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Canonical variate analysis-based monitoring of process correlation structure using causal feature representation

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ABSTRACT

Although the monitoring of process variables has been extensively studied, techniques for monitoring faults in the process correlation structures have not yet been fully investigated. The typical methods based on the covariance matrix of the process data for process monitoring have limited capability to effectively monitor underlying structural changes. This paper proposes a canonical variate analysis (CVA) approach based on the feature representation of causal dependency (CD) for the monitoring of faults associated with changes in process structures, which employs CD for pretreating the data and subsequently utilizes CVA for quantifying dissimilarity. Apart from the improved performance of capturing the underlying connective structure information, the utilization of the CD feature in the first step provides more application-dependent representations compared with the original data, as well as decreased degree of redundancy in the feature space by incorporating causal information. The effectiveness of the proposed CD-based approach for the monitoring of structural changes is demonstrated for both single faults and multiple faults in simulation studies of a networked system. In the simulation results, the CD-based method performs the best, followed by correlation-based and then variable-based methods.

1. Introduction

As manufacturing facilities become increasingly integrated and large scale, the potential for faults to dynamically propagate in non-intuitive ways to produce significant harm to equipment, life, and the environment has increased. The rapid detection of faults and associated identification of their causes are, therefore, of outmost importance, which has attracted the interest of many researchers and practitioners. However, most of the process monitoring methods developed so far, including the multivariate statistical control chart approaches [1–3], dimensionality reduction techniques [4–8], and time-series or state-space methods [9,10], focus on the monitoring of process variable faults [11,12].

Compared with the achievements in the monitoring of process variable faults, limited exploration has been done on the important complementary problem of monitoring the faults of process correlation structures [13]. With the emerging big data concept, the monitoring of correlation structures has become of increased interest [14]. The explosive growth of process data along with the increasingly large-scale industries provides a valuable resource for the analysis and operations of industrial processes. This paper aims to develop a new approach for monitoring changes in the process structure.

Typical approaches adopted for monitoring the process correlations are based on the process information described by the covariance matrix. Example approaches include the generalized variance [15,16,18], the conditional entropy [17], and the likelihood ratio test (LRT) [19,20]. The covariance-based methods experience inherent limitations in the detection of local anomalies as well as the subsequent identification of the fault origins. In other words, the inherent structure of the process is not explicitly taken into account in the covariance-based methods. For instance, two variables, x and y, can be connected in several different ways such as (i) direct connection $x \to y$, (ii) indirect connection $x \to z \to y$ or (iii) co-regulated by a third variable z ($z \to x$ and $z \to y$). In all these cases, the variability between x and y may be similar, and a deviation on their underlying causal relationship may pass undetected and undiscerned by only monitoring the covariance. In order to access and use the underlying information of the process correlation structure, alternative measures of structural relationships should be adopted in the process monitoring procedures.

An efficient way to explore the relationship for the underlying structure amongst variables is using causal information. A

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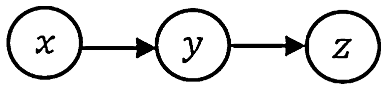

Fig. 1. Causal linkage of the variables x, y, and z.

causal map can clearly reflect the directional linkages between any two variables. In addition, the information of causal connectivity can be used to reduce the correlated degree for the feature space of correlation, thereby enhancing the performance of fault monitoring. It was shown in [21] that the monitoring performance was more sensitive in a space of uncorrelated features. For example, in Fig. 1, without considering the causal connectivity among the three variables, the feature representation of correlation contains three components, i.e., $r_{x,y}$, $r_{y,z}$, and $r_{x,z}$. From the causal links in Fig. 1, $r_{x,z}$ is redundant with ($r_{x,y}$, $r_{y,z}$). In other words, the inclusion of $r_{x,z}$ in the feature representation of correlation does not provide more information but increases the degree of correlation.

