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Reconstruction-based Contribution for Process Monitoring

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Abstract: This paper presents a new method to perform fault diagnosis for data-correlation based process monitoring. As alternative to the traditional contribution plot method, reconstruction-based contribution of fault detection indices is proposed. The monitored indices are SPE, T^2 and a combined index φ. The lack of diagnosability of traditional contributions is analyzed for the case of single sensor faults with large fault magnitudes, whereas for the same case the proposed reconstruction-based contributions guarantee correct diagnosis. Monte Carlo simulation results are provided for the case of modest fault magnitudes by randomly assigning fault sensors and fault magnitudes.

Keywords: process monