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# Canonical variate analysis-based contributions for fault identification

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ABSTRACT

While canonical variate analysis (CVA) has been used as a dimensionality reduction technique to take into account serial correlations in the process data with system dynamics, its effectiveness in fault identification (i.e., identification of variables most closely associated with a fault) in industrial processes has not been extensively investigated. This paper proposes CVA-based contributions for fault identification, where two types of contributions are developed based on the variations in the canonical state space and in the residual space. The two contributions are used to categorize faulty variables into state-space faulty variables (SSFVs) and residual-space faulty variables (RSFVs), which enhances the understanding of the character of each fault as well as the performance of fault monitoring based on different statistics. The effectiveness of the proposed approach is demonstrated on the Tennessee Eastman process. The simulation results show that the faulty variables identified by the CVA-based contributions can impact the statistics of the state space, the residual space, or both; and abnormal events are observed to be more often linked to faulty variables in the residual space rather than in the state space.



## 1. Introduction

A *fault* is defined as any abnormal event that occurs during process operations. Investigating the causes of faults is critical for the efficient and optimal operation of industrial processes. As manufacturing facilities become increasingly integrated and large-scale – largely due to efforts to reduce energy costs, maximize profit, and reduce environmental releases – the potential for faults to dynamically propagate in nonintuitive ways to produce significant harm to equipment, life, and the environment has increased. These trends motivate the development of methods to quickly identify variables associated with a fault as quickly as possible, preferably before its effects propagate to the extent of becoming a major safety concern. Such methods are collectively referred to as *fault identification*, in contrast to *fault detection*, which is the first step in a data-based process monitoring scheme that detects whether some fault has occurred, and *fault diagnosis*, in which the specific cause of the fault is determined.

Accurate first-principles dynamic models do not exist for most manufacturing facilities, which is why existing process monitoring systems in industry are typically constructed based on measured data collected and stored in a historical database. In this approach, information about the process operations needs to be abstracted from the historical data. This task of fault identification can be rather challenging when there are a large number of strongly correlated process variables, as is typical in most chemicals, petrochemicals, and refining operations.

The proficiency of identifying faults from data can be improved using dimensionality reduction techniques, such as principal component analysis (PCA) [1,2], partial least-squares (PLS) analysis [3,4], and canonical variate analysis (CVA) [5–7]. In statistical process monitoring, the PCA and PLS methods has been observed to perform well for process measurements when the in-control variations are independent and identically distributed (i.i.d.). With the i.i.d. assumption, the entire variability of the observations can be explained by estimating the covariance without time lags. If the vectors of observations are serially correlated, that is, the observations at one time instant are correlated with those at past time instants, the zero-lag covariance matrix cannot fully represent the entire variation.

To handle serially correlated multivariate observations, PCA [8] and PLS techniques [9] have been utilized by constructing a covariance matrix with time lags. A dynamic model is extracted directly from data by performing the time lagged version of PCA [10,11]. Utilizing the eigenvector of the covariance matrix that corresponds to the zero eigenvalue, a multivariate autoregressive with exogenous input (ARX) model is developed in [10]. The eigenvector corresponding to a nearly zero eigenvalue is an approximate representation of the ARX model [5,10]. A drawback of this approach

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is the inflexibility of the ARX model for the description of dynamic processes [12].

Aside from methods derived from PCA and PLS, CVA is also a dimensionality reduction technique that selects pairs of variables from the inputs and outputs that maximizes a correlation statistic [12–14]. This method takes serial correlations into account during the dimensionality reduction procedure. In the CVA approach, the statistical model extracted by the CVA approach is in the form of a state-space model where the state variables are statistically independent at zero lag [5].

Contribution plots [15] are the most popular technique for determining which variables are most strongly associated with the statistics no longer being within the normal operating condition (NOC). A higher contribution of a process variable indicates that the fault-related deviations in the specific variable are larger. Several efforts have been published that identified weaknesses and/or proposed modifications of contribution charts to improve their ability to identify the variables of most value in identifying the location of the fault (aka “faulty variables”). Utilizing a scheme of PCA-based contribution plot, Kourti and MacGregor [16] determined faulty variables of a high-pressure low-density polyethylene reactor, and reported that the PCA-based contribution plots may not always correctly identify the most important variables associated with a fault. Yue and Qin [17] proposed an index that combines $T^2$ and $Q$ statistics during fault identification, which was shown to be more effective than using a single statistic [18]. By introducing confidence limits into contribution plots, Westerhuis et al. [19] improved the statistical analysis of faulty variables, and concluded that the contribution plots should be carefully interpreted due to a smearing effect in the residuals of PCA. Since the smearing effect may mislead the determination of faulty variables, Liu [20] proposed contribution plots without the smearing effect on non-faulty variables by maximizing the reduction of a combined index through a missing data method. The data-driven and model-based methods for fault identification were comprehensively compared in [21], which reported that the identification of simple faults can be easily provided by contribution plots, while the determination of complicated faults needs additional information about the process operations. Furthermore, a reconstruction-based approach for determining faulty variables from the subspace of abnormal events is developed in [18,22], where an identification index is utilized to identify faults. The identification index is defined as the ratio of the reconstructed squared prediction error (SPE) to the faulty SPE.

Both PCA- and PLS-based contribution plots are limited in their ability to quickly identify faults because the underlying PCA and PLS methods do not produce the most accurate dynamic models, even when lagged data are used in their construction. This drawback has been recognized, and contribution plots in conjunction with state-space models have been carried out to better take into account the process dynamics [23–26,29]. In a few studies [23–25], subspace system identification based on N4SID has been utilized to obtain a state-space model that was used to construct contribution plots. Although CVA has been demonstrated to outperform N4SID for subspace identification in terms of stability and parsimony (fewer parameters) in the representation of dynamic systems [26–28], investigation on the application of contribution plots to CVA is limited. In one study where contribution plots and CVA-based state-space models were investigated [29], contributions were calculated based on the statistics of the states in the state-space model. In the study [29], process inputs were not considered in the state-space model.

