Variable Elimination-Based Contribution for Accurate Fault Identification

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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.

Keywords: Fault identification, fault diagnosis, multivariate statistical process control (MSPC), process monitoring, contribution plot, kernel principal component analysis, nonlinear systems.

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 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,
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 following 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 (Duina 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 \( x \) that has measurements of \( M \) variables, SPE is defined as

\[
SPE = \| (I_m - PP^T) x \|^2 = x^T (I_m - PP^T) x = x^T C x
\]

(1)

where \( I_m \in \mathbb{R}^{M \times M} \) is an identity matrix, \( P \in \mathbb{R}^{M \times R} \) is the PCA loading matrix, and \( C \in \mathbb{R}^{M \times M} \) represents the projection matrix to the RS. The other index is \( T^2 \), which is described as

\[
T^2 = t^T \Sigma^{-1} t = x^T P \Sigma^{-1} P^T x = x^T D x
\]

(2)

where \( t \in \mathbb{R}^R \) is the score vector for the new sample \( x \) and \( \Sigma \in \mathbb{R}^{R \times R} \) 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

\[
\psi = \frac{\delta^2 SPE + \tau^2 T^2}{\delta^2 + \tau^2} = x^T \left( \frac{C}{\delta^2} + \frac{D}{\tau^2} \right) x = x^T \Phi x
\]

(3)

where \( \delta^2 \) and \( \tau^2 \) 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 \( x_f \in \mathbb{R}^M \) is reconstructed by sliding \( x_f \) along a variable direction as follows:

\[
z_m = x_f - f_m \xi_m
\]

(4)

where \( \xi_m \in \mathbb{R}^M \) is the \( m \)th natural basis and describes the direction of the \( m \)th variable, and \( f_m \) is the magnitude of the fault along the \( m \)th variable direction. As shown in Eqs. (1) - (3), the general form of the fault detection index for the reconstructed sample \( z_m \) is described as

\[
I(z_m) = z_m^T G z_m
\]

(5)

where \( G \) represents \( C \) for SPE, \( D \) for \( T^2 \), and \( \Phi \) for \( \psi \). The fault magnitude \( f_m \) is derived by minimizing \( I(z_m) \):

\[
f_m = (\xi_m^T G \xi_m)^{-1} \xi_m^T G x_f.
\]

(6)

The reconstruction-based contribution of the \( m \)th variable, \( RBC_m \), is the fault detection index of the reconstructed portion along the \( m \)th variable direction.

\[
RBC_m = (f_m \xi_m)^T G (f_m \xi_m).
\]

(7)

Substituting Eq. (6) into Eq. (7), \( RBC_m \) of \( x_f \) is given as

\[
RBC_m = \frac{\xi_f^T G x_f}{\xi_m^T G \xi_m}.
\]

(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.
In KPCA, the $n$th sample $x_n \in \mathbb{R}^M$ is mapped onto the feature space by a mapping function $\phi_n = \phi(x_n)$, and the dot product is calculated with the kernel function $k$ as
\[
(\phi_i, \phi_j) = k(x_i, x_j).
\]
(9)

The kernel function plays an important role for linking the measurement to the corresponding feature mapping. Hence, the nonlinear mapping function $\phi$ does not have to be explicitly describe.

In the same way of applying PCA to the data matrix $X \in \mathbb{R}^{N \times M}$ which contains $N$ measurements of $M$ variables, PCA is applied to the feature matrix $X \in \mathbb{R}^{N \times P}$ which contains $N$ feature mappings in KPCA. Here, $P$ is the dimension of the feature space. The KPCA loading matrix $P_f \in \mathbb{R}^{P \times R}$ is given as
\[
P_f = X^T A \Sigma_f^{-\frac{1}{2}}
\]
(10)
where $A \in \mathbb{R}^{N \times R}$ is a matrix whose columns are eigenvectors of the kernel matrix $K \in \mathbb{R}^{N \times N}$ that composes of dot products of all pairs of $N$ feature mappings, and $\Sigma_f \in \mathbb{R}^{R \times R}$ is a diagonal matrix that contains eigenvalues. Here, $R$ is the number of principal components retained in the KPCA model.