It is important to note that the directional connectivity of the components within the plant can play a significant role in fault monitoring [22–24]. Several papers describe the construction of the causal map from a process flow diagram or piping and instrumentation diagram [23,25,40]. Their results showed that data-driven techniques in combination with cause-and-effect relationships among process variables can lead to efficient monitoring of faults. The linkage of data-driven analysis with a causal relationship of the process has been identified as a promising approach to fault monitoring [22,23,25].

Previously, the authors introduced a feature representation of causal dependency (CD) to incorporate the data-driven techniques in conjunction with the causal information [26–28]. The CD is utilized to quantify the similarity between the relationship of two causally related variables under current operating conditions and historical operating conditions. It was reported in [29] that better fault monitoring results are achieved for features that are more application-dependent. In terms of application-dependence in process facilities, the CD is an appropriate feature to represent deviations in the process structure. In this article, an approach based on the CD feature representation is proposed for the monitoring of process structural faults. The proposed CD-based approach can potentially facilitate to detect process structural faults and to identify the root causes, owing to the finer description of the underlying structure and the less correlated feature space of the CD by utilizing causal information. Different from the previous work [27] and [28] which focused on the monitoring of *process variable faults*, this article investigates the monitoring of *process correlation structures*. In addition, this work incorporates a dimensionality reduction step based on Canonical Variate Analysis (CVA), which generates dynamic state-space models from the process data to improve the monitoring proficiency.

The rest of this paper is organized as follows. Section 2 briefly reviews the traditional CVA-based data-driven monitoring method. Section 3 describes the CD-based approach for monitoring process structural faults. The effectiveness of the proposed method is demonstrated by a gene network system in Section 4. Section 5 summarizes the conclusions.

2. Canonical variate analysis

The Canonical Variate Analysis (CVA) method, which serves as the technique in the step of dissimilarity quantification, is briefly reviewed in this section. More details of CVA can be found in [30,31].

2.1. CVA theorem

CVA is a dimensionality reduction technique in multivariate statistical analysis which maximizes the correlation between two selected sets of variables. Consider vectors of process variables $\boldsymbol{x} \in R^m$ and $\boldsymbol{y} \in R^n$ with covariance matrices $\Sigma_{\boldsymbol{xx}}$ and $\Sigma_{\boldsymbol{yy}}$ and cross-covariance matrix $\Sigma_{\boldsymbol{xy}}$. The orthogonal basis is chosen as those linear combinations of a variable set $\boldsymbol{x}$ that are more correlated with the linear combinations of another variable set $\boldsymbol{y}$ in the CVA approach, where these linear combinations are named *canonical variables* and are represented as $\boldsymbol{c}$ and $\boldsymbol{d}$, namely

$$\boldsymbol{c} = \boldsymbol{J}\boldsymbol{x} \tag{1}$$

$$\boldsymbol{d} = \boldsymbol{L}\boldsymbol{y} \tag{2}$$

where $\boldsymbol{J}$ and $\boldsymbol{L}$ are projection matrices that can be calculated by solving the SVD [31]:

$$\Sigma_{\boldsymbol{xx}}^{-1/2}\Sigma_{\boldsymbol{xy}}\Sigma_{\boldsymbol{yy}}^{-1/2} = \boldsymbol{U}\Sigma\boldsymbol{V}^{\mathrm{T}} \tag{3}$$

where Σ is the diagonal matrix of nonnegative singular values in descending order, and $\boldsymbol{U}$ and $\boldsymbol{V}$ are matrices of the right and left singular vectors. Then the projection matrices $\boldsymbol{J}$ and $\boldsymbol{L}$ are obtained by

$$\boldsymbol{J} = \boldsymbol{U}^{\mathrm{T}}\Sigma_{\boldsymbol{xx}}^{-1/2} \tag{4}$$

$$\boldsymbol{L} = \boldsymbol{V}^{\mathrm{T}}\Sigma_{\boldsymbol{yy}}^{-1/2} \tag{5}$$

The matrices $\boldsymbol{U}^{\mathrm{T}}$ and $\boldsymbol{V}^{\mathrm{T}}$ guarantee that the canonical variables are only pairwise correlated, and the matrices $\Sigma_{\boldsymbol{xx}}^{-1/2}$ and $\Sigma_{\boldsymbol{yy}}^{-1/2}$ scale the canonical variables so that $\boldsymbol{c}$ and $\boldsymbol{d}$ have unit variance.

