is out-of-control. The second one is referred to as a *conditional component*, is used to determine if an observation vector generating a signal supplies the linear relationships between the variables. Jackson (1991) supposed that when the variables are transformed to be uncorrelated principal components, they might ensure some intuition about the structure of the out-of-control process so that certain original observations can be examined. Nevertheless, when the number of observed variables increases, these traditional methods require more computations and more detailed separation procedure. Therefore, more feasible methods should be developed to overcome this complexity.

2. METHOD

This study uses ICA to detect variable(s) that caused any signal(s) in a multivariate process. There are some applications of using ICA in-process monitoring. For example, Kano et al. (2003) proposed a new SPC method based on ICA and they have demonstrated the idea of monitoring based on the independent components (ICs) instead of the observed data. The utilization of kernel density estimation to define the control limits of ICs that do not satisfy Gaussian distribution is investigated by Lee et al. (2003). Also, Lee et al. (2004) extended their original method to multi-way ICA that to monitor the batch processes which combine ICA and kernel estimation.

However, there is a gap abandon by these studies in practice. This gap is about determining which quality variable(s) that cause the generation of the signal. In the present work, a new approach called IC-USPC is proposed to handle this problem. The Hotelling T^2 chart does not provide information about the source of the out-of-control signal. Looking at the individual control charts of the observed variables can be misleading due to the dependency between the variables. The main advantage of the proposed approach is that converting the observed variables into ICs and monitor the individual USPC charts of the ICs. For this purpose, the performance of the IC-USPC is evaluated and compared with conventional MYT decomposition findings. Simulation results have shown that IC-USPC can achieve the same results with MYT decomposition more easily and practically in terms of computation.

2.1. MYT Decomposition

The MYT decomposition is defined as the separation of T^2 value into independent and orthogonal components. The decomposed components are divided into two types that conditional component and unconditional component. A possible T^2 decomposition can be shown as in the following equation:

$$T^2 = T_1^2 + T_{2.1}^2 + T_{3.12}^2 + \cdots + T_{p.12\ldots p-1}^2 \tag{1}$$

where unconditional terms are represented by T_j^2, while conditional terms are indicated by $T_{j.12\ldots j-1}^2$. The T^2 value is the statistical distance from the observed data vector to the mean vector. Although the same T^2 value is obtained for each sequence derived for the components of the vector **X**, they differ in the decomposition of this value into p independent terms. Since the MYT decomposition of T^2 requires p terms for decomposition in each division, , $p \times p!$ possible terms are generated with together $p!$ possible division (Mason and Young, 2002).

The unconditional components in any decomposition are calculated as in (2):

$$T_j^2 = \frac{\left(x_j - \bar{x}_j\right)^2}{s_j^2} \tag{2}$$

where x_j is the jth component of the observed vector, $\bar{x}_j$ and s_j^2 mean and variance of this component, respectively. Similarly, the conditional components can be obtained as follows:

$$T_{j.1,2,\ldots,j-1}^2 = \frac{\left(x_j - \bar{x}_{j.1,2,\ldots,j-1}\right)^2}{s_{j.1,2,\ldots,j-1}^2} \tag{3}$$

Detection of variable(s) contributing to the signal is possible by comparing each term of the MYT decomposition of the signal value with its critical value. When it is assumed that the sample size is n and the number of variables is p, the critical value of the unconditional terms and conditional terms are $\left(\frac{n+1}{n}\right) F_{(1-\alpha;1,n-1)}$ and $\left[\frac{p(n+1)(n-1)}{n(n-p)}\right] F_{(1-\alpha;p,n-p)}$, respectively.

2.2. Independent Component Analysis

ICA (Jutten and Herault, 1991; Girolami, 1999) is a signal processing technique for transforming observed multivariate data into statistically independent components, which are expressed as linear combinations of observed variables. ICA is a powerful and useful statistical tool for extracting independent sources given only observed data that are mixtures of unknown sources. The implementation of ICA in extracting the characteristic signals is based on the difference of higher-order statistical characteristics. Several applications of ICA have been reported in speech processing, biomedical signal processing, machine vibration analysis, nuclear magnetic resonance spectrocopy, infrared optical source separation, radio communications, and so on (Girolami, 1999).