For a new sample $x \in \mathbb{R}^M$, the fault detection indices, $\text{SPE}_f$ and $T_f^2$, are defined as
\[
\text{SPE}_f = \| (I - P_f P_f^T) \phi(x) \|^2
= k(x, x) - k(x)^T A \Sigma_f^{-1} A^T k(x)
= k(x, x) - k(x)^T C_f k(x)
\]
(11)
\[
T_f^2 = t_f^T \Sigma_f^{-1} t_f
= \phi(x)^T P_f \Sigma_f^{-1} P_f^T \phi(x)
= k(x)^T A \Sigma_f^{-1} A^T k(x)
= k(x)^T D_f k(x)
\]
(12)
where $t_f \in \mathbb{R}^R$ is the score vector for the sample $x$, and $k(x) \in \mathbb{R}^N$ composes of kernel functions of $x$ and $x_n \ (n = 1, 2, \ldots, N)$.

A combined index was proposed by Alcala and Qin (2010) in the same way as the PCA-based combined index.
\[
\psi_f = \frac{\text{SPE}_f}{\delta_f^2} + \frac{T_f^2}{\tau_f^2}
= \frac{k(x, x)}{\delta_f^2} + k(x)^T C_f k(x)
\]
(13)
\[
\Phi_f = \frac{D_f}{\tau_f^2} - \frac{C_f}{\delta_f^2}
\]
(14)
where $\delta_f^2$ and $\tau_f^2$ are control limits for $\text{SPE}_f$ and $T_f^2$. The control limits are determined by assuming that feature mappings follow a multivariate normal distribution.

A faulty sample $x_f \in \mathbb{R}^M$ is reconstructed along the $m$th variable direction as Eq. (4), and the fault detection index for the reconstructed sample $z_m$ is calculated through Eqs. (11) - (13). The fault magnitude $f_m$ that minimizes $\psi_f$ is derived as
\[
f_m = \frac{\xi_m B^T}{\delta_f^2} \left[ \frac{1}{N} - F \Phi_f k(z_m) \right]
\]
(15)
\[
k(z_m)^T \left[ \frac{1}{N} - F \Phi_f k(z_m) \right]
\]
where
\[
B = \left[ \begin{array}{ccc}
k(z_m, x_1)(x_f - x_1)^T \\
k(z_m, x_2)(x_f - x_2)^T \\
\vdots \\
k(z_m, x_N)(x_f - x_N)^T \\
\end{array} \right]
\]
(16)
\[
F = I - E.
\]
(17)

$E \in \mathbb{R}^{N \times N}$ is a matrix with all elements $1/N$. $\tilde{k}$ represents the kernel function of a pair of mean-centered feature mappings. However, $f_m$ is not explicitly solved because the right hand of Eq. (15) has the kernel functions of the reconstructed sample $z_m$, therefore Eq. (15) has to be solved iteratively. The RBC for the $n$th variable is $f_m^n$, which is used for identifying the faulty variable.

### 3. VARIABLE ELIMINATION-BASED CONTRIBUTION (VEC)

The proposed variable elimination-based contribution (VEC) method builds not only the fault detection model using all variables but also the fault identification models by eliminating one variable at a time. After a fault is detected with the fault detection model, the fault detection index is calculated by each of the fault identification models. Then, the eliminated variable corresponding to the index that does not change before and after occurrence of the fault is identified as a faulty variable.

Given a data matrix $X \in \mathbb{R}^{N \times M}$, which represents normal operating condition (NOC), with $N$ samples of $M$ variables, the VEC method builds fault identification models $M^{[n]} (m = 1, 2, \ldots, M)$ by eliminating the measurements of the $m$th variable. The fault identification models can be built by using PCA, KPCA, or any other method, which is used to build a fault detection model. The difference between the fault detection model and the fault identification models is the variables used for modeling. All $M$ variables are used in the fault detection model, while $M - 1$ variables are used in the fault identification models. If multiple variables need to be identified simultaneously, more than one variables are eliminated when fault identification models are constructed.