2.2. CVA algorithm

Hotelling initially proposed the CVA concept for multivariate statistical analysis, which was not employed to system identification until Akaike's work on ARMA models [30]. The CVA method was further developed for identifying state-space models by Larimore [30]. Given time series output data $\boldsymbol{y}(t) \in R^{m_y}$ and input data $\boldsymbol{u}(t) \in R^{m_u}$, the linear state-space model is given by

$$\boldsymbol{x}(t+1) = \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{v}(t) \tag{6}$$

$$\boldsymbol{y}(t) = \boldsymbol{C}\boldsymbol{x}(t) + \boldsymbol{D}\boldsymbol{u}(t) + \boldsymbol{E}\boldsymbol{v}(t) + \boldsymbol{w}(t) \tag{7}$$

where $\boldsymbol{x}(t)$ is a state vector, $\boldsymbol{v}(t)$ and $\boldsymbol{w}(t)$ are independent white noise processes, and $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$, $\boldsymbol{D}$ and $\boldsymbol{E}$ are coefficient matrices.

Important to the CVA algorithm is the concept of past and future vectors. At a particular time instant $t \in (1, \cdots, n)$, the past vector $\boldsymbol{p}(t)$ containing the past outputs and inputs is

$$\boldsymbol{p}(t) = \left[\boldsymbol{y}^{\mathrm{T}}(t-1), \boldsymbol{y}^{\mathrm{T}}(t-2), \cdots, \boldsymbol{y}^{\mathrm{T}}(t-l), \boldsymbol{u}^{\mathrm{T}}(t-1), \boldsymbol{u}^{\mathrm{T}}(t-2), \cdots, \boldsymbol{u}^{\mathrm{T}}(t-l)\right]^{\mathrm{T}} \tag{8}$$

and the future vector $\boldsymbol{f}(t)$ comprising of the outputs in the present and future is

$$\boldsymbol{f}(t) = \left[\boldsymbol{y}^{\mathrm{T}}(t), \boldsymbol{y}^{\mathrm{T}}(t+1), \cdots, \boldsymbol{y}^{\mathrm{T}}(t+h)\right]^{\mathrm{T}} \tag{9}$$

where l and h are the numbers of lags in vectors $\boldsymbol{p}(t)$ and $\boldsymbol{f}(t)$, respectively.

By substituting the matrix $\Sigma_{\boldsymbol{xy}}$ with Σ_{pf}, $\Sigma_{\boldsymbol{xx}}$ with $\Sigma_{\boldsymbol{pp}}$, and $\Sigma_{\boldsymbol{yy}}$ with $\Sigma_{\boldsymbol{ff}}$, the matrices $\boldsymbol{J}$, $\boldsymbol{L}$, and $\boldsymbol{D}$ can be calculated via the SVD as (3). The states $\boldsymbol{x}(t)$ in (6) and (7) can be obtained from the data using the CVA states as

$$\boldsymbol{x}_d(t) = \boldsymbol{J}_d\boldsymbol{p}(t) = \boldsymbol{U}_d^{\mathrm{T}}\widehat{\Sigma}_{\boldsymbol{pp}}^{-1/2}\boldsymbol{p}(t) \tag{10}$$

where $\boldsymbol{J}_d = \boldsymbol{U}_d^{\mathrm{T}}\widehat{\Sigma}_{\boldsymbol{pp}}^{-1/2}$ and $\boldsymbol{U}_d$ contains the first d columns of $\boldsymbol{U}$ in (3) [31].