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Variable Elimination-Based Contribution for Accurate Fault Identification ⋆

Yusuke Satoyama * **Koichi Fujiwara** * **Manabu Kano** *

* *Department of Systems Science, Kyoto University, Kyoto 606-8501, JAPAN (e-mail: manabu@human.sys.i.kyoto-u.ac.jp).*

Abstract: We propose a new fault identification method, which can describe the contribution of each process variable to a detected fault and identify a faulty variable more accurately than conventional methods. In the proposed method, in addition to a fault detection model that describes normal operating condition (NOC), multiple fault identification models that describe the same NOC are also constructed by eliminating one variable from all monitored variables at a time. After a fault is detected with the fault detection model, the fault detection index, e.g. a combined index of the T^2 and Q statistics, is calculated by using each of the fault identification models. When the faulty variable is eliminated, the index does not change before and after the fault occurs. On the other hand, when the normal variable is eliminated, the index is affected by the fault and increases after the fault occurs. Thus, the eliminated variable corresponding to the index that does not increase after the occurrence of the fault is identified as a faulty variable. In the proposed method, the ratio of the average index in NOC to the current index is used as a fault identification index or a contribution. To validate the proposed method, VEC was compared with the reconstruction-based contribution (RBC) through numerical examples. The results have demonstrated that VEC outperformed RBC in fault identification performance both in the linear case and in the nonlinear case.

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1. INTRODUCTION

To safely operate processes and consistently produce high-quality products, process monitoring is crucial in any industry. Because of the practicability, data-driven approaches have been widely investigated and used for fault detection, identification, and diagnosis. In particular, multivariate statistical process control (MSPC), which was proposed by Jackson and Mudholkar (1979), has been successfully applied to various industrial processes as a dominant tool of statistical process monitoring (Kresta et al., 1991; Nomikos and MacGregor, 1995; Kano and Nakagawa, 2008; Qin, 2012). In MSPC, principal component analysis (PCA) is applied to normal operation data to construct a PCA model that describes correlation among variables when process is operated in normal operating condition (NOC), and measurement samples are projected onto a principal component subspace (PCS) that represents variable correlation in NOC and a residual subspace (RS) that contains abnormality or noise. Then, two statistics are calculated as fault detection indices: T^2 and squared prediction error (SPE). The T^2 statistic is the mahalanobis distance from the origin to the sample projected onto the PCS, and the SPE, or Q statistic, is the distance to the sample projected onto the RS. The process is judged to deviate from NOC, that is, a fault is detected, when either T^2 or SPE exceeds the control limit.

Once a fault is detected, diagnosing the root cause is crucial for taking an appropriate action to recover process condition. PCA-based methods for fault identification or diagnosis have been developed. A contribution plot is a conventional method and has been widely used (MacGregor et al., 1994; Nomikos, 1996; Westerhuis et al., 2000). This method examines the contribution of each process variable to T^2 or SPE and identifies the variable corresponding to the largest contribution as the variable related to the root cause. However, Alcala and Qin (2009) pointed out that the faulty variable does not always have the largest contribution, and they proposed the alternative method using reconstruction-based contribution (RBC). In this method, after a fault is detected, the faulty sample is reconstructed by sliding the sample vector along each variable direction at a time so that the fault detection index is minimized, then the variable direction corresponding to the minimum index is identified as a faulty direction. The result of a numerical example showed that the diagnosability of this RBC method was higher than that of the conventional contribution plot.

The RBC method was extended to cope with nonlinear processes using kernel principal component analysis (KPCA), which can extract a nonlinear relationship among input variables by mapping the measurements from the original space to the feature space where linear PCA is performed (Alcala and Qin, 2010). KPCA has been used as a nonlinear process monitoring tool (Lee et al., 2004; Choi et al., 2005). In KPCA-based process monitoring,

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fault detection indices are defined in a similar way as PCA-based process monitoring, but the contribution is not used because the mapping function is not explicitly described. In the RBC method, the fault detection indices based on KPCA before and after reconstruction of each variable are used for the nonlinear fault identification.

However, as demonstrated through a case study in the fallowing section, the contribution of a normal variable may be estimated large, comparable with that of a faulty variable. In such a situation, the result of the RBC method can be misleading.

To overcome such weakness of the RBC methods, in the present work, we propose a new fault identification method which can accurately describe the contribution of each process variable to a detected fault and clearly identify a faulty variable. In addition to a fault detection model that describes normal operating condition (NOC), the proposed method constructs multiple fault identification models that describe the same NOC by eliminating one variable (or multiple variables if necessary) from all monitored variables at a time. After a fault is detected with the fault detection model, the fault detection index for a faulty sample is calculated by using each of the fault identification models and is compared to the corresponding fault detection index in NOC. The index calculated by eliminating the normal variable increases after a fault occurs, since it is still affected by the fault. On the other hand, the index calculated by eliminating the faulty variable does not change from that in NOC. Hence, the eliminated variable corresponding to the index that is kept small in faulty operating condition is identified as a faulty variable. In this work, the ratio of the average index in NOC to the index after a fault occurs is used for fault identification as a contribution of each variable. The proposed contribution is referred to as variable elimination-based contribution (VEC). The VEC-based fault identification method can be used with any modeling method or index. In addition, it is more intuitive and simple than the RBC method. To validate the proposed VEC method, it is compared with the RBC method in fault identification performance through several numerical examples.