When a fault is detected, the fault detection index $I(x_f^{[m]})$ for the faulty sample $x_f \in \mathbb{R}^M$ is calculated using the fault identification models $M^{[m]}$. Here, $x_f^{[m]} \in \mathbb{R}^{M-1}$ represents the faulty sample whose measurement of the $m$th variable is eliminated.

The variable elimination-based contribution (VEC) of the $m$th variable, $VEC_m$, is defined as
\[
VEC_m = \frac{1}{N} \sum_{n=1}^{N} \frac{I(x^{[m]}_{\text{NOC}, n})}{I(x_f^{[m]})}
\]
(18)
where \( x^{[m]}_{\text{NOC},n} \) is the \( n \)th sample in NOC whose measurement of the \( m \)th variable is eliminated. The denominator of Eq. (18) is the fault detection index, and the numerator represents the mean fault detection index during NOC. The contribution \( VEC_m \) is used as the fault identification index. If the \( i \)th variable is the true cause of a fault, the fault detection index re-calculated by eliminating the \( i \)th variable does not change before and after the occurrence of the fault. On the other hand, the index re-calculated by eliminating the \( j \) (\( j \neq i \))th variable increases after the occurrence of the fault since it is affected by the \( i \)th faulty variable. Hence, the \( i \)th contribution \( VEC_i \) becomes much larger than \( j \)th contribution \( VEC_j \). Consequently, the VEC method can derive the contribution of each variable and identify the faulty variable(s) accurately.

## 4. NUMERICAL EXAMPLES

The proposed VEC method is compared with the conventional RBC method through numerical examples of a linear system and a nonlinear system based on the success rate of fault identification.

### 4.1 Linear system

As a numerical example of a linear system, the example provided by Alcala and Qin (2009) was adopted. The system with 6 measured variables is described as

\[
\begin{bmatrix}
    x_1 \\
    x_2 \\
    x_3 \\
    x_4 \\
    x_5 \\
    x_6
\end{bmatrix} =
\begin{bmatrix}
    -0.2310 & -0.0816 & -0.2662 \\
    -0.3241 & 0.7055 & -0.2158 \\
    -0.2170 & -0.3056 & -0.5207 \\
    -0.4089 & -0.3442 & -0.4501 \\
    -0.6408 & 0.3102 & 0.2372 \\
    -0.4655 & -0.4330 & 0.5938
\end{bmatrix}
\begin{bmatrix}
    s_1 \\
    s_2 \\
    s_3 \\
    s_4 \\
    s_5 \\
    e
\end{bmatrix} +
\begin{bmatrix}
    e_1 \\
    e_2 \\
    e_3 \\
    e_4 \\
    e_5 \\
    e_6
\end{bmatrix}
\] (19)

where \( s_1, s_2, \) and \( s_3 \) follow \( N(0,1^2), N(0,0.8^2), \) and \( N(0,0.6^2), \) respectively. Here, \( N(m, \sigma^2) \) is a normal distribution with the mean \( m \) and the variance \( \sigma^2 \). Measurement noise \( e_i (i = 1, 2, \ldots, 6) \) follow \( N(0,0.2^2) \). 100 samples were generated as normal operation data, and they were used to construct the PCA model representing NOC and determine the control limit for the combined index \( \psi \). The number of principal components was determined so that the model captured more than 90% of the variance of the data. The control limit for the fault detection index was determined at a confidence level of 0.95.

When a fault occurs at the \( m \)th sensor, the faulty sample \( x_f \in \mathbb{R}^6 \) is expressed as

\[
x_f = x^* + f_m \xi_m
\] (20)

where \( x^* \) is a normal portion of \( x_f \). In this example, 1000 test samples were generated under the assumption that the second variable was the root cause of the fault, that is, the fault occurs in the second variable direction \( \xi_2 = [0 \ 1 \ 0 \ 0 \ 0 \ 0]^T \), and the fault magnitude \( f_2 \) was a random number following \( U(0,5) \). Here, \( U(a,b) \) is a uniform distribution between \( a \) and \( b \). The test samples were monitored by using the fault detection model, then the faulty samples whose index exceeded the control limit were examined by the proposed VEC method and the conventional RBC method. The number of faulty samples was 805.