In this article, the contribution plots are proposed to be applied to both the state space (retained states in the state-space model obtained via CVA) and the residual space (the rest of the states in the CVA model), to examine the utility of the two different measures for fault identification. The two types of contributions (state space and residual space) correspond to different characteristics of the process and can potentially provide more insights into the fault. This article plots the contributions as two-dimensional color maps, which allows improved fault identification compared to the traditional one-dimensional plots [30].

The rest of this paper is organized as follows. The CVA approach is briefly described in Section 2. The contribution maps for CVA-based state and residual spaces are developed in Section 3. The effectiveness of the proposed scheme is demonstrated in the Tennessee Eastman process in Section 4, followed by conclusions in Section 5.

## 2. Canonical variate analysis (CVA) revisited

### 2.1. The CVA statistical method

CVA is a dimensionality reduction technique in multivariate statistical analysis, which maximizes a correlation statistic with selected two sets of variables. Assuming process input and output vectors $\boldsymbol{x} \in R^m$ and $\boldsymbol{y} \in R^n$ with covariance matrices $\boldsymbol{\Sigma_{xx}}$ and $\boldsymbol{\Sigma_{yy}}$ and cross-covariance matrix $\boldsymbol{\Sigma_{xy}}$, matrices $\boldsymbol{J} \in R^{m\times m}$ and $\boldsymbol{L} \in R^{n\times n}$ can be obtained under the condition that

$$\begin{cases} \boldsymbol{J}\boldsymbol{\Sigma}_{xx}\boldsymbol{J}^{\mathrm{T}} = \boldsymbol{I}_{\overline{m}} \\ \boldsymbol{L}\boldsymbol{\Sigma}_{yy}\boldsymbol{L}^{\mathrm{T}} = \boldsymbol{I}_{\overline{n}} \end{cases} \tag{1}$$

and

$$\boldsymbol{J}\boldsymbol{\Sigma}_{xy}\boldsymbol{L}^{\mathrm{T}} = \boldsymbol{D} = \mathrm{diag}(\gamma_1, \ldots, \gamma_r, 0, \ldots, 0) \tag{2}$$

where $\overline{m} = \mathrm{rank}(\boldsymbol{\Sigma_{xx}})$, $\overline{n} = \mathrm{rank}(\boldsymbol{\Sigma_{yy}})$, $r = \mathrm{rank}(\boldsymbol{\Sigma_{xy}})$, $\gamma_i$ ($i = 1, 2, \ldots, r$) are canonical correlations with $\gamma_1 \geq \cdots \geq \gamma_r$, and $\boldsymbol{I}_k$ is a block-diagonal matrix with a $k \times k$ identity matrix as the first block and a zero matrix as the second block [13]. The vectors of canonical variables $\boldsymbol{c} = \boldsymbol{Jx}$ and $\boldsymbol{d} = \boldsymbol{Ly}$ contain a set of independent variables with the covariance matrix $\boldsymbol{\Sigma_{cc}} = \boldsymbol{I}_{\overline{m}}$ and $\boldsymbol{\Sigma_{dd}} = \boldsymbol{I}_{\overline{n}}$, respectively.

By solving the singular value decomposition (SVD)

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

the matrix of canonical correlations $\boldsymbol{D}$ can be computed as $\boldsymbol{D} = \boldsymbol{\Sigma}$; and the projection matrices $\boldsymbol{J}$ and $\boldsymbol{L}$ can be obtained as $\boldsymbol{J} = \boldsymbol{U}^T \boldsymbol{\Sigma_{xx}}^{-1/2}$ and $\boldsymbol{L} = \boldsymbol{V}^T \boldsymbol{\Sigma_{yy}}^{-1/2}$, respectively. The matrices $\boldsymbol{U}^{\mathrm{T}}$ and $\boldsymbol{V}^{\mathrm{T}}$ rotate the canonical variables to be pairwise correlated, and the matrices $\boldsymbol{\Sigma_{xx}}^{-1/2}$ and $\boldsymbol{\Sigma_{yy}}^{-1/2}$ scale the canonical variables to be unit variance.

### 2.2. CVA state vector

Hotelling proposed the CVA concept for multivariate statistical analysis, but CVA was not utilized for stochastic realization theory and system identification until Akaike's work on ARMA models [13]. The CVA approach was further developed using state-space models by Larimore [13]. 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 [31,33]

$$\boldsymbol{x}(t+1) = \boldsymbol{Ax}(t) + \boldsymbol{Bu}(t) + \boldsymbol{v}(t) \tag{4}$$

$$\boldsymbol{y}(t) = \boldsymbol{Cx}(t) + \boldsymbol{Du}(t) + \boldsymbol{Ev}(t) + \boldsymbol{w}(t) \tag{5}$$

where $\boldsymbol{x}(t) \in R^d$ is a $d$-dimensional 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.

At a particular time instant $t = 1, 2, \ldots$, the vector including the past information is given by

$$\boldsymbol{p}(t) = [\boldsymbol{y}^{\mathrm{T}}(t-1), \boldsymbol{y}^{\mathrm{T}}(t-2), \ldots, \boldsymbol{u}^{\mathrm{T}}(t-1), \boldsymbol{u}^{\mathrm{T}}(t-2), \ldots]^{\mathrm{T}} \tag{6}$$