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Non-causal data-driven monitoring of the process correlation structure: A comparison study with new methods

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ABSTRACT

Current approaches for monitoring the process correlation structure lag significantly behind the effectiveness already achieved on the detection of changes in the mean levels of process variables. We demonstrate that this is true, even for well-known methodologies such as MSPC-PCA and related approaches. On the other hand, data-driven process monitoring approaches are typically non-causal and based on the marginal covariance between process variables. We also show that such global measure of association is unable, by design, to effectively discern changes in the local correlation structure of the system and propose, for the first time, the explicit use of partial correlations in process monitoring. As a second contribution, we introduce the use of sensitivity enhancing data transformations (SET) with the ability to maximize the detection ability of all monitoring procedures based on (partial or marginal) correlation, and show how they can be constructed. Results confirm the added-value of the proposed monitoring scheme.

1. Introduction

The optimized and safe operation of current industrial processes requires the simultaneous monitoring of a large number of multiple related variables. A variety of multivariate statistical process control (MSPC) methods, namely control charts, have been developed and applied in order to determine whether the process is only subject to common causes of variability or if a special or assignable cause, related with some abnormality inside or outside the process, has occurred. Analysing the literature, one can verify that most multivariate process monitoring methodologies developed so far, including the latent variables methodologies (Jackson, 1959; Jackson and Mudholkar, 1979; Ku et al., 1995; Li et al., 2000; MacGregor et al., 1994; Wise and Gallagher, 1996) and state-space or time-series approaches (Negiz and Çinar, 1997a,b), are essentially non-causal and focused on detecting changes in the process mean (Abbasi et al., 2009; Ghute and Shirke, 2008; Yeh et al., 2006; Yen et al., 2012). The important complementary problem of monitoring the process correlation structure has been almost absent from the research efforts, creating a significant gap in what regards to the high level of performance achievable today in detecting changes in the mean levels of the process variables, contrasting with the rather limited ability to effectively signal out perturbations in the correlation structure. In fact, even though this situation has been pointed out several times, including in the recent literature, as for instance by Xiao (2013) and Liu et al. (2013), only a few contributions have been put forward for explicitly monitoring the process correlation structure (also called multivariate dispersion).

Therefore, this article is devoted to the analysis and development of new process monitoring methods specifically designed for detecting changes in the process correlation structure and for finding out, in a second stage, the associated root causes. With this effort, we aim to significantly contribute to shorten the gap between the expected performances of the approaches available for monitoring the variables mean levels and those for monitoring multivariate dispersion, providing a more balanced set of tools to practitioners that have to deal with both aspects in real world problems.

In this regard, some causal methodologies were proposed, such as those developed by Bauer et al. (2007), that uses transfer entropy in order to identify the directionality of the fault's propagation path, and the methodology proposed by Yuan and Qin (2012), where a combination of Granger causality and principal component analysis is employed to perform feature selection for locating the origin of faults with oscillatory characteristics. However, these methodologies are strongly oriented to fault diagnosis rather than fault detection, which is an obvious pre-requirement before their application. Chiang and Braatz (2003) also suggested the combined use

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of the Kullback–Leibler information distance and the process causal map to detect and diagnose faults. Yet, this approach requires the knowledge of the causal map in the form of a digraph. Thus, given their pervasive use, shorter development times, good performance and the fact of not relying on a priori information about the system structure, this paper will focus on the class of non-causal approaches for monitoring the process correlation structure.

Among the non-causal procedures specifically developed for monitoring the process covariance, the most widely adopted ones are based on the generalized variance, for which several approaches were proposed, namely by Alt (1984), Aparisi et al. (2001) and Djauhari (2005). However, the generalized variance is a rather ambiguous measure of multivariate variability, as quite different covariance matrices can lead to similar values for the determinant. Other approaches are based on the likelihood ratio test (LRT), as for example those found in the works of Alt and Smith (1988) and Levinson et al. (2002). More recently, Yen and Shiau (2010) presented a control chart, based on LRT, specifically designed to detect an increase in process dispersion, which was later on extended to variations in both directions (increase and decrease) (Yen et al., 2012).

Analysing all these contributions for non-causal monitoring of the correlation structure it is possible to verify that all of them are strictly based on the process general information described by the covariance matrix, also referred as the marginal covariance matrix. Even multivariate statistical process control based on principal component analysis (MSPC-PCA) (Jackson, 1959; Jackson and Mudholkar, 1979; Kresta et al., 1991), which implicitly has the potential to detect changes in the correlation structure of data through the *Q* or *SPE* statistics, is based on the marginal covariance matrix and therefore lacks the ability to effectively detect local structural changes. This situation arises from the fact that MSPC-PCA mainly considers changes in the variables' mean and variance, which might not occur during a structural change (Wang and He, 2010). The belief that the *Q*/*SPE* statistics may be enough for detecting changes in the process correlation structure will be challenged in Section 5.1, where we will demonstrate that MSPC-PCA is easily outperformed by monitoring statistics devoted to monitor the correlation structure, when problems are really located at this level.