### 4.2 Nonlinear system

The proposed VEC method and the conventional RBC method were compared through a numerical example of a nonlinear system in the same way as the linear system. The system is described as

\[
\begin{bmatrix}
    x_1 \\
    x_2 \\
    x_3
\end{bmatrix} =
\begin{bmatrix}
    s_1 \\
    s_2 \\
    s_3
\end{bmatrix}
\] (21)

where \( s_1 \) and \( s_2 \) follow \( N(0,1^2) \). The measurement noise \( e_i (i = 1, 2, 3) \) follows \( N(0,1^2) \). 1000 test samples were generated using Eq. (21) for constructing the KPCA model of NOC and determining the control limit of the combined index \( \psi_f \). The KPCA model was built so that more than 90% of the variance of data was captured, and the control limit for the fault detection index was determined at a confidence level of 0.95. The Gaussian kernel with the parameter \( \sigma = 1 \) was used. 1000 test samples were generated using Eq. (20) by assuming that the third variable was the root cause of the fault and the fault magnitude was a random number following \( U(0,5) \). 932 samples were

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Table 1. Comparison between RBC and VEC in the linear case. Fault identification performance was evaluated on the basis of the rate for each variable to be identified as the faulty variable.

| Variable | RBC (%) | VEC (%) |
|----------|---------|---------|
| 1        | 0.8     | 0.4     |
| 2        | 93.8    | 94.7    |
| 3        | 0.1     | 0.0     |
| 4        | 0.5     | 0.9     |
| 5        | 2.6     | 2.3     |
| 6        | 2.2     | 1.7     |

The rate for each variable to be identified as the faulty variable is summarized in Table 1. The success rate of fault identification was 93.8% by the RBC method and 94.7% by the proposed VEC method. Both methods successfully identified the faulty variable 2. Figure 1 shows the box-and-whisker plots that describe the range of RBC and VEC for each variable. The lower and upper lines of each box correspond to the lower and upper quartiles and the center line is the median. The whiskers extending from the edges of the box show remaining samples and the cross plots are outliers. In the proposed VEC method, the contribution VEC of variable 2 is considerably larger than those of the other variables. Hence, variable 2 is judged as a faulty variable with confidence. On the other hand, in the conventional RBC method, the difference between the contribution RBC of variable 2 and those of variables 5 and 6 is not large in comparison with the VEC method. These results have shown that VEC is more reliable than RBC.
detected as faulty samples by the fault detection index $\psi_F$ and examined by the proposed VEC method and the RBC method.

The rate for each variable to be identified as the faulty variable is shown in Table 2. The proposed method successfully identified the faulty variable 3 in significantly high rate and outperformed the conventional RBC method. Figure 2 shows the range of RBC and VEC by using the box-and-whisker plots. It is clear that the difference between VEC of variable 3 and the others are significantly large, while the difference between RBC of variable 3 and the others are small.

### Table 2. Comparison between RBC and VEC in the nonlinear case. Fault identification performance was evaluated on the basis of the rate for each variable to be identified as the faulty variable.

| Variable | RBC (%) | VEC (%) |
|----------|---------|---------|
| 1        | 24.2    | 0.9     |
| 2        | 9.8     | 9.0     |
| 3        | 66.0    | 90.1    |

5. CONCLUSION

In the present work, we proposed a new fault identification method, which is referred to as the variable elimination-based contribution (VEC) method. The proposed method builds fault identification models by eliminating one variable from all monitored variables at a time in addition to the fault detection model describing the normal operating condition (NOC). When a fault is detected with the fault detection model, monitored variables are examined with the fault identification models. They can be constructed with any modeling method, which is used to build a fault detection model. The proposed VEC method was compared with the conventional RBC method in fault identification performance through numerical examples of the linear system and the nonlinear system. The results have demonstrated that the proposed VEC method outperformed the conventional RBC method in both linear
and nonlinear cases. The VEC method is effective for fault identification.

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