The limitations of ICA are: (1) only non-Gaussian ICs can be estimated (just one of them can be Gaussian); and (2) neither signs, powers, nor orders of ICs can be estimated (Kano et al., 2003).

In the ICA algorithm, it is assumed that p observed variables $x_1, x_2, \dots, x_p$ are expressed as linear combinations of m ($\leq p$) unknown ICs $s_1, s_2, \dots, s_m$. The observed variables and the ICs have zero mean. The relation between the observed data and the independent component matrices is given as in (4),

$$\mathbf{x} = \boldsymbol{A}\boldsymbol{s} \tag{4}$$

where $\mathbf{x} = [x_1, x_2, \dots, x_p]^T$, $\mathbf{s} = [s_1, s_2, \dots, s_m]^T$, and $\mathbf{A} \in R^{p\times m}$ is an unknown mixing matrix. When n samples are considered, the above equation can be rewritten as:

$$\mathbf{X} = \mathbf{AS} \tag{5}$$

where $\mathbf{X} \in R^{p\times n}$ is the observed-variable data matrix and $\mathbf{S} \in R^{m\times n}$ is the independent-component data matrix. The main idea of ICA is to estimate both mixing matrix $\mathbf{A}$ and the independent component matrix $\mathbf{S}$ from only the information of the observed data matrix $\mathbf{X}$. The practical problem of ICA is to calculate a separating matrix $\mathbf{W} \in R^{m\times p}$ so that components of the estimated independent-component data matrix $\widehat{\boldsymbol{S}}$ is obtained as follows:

$$\widehat{\boldsymbol{S}} = \mathbf{WX} \tag{6}$$

It must be said that the ICs must be become as independent of each other as possible.

3. THE SIMULATED EXAMPLE

3.1.Problem Definition

This study considers a simulated example to demonstrate the use of our proposed approach. In our simulation, we assume that a multivariate process is initially in control, and the sample observations come from a multivariate normal distribution with known mean vector $\boldsymbol{\mu}_0$ and covariance matrix $\boldsymbol{\Sigma}_0$. This study applies the Hotelling T^2 control chart to monitor a multivariate process with two quality characteristics. We consider the types of correlation, ρ, between two quality variables as no correlation (i.e., $\rho = 0$), moderate correlation (i.e., $\rho = 0.6$), and high correlation (i.e., $\rho = 0.9$). Since the process has 2 quality characteristics (i.e., $p = 2$), the possible sets of quality variables at signal would be $2^p - 1 = 3$. In our study, we use the following notations: $(1,0), (0,1)$, and $(1,1)$ to represent the 3 possible sets, in which "0" stands for the "in-control" state and "1" stands for the "out-of-control" state. The meaning of $(1,0)$ stands for the first quality variable (X_1) that is at fault while the second quality variable (X_2) is not at fault.

For mathematical convenience, we assume that each quality variable for an in-control process follows a normal distribution with zero mean and one standard deviation. Also, we assume that the out-of-control process follows a normal distribution with mean of one and one standard deviation. The data are structured only as individual observations. Under these conditions, the Hotelling T^2 statistics are computed as follows:

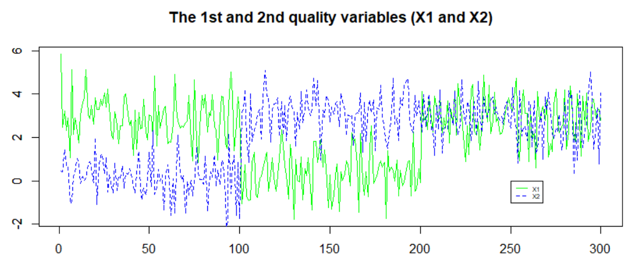
$$T_i^2 = (\mathbf{X}_i - \overline{\mathbf{X}})^T \mathbf{S}^{-1} (\mathbf{X}_i - \overline{\mathbf{X}}) \tag{7}$$

where $\overline{\mathbf{X}} = \frac{1}{n}\sum_{j=1}^{n} \mathbf{X}_j$ and $\mathbf{S} = \frac{1}{n-1}\sum_{j=1}^{n} (\mathbf{X}_j - \overline{\mathbf{X}})(\boldsymbol{X}_j - \overline{\boldsymbol{X}})^T$ are estimated mean and variance-covariance matrix, respectively.