As process variables may present a significant mutual marginal covariance even though they do not directly interact in a causal way (as long as they are affected by some common causes of variation), monitoring procedures based on this quantity are unable, by design, to effectively detect and discern changes in the local causal correlation structure. They lack the necessary resolution to perform such an analysis, and any change detected in the marginal covariance between two variables may be due to changes directly related to them, or that happened in any other variables whose variation may, directly or indirectly, affect them. Moreover, some structural changes might not even have an impact on the marginal covariance, especially if several deviations occur at the same time and compensate each other. Therefore, in order to access and use the local information of the variables correlation structure, alternative measures of association must be adopted in the process monitoring procedures. Partial correlation (PC) is one such quantity (Sokal and Rohlf, 1995), as it evaluates the correlation between pairs of variables, after controlling for the effect of others, i.e., after removing their indirect effect in inducing any association between the variables under analysis. This leads us to the following premise: as partial correlation coefficients are able to retain, to a larger extent, information about the local association of variables (even though in a non-causal sense, i.e., without the associated causal directionality), they can provide a finer map of the inner connective structure of variables. Thus, statistical process monitoring (SPM) based on partial correlations should be able to detect changes in the local association structure of variables (fault detection) and to identify the root causes of specific process upsets (fault diagnosis), in a more effective way. Therefore, the total time invested in fault detection and diagnosis activities may be improved using such an alternative measure of local association, as both the primary detection and especially the diagnosis process, will be improved.

We would like to point out that, even though partial correlations have been proposed a short time after PCA, their potential to improve process monitoring and fault detection activities have not yet been explored. This fact is quite surprising, as detection and, in particular, diagnosis tasks, can potentially benefit significantly from the use of local measurements of association. This is in major contrast with the widely explored use of marginal correlation approaches such has PCA and most of the current monitoring methodologies.

In this context, we propose in this work two new contributions to the process monitoring field. Firstly, a new set of methodologies is proposed for monitoring changes in the process correlation structure, that are based on the use of partial correlation information. Secondly, we introduce the use of sensitive enhancing transformations (SET) for maximizing the ability of the methodologies to detect changes in the process correlation structure, independently of their marginal or local nature. The proposed methods based on the use of partial correlations are applied to multivariate systems and their performances compared to the marginal-based approaches available in the literature. The results obtained indicate that partial correlation based statistics were indeed able to improve the detection of changes in the systems structure. However, the greatest contribution to this outcome is the use of a proper variable transformation (the SET) that efficiently increases the sensitivity to small changes on the correlation structure of processes.

This article is organized as follows. In the next section, we review the current monitoring statistics based on marginal covariance. Then, we describe the new proposed monitoring statistics based on partial correlations and introduce the set of sensitivity enhancing transformations, which play a critical role in the methods' performance. Next, we present and discuss the results obtained from the application of all methods considered to systems with different degrees of complexity. Finally, we summarize the contributions proposed in this paper and present the main conclusions.

2. Statistical process monitoring based on marginal covariance

As the topic of this article is on the monitoring of the multivariate process dispersion, we devote this section to a review of the methodologies that were proposed for specifically addressing this problem. These approaches will constitute the benchmarks against which the performance of the new proposed methodologies will be assessed and compared in Section 5.

2.1. W Statistic

Alt and Smith (1988) presented three procedures for monitoring process variability by following its marginal covariance. One of the schemes is based on the likelihood ratio test, which is defined as,

$$W = -p(n-1) - (n-1)\ln\left(\frac{|\mathbf{S}|}{|\mathbf{\Sigma}_0|}\right) + (n-1)tr(\mathbf{\Sigma}_0^{-1}\mathbf{S}) \tag{1}$$

where p is the number of variables, n the number of observations, $\mathbf{\Sigma}_0$ the in-control covariance matrix and $\mathbf{S}$ the sample covariance matrix. Anderson (2003) showed that W is asymptotically distributed as $\chi^2_{p(p+1)/2}$, and therefore the process dispersion is considered to be out-of-control if W exceeds the $UCL = \chi^2_{p(p+1)/2,\alpha}$ ($\chi^2_{d,\alpha}$ is the $100\times(1-\alpha)$th percentile of a Chi-squared distribution with d degrees of freedom).