2. RECONSTRUCTION-BASED CONTRIBUTION (RBC)

2.1 RBC with PCA

The RBC method is based on the idea of *fault identification via reconstruction* (Dunia and Qin, 1998). This method reconstructs a faulty sample by sliding it along each variable direction so that the SPE index is minimized, then it identifies the variable direction corresponding to the minimum index as a faulty direction.

In MSPC based on PCA, two fault detection indices are defined on the basis of the PCA model constructed from normal operation data. One is SPE, which detects abnormality that cannot be described by the PCA model representing NOC. For a new sample $\boldsymbol{x} \in \mathcal{R}^M$ that has measurements of M variables, SPE is defined as

$$\begin{aligned}\mathrm{SPE} &= \|(\boldsymbol{I}_M - \boldsymbol{P}\boldsymbol{P}^T)\boldsymbol{x}\|^2 \\ &= \boldsymbol{x}^T(\boldsymbol{I}_M - \boldsymbol{P}\boldsymbol{P}^T)\boldsymbol{x} \\ &= \boldsymbol{x}^T\tilde{\boldsymbol{C}}\boldsymbol{x} \end{aligned} \tag{1}$$

where $\boldsymbol{I}_M \in \mathcal{R}^{M\times M}$ is an identity matrix, $\boldsymbol{P} \in \mathcal{R}^{M\times R}$ is the PCA loading matrix, and $\tilde{\boldsymbol{C}} \in \mathcal{R}^{M\times M}$ represents the projection matrix to the RS. The other index is T^2, which is described as

$$\begin{aligned}T^2 &= \boldsymbol{t}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{t} \\ &= \boldsymbol{x}^T\boldsymbol{P}\boldsymbol{\Sigma}^{-1}\boldsymbol{P}^T\boldsymbol{x} \\ &= \boldsymbol{x}^T\boldsymbol{D}\boldsymbol{x} \end{aligned} \tag{2}$$

where $\boldsymbol{t} \in \mathcal{R}^R$ is the score vector for the new sample $\boldsymbol{x}$ and $\boldsymbol{\Sigma} \in \mathcal{R}^{R\times R}$ is a diagonal matrix that contains variances of principal components. Here, R is the number of principal components retained in the PCA model. The T^2 index shows whether or not the process operating condition is included in the range of NOC. The combined index of SPE and T^2 has been developed since it is preferred to monitor a single index rather than two indices simultaneously (Raich and Cinar, 1996). The combined index proposed by Yue and Qin (2001) is described as

$$\psi = \frac{\mathrm{SPE}}{\delta^2} + \frac{T^2}{\tau^2} = \boldsymbol{x}^T\left(\frac{\tilde{\boldsymbol{C}}}{\delta^2} + \frac{\boldsymbol{D}}{\tau^2}\right)\boldsymbol{x} = \boldsymbol{x}^T\boldsymbol{\Phi}\boldsymbol{x} \tag{3}$$

where δ^2 and τ^2 are control limits for SPE and T^2, and they are determined under the assumption that monitored variables follow a multivariate normal distribution.

A faulty sample $\boldsymbol{x}_f \in \mathcal{R}^M$ is reconstructed by sliding $\boldsymbol{x}_f$ along a variable direction as follows:

$$\boldsymbol{z}_m = \boldsymbol{x}_f - f_m\boldsymbol{\xi}_m \tag{4}$$

where $\boldsymbol{\xi}_m \in \mathcal{R}^M$ is the mth natural basis and describes the direction of the mth variable, and f_m is the magnitude of the fault along the mth variable direction. As shown in Eqs. (1) - (3), the general form of the fault detection index for the reconstructed sample $\boldsymbol{z}_m$ is discribed as

$$I(\boldsymbol{z}_m) = \boldsymbol{z}_m^T\boldsymbol{G}\boldsymbol{z}_m \tag{5}$$

where $\boldsymbol{G}$ represents $\tilde{\boldsymbol{C}}$ for SPE, $\boldsymbol{D}$ for T^2, and $\boldsymbol{\Phi}$ for ψ. The fault magnitude f_m is derived by minimizing $I(\boldsymbol{z}_m)$:

$$f_m = (\boldsymbol{\xi}_m^T\boldsymbol{G}\boldsymbol{\xi}_m)^{-1}\boldsymbol{\xi}_m^T\boldsymbol{G}\boldsymbol{x}_f. \tag{6}$$

The reconstruction-based contribution of the mth variable, RBC_m, is the fault detection index of the reconstructed portion along the mth variable direction.

$$\mathrm{RBC}_m = (f_m\boldsymbol{\xi}_m)^T\boldsymbol{G}(f_m\boldsymbol{\xi}_m). \tag{7}$$

Substituting Eq. (6) into Eq. (7), RBC_m of $\boldsymbol{x}_f$ is given as

$$\mathrm{RBC}_m = \frac{\left(\boldsymbol{\xi}_m^T\boldsymbol{G}\boldsymbol{x}_f\right)^2}{\boldsymbol{\xi}_m^T\boldsymbol{G}\boldsymbol{\xi}_m}. \tag{8}$$

2.2 RBC with KPCA

Alcala and Qin (2010) extended the RBC method for nonlinear processes with KPCA. KPCA models a nonlinear relationship among variables by mapping measurements from the original space to the feature space where linear PCA functions well. In a similar way as the RBC method with PCA, RBC of each variable is calculated on the basis of the KPCA model.

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