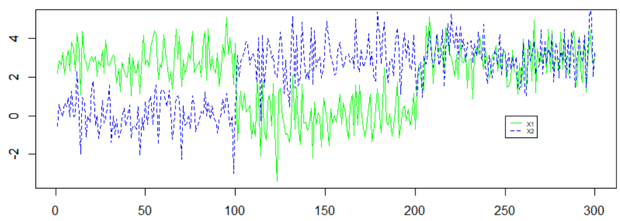
In the literature, generally, the use of multivariate control charts are seen as more important when data set are correlated, and univariate control charts can be performed as a complement to them (Fuchs and Kenett, 1998). However, considering the relationship between variables, the use of univariate SPC charts may yield misleading results. Therefore, in this study, it was proposed that the USPC chart of independent variables (S_1 and S_2) could be used instead of the univariate SPC chart of observed variables to detect the signal variable(s).

This study generates 100 data sets of observations for every possible combination of fault sets. Since there are 3 possible sets of quality variables at fault in the case of $p = 2$, we have 300 data sets in a simulation run. Those 300 data sets are initially used to serve as the Phase I. Another 300 data sets are generated for Phase II.

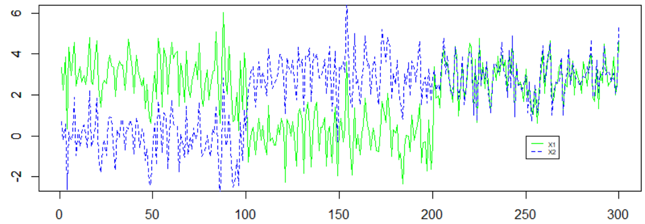
Figure 1 shows the 300 data sets of X_1 and X_2 in the cases of $\rho = 0$, $\rho = 0.6$, and $\rho = 0.9$, respectively.



(a) no correlation



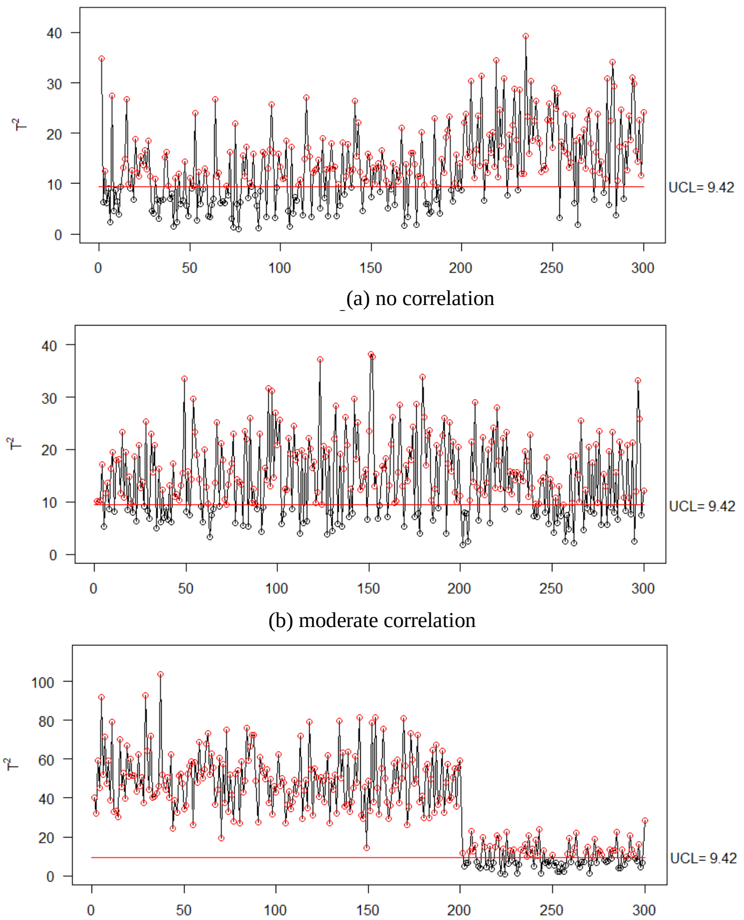
(b) moderate correlation



(c) high correlation

Figure 1. The 300 data vectors (X_1, X_2, X_3) for 3 combinations of possible fault sets, : $(1{,}0)$, $(0{,}1)$, and $(1{,}1)$, in the cases of $\rho = 0$, $\rho = 0.6$, and $\rho = 0.9$.

We also use the same data set to calculate out-of-control Hotelling T^2 statistics which is shown in Figure 2.



(a) no correlation

(b) moderate correlation

(c) high correlation

Figure 2. The corresponding Hotelling T^2 statistics for the data sets in Figure 1.

If the study includes all results of 3 types of correlations, it could exceed the scope of a paper. Also, as shown in Figure 1 and Figure 2, the out-of-control process is more distinct in the highly correlated data set. Therefore, the next part of the study has been limited to the findings obtained by using high correlation data set.

Monitoring Results

The procedure of the proposed IC-USPC scheme is similar to typically USPC. The only difference between the schemes is monitored variables and control limits . In the IC-USPC chart, ICs are monitored instead of original observed variables. Besides, because of the ICs are non-normal, the control limits of IC-USPC are generated using kernel density estimation, unlike conventional USPC.

To apply the proposed IC-USPC method for determination of signal variable(s), the following procedure is implemented:

(1) One data set, including 100,000 simulated samples, under in-control process condition is used to determine control limits.
(2) A new sample is obtained under the condition of $\rho = 0.9$ to demonstrate the example more clearly. This new monitoring data set is consisting of 40 samples that have 20 samples from the in-control and 20 samples from the out-of-control process.
(3) Observed variables are monitored in USPC.
(4) Hotelling's T^2 analysis is applied for MSPC, and then MYT decomposition outcome are obtained.
(5) Then, the observed variables are transformed into ICs.
(6) Each IC is independently monitored in the proposed IC-USPC chart.
(7) IC-USPC chart is compared with MYT decomposition results.

To understand the need to use ICs instead of observed variables, the independence of both of them is shown in Figure 3. Referring to Figure 3, there is a positive correlation between the observed variables, whereas there is no correlation between the ICs. Therefore, it would be better to monitor uncorrelated ICs instead of correlated observed variables.

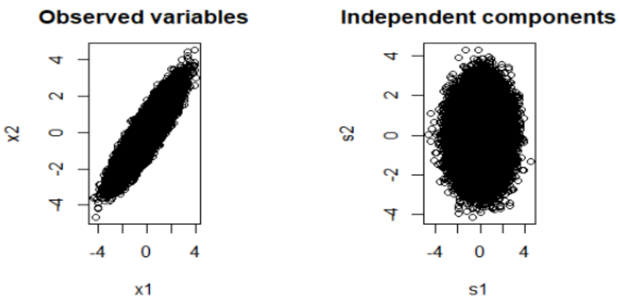
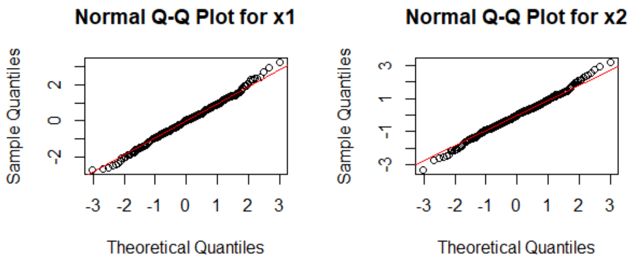
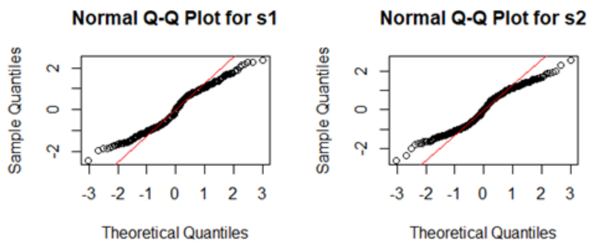


Figure 3. Independency of observed variables and independent components

Also, as shown in Figure 4, the observed variables follow the normal distribution, whereas the ICs are not normally distributed. For this reason, to establish control limits in the proposed IC-USPC, the kernel density estimations have been used.



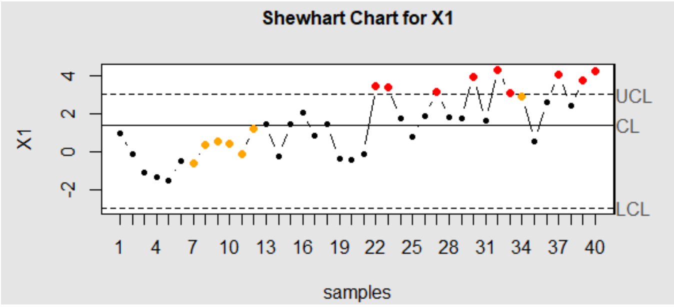
(a) Observed variables



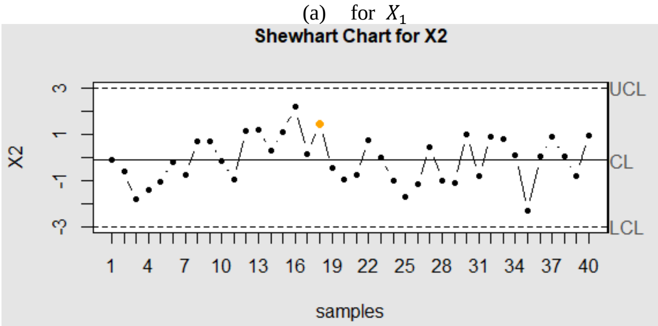
(b) Independent components

Figure 4. Normality plots of (a) observed variables and (b) independent components

Figure 5 shows the individual USPC charts of the observed variables. Accordingly, it can be said that the first variable is out of control while the second variable is in-control. However, this result will not be very reliable due to the dependency structure between the variables.



(a) for X_1



(b) for X_2

Figure 5. Individual USPC chart for (a) X_1 and (b) X_2

Two process individual variables were used to construct Hotelling's T^2 control chart and Figure 6 is obtained. It can be confirmed from Figure 6 that the process is out-of-control because the statistics T^2 exceeds its control limit. However, the detection of signalling (source) variable(s) remains a question to be investigated.

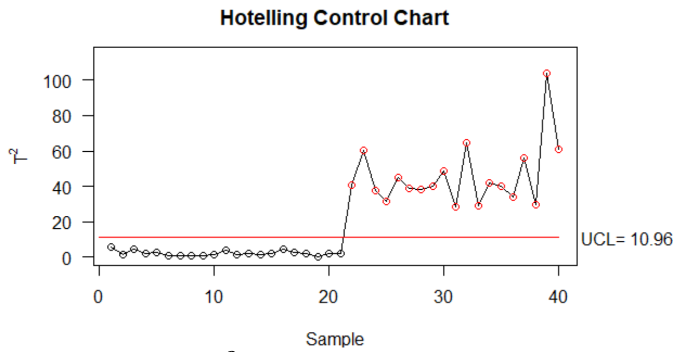


Figure 6. Hotelling T^2 Control Chart for observed data (X_1, X_2)

It is noticed that nineteen points were outside the upper control limit (points 22-40). We will use the MYT decomposition method to demonstrate how to identify the variable(s) that cause this out of control situation.

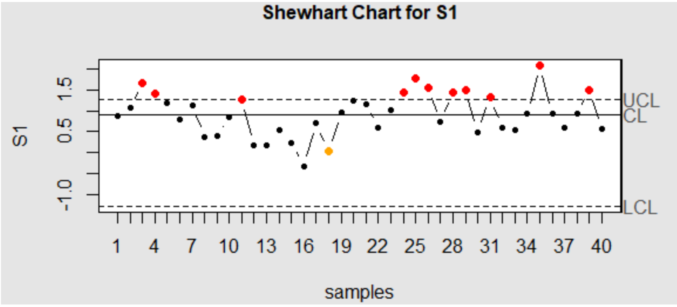
The Table 1 shows the decomposed components of T^2 for the out-of-control process given in Figure 6. MYT decomposition is a procedure that considers each out-of-control point, each variable and the relationship between the variables. For example, as shown in Table 1, T^2 decomposition is assesed separately for each observation exceeding the control limit for both variables and the dependence between the variables. This shows that as the sample size and/or the number of variables increases, it will be more difficult to work with this method.

In Table 1, column 1 shows out-of-control points, while column 3 shows the T^2 decomposition values. In column 2, T_1^2 and T_2^2 represent unconditional components while $T_{1.2}^2$ represents conditional component. UCL values in column 4 are critical values for the corresponding T^2 components. When the number of the quality characteristics is $p = 2$, the sample size is $n = 40$ and %99 confidence level $(1 - \alpha = 0.99)$ are considered, the critical value for the unconditional components (T_1^2 and T_2^2) is calculated as $\left(\frac{40+1}{40}\right) F_{0.99;1,40-1} = 7.5161$ and the critical value for the conditional component ($T_{1.2}^2$) is calculated as $\frac{2(40+1)(40-1)}{40(40-2)} F_{0.99;2,40-2} = 10.9641$. If the T^2 decomposition value is greater than the corresponding critical value, it is said that the variable(s) that contribute to this out of control situation. For example, for point 22, since $T_1^2 = 21.6705 > UCL = 7.5161$ and $T_{1.2}^2 = 49.4811 > UCL = 10.9641$, it can be interpreted as both the first variable and the dependency between the first and second variables cause the out of control situation at this point. The variable(s) that causes the process which is in out-of-control are shown as bold in Table 1. Examining the results of T^2 decomposition, mostly, it is seen that the out of control state is not only caused by the first variable but also by the dependency structure between the first and second variables.

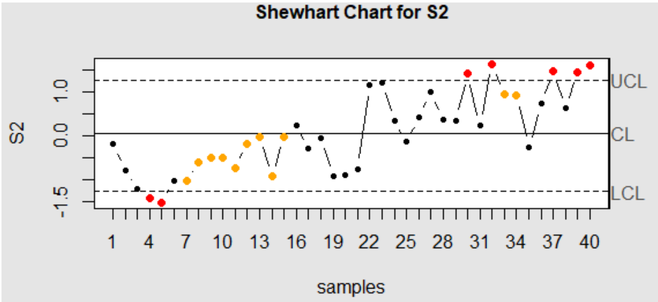
Table 1. MYT Decomposition results

Out-of-control points	T^2 comp.	T^2 decomp.	UCL	p-value	1	2	Out-of-control points	T^2 comp.	T^2 decomp.	UCL	p-value	1	2
	T_1^2	**21.6705**	7.5161	**0.0000**	1	0		T_1^2	**32.9524**	7.5161	**0.0000**	1	0
22	T_2^2	3.5757	7.5161	0.0661	2	0	32	T_2^2	5.1071	7.5161	0.0295	2	0
	$T_{1.2}^2$	**49.4811**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**77.4136**	10.9641	**0.0000**	1	2
	T_1^2	**16.4458**	7.5161	**0.0002**	1	0		T_1^2	**18.8263**	7.5161	**0.0001**	1	0
23	T_2^2	0.9361	7.5161	0.3393	2	0	33	T_2^2	1.1741	7.5161	0.2852	2	0
	$T_{1.2}^2$	**54.3541**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**60.7250**	10.9641	**0.0000**	1	2
	T_1^2	**15.5522**	7.5161	**0.0003**	1	0		T_1^2	**13.5971**	7.5161	**0.0007**	1	0
24	T_2^2	0.0019	7.5161	0.9651	2	0	34	T_2^2	0.9384	7.5161	0.3387	2	0
	$T_{1.2}^2$	**80.2190**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**42.6625**	10.9641	**0.0000**	1	2
	T_1^2	**12.2808**	7.5161	**0.0012**	1	0		T_1^2	**10.8469**	7.5161	**0.0021**	1	0
25	T_2^2	0.0548	7.5161	0.8161	2	0	35	T_2^2	0.1511	7.5161	0.6996	2	0
	$T_{1.2}^2$	**57.1527**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**45.7566**	10.9641	**0.0000**	1	2
	T_1^2	5.1714	7.5161	0.0285	1	0		T_1^2	3.2249	7.5161	0.0803	1	0
26	T_2^2	1.0325	7.5161	0.3158	2	0	36	T_2^2	2.9211	7.5161	0.0954	2	0
	$T_{1.2}^2$	**54.5432**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**61.4244**	10.9641	**0.0000**	1	2
	T_1^2	**8.3369**	7.5161	**0.0063**	1	0		T_1^2	**15.1652**	7.5161	**0.0004**	1	0
27	T_2^2	0.0154	7.5161	0.9018	2	0	37	T_2^2	1.5386	7.5161	0.2222	2	0
	$T_{1.2}^2$	**40.5609**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**42.1530**	10.9641	**0.0000**	1	2
	T_1^2	5.9303	7.5161	0.0196	1	0		T_1^2	6.0624	7.5161	0.0183	1	0
28	T_2^2	0.0047	7.5161	0.9458	2	0	38	T_2^2	0.0119	7.5161	0.9136	2	0
	$T_{1.2}^2$	**29.6575**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**34.5176**	10.9641	**0.0000**	1	2
	T_1^2	**15.9412**	7.5161	**0.0003**	1	0		T_1^2	**16.3755**	7.5161	**0.0002**	1	0
29	T_2^2	0.8884	7.5161	0.3517	2	0	39	T_2^2	0.2883	7.5161	0.5944	2	0
	$T_{1.2}^2$	**52.9245**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**67.1198**	10.9641	**0.0000**	1	2
	T_1^2	**39.1357**	7.5161	**0.0000**	1	0		T_1^2	**9.8531**	7.5161	**0.0032**	1	0
30	T_2^2	7.3059	7.5161	0.0101	2	0	40	T_2^2	0.0697	7.5161	0.7932	2	0
	$T_{1.2}^2$	**84.2371**	10.9641	**0.0000**	1	2		$T_{1.2}^2$	**44.3743**	10.9641	**0.0000**	1	2
	T_1^2	7.2502	7.5161	0.0104	1	0							
31	T_2^2	0.0501	7.5161	0.8241	2	0							
	$T_{1.2}^2$	**44.1305**	10.9641	**0.0000**	1	2							

The USPC charts of the ICs are presented in Figure 7. As shown in Figure 7, both independent variables exceed control limits. Thus, the hidden information about the out-of-control state that cannot be observed in the USPC charts of the second variable has been revealed with ICs. Also, although the T^2 values corresponding to the 26, 28 and 31 observations were not observed as out-of-control according to the MYT decomposition, it can be seen that the ICs corresponding to these observations exceeded the control limits in the USPC for S_1. Thus, it can be concluded that IC-USPC has reached hidden information that cannot be obtained by conventional methods.



(a) for S_1



(b) for S_2

Figure 7. Individual USPC chart for independent components (a) S_1 and (b) S_2

4. CONCLUSION

The main purpose of the present work is that the process monitoring performance can be improved by determining signal variables by using ICA. To expose the applicability of the proposed IC-USPC method, its signal variable detection performance is evaluated and compared with the conventional USPC $\bar{x}$-chart and the MYT decomposition. The simulated results show that IC-USPC can detect the signal variable(s) more functional and more accurate than the others.

As a result, the proposed IC-USPC chart is more advantageous than the conventional USPC $\bar{x}$-chart and MYT decomposition methods. It can be said that the IC-USPC chart, which has more reliable results than USPC $\bar{x}$-charts, is more practical than MYT decomposition.

IC-USPC is still under development. For example, to make the proposed method more applicable, a multivariate process with 3 or more quality characteristics can be discussed in future research. Since the signal variable(s) can be monitored, the IC-USPC has the potential for signal identification. As the requirements for process monitoring increase, there would be a greater need for the SPC to develop methods that can include the detection of the signal and the detection of the source of the signal. Therefore, the IC-USPC is a promising approach and further efforts are needed in this issue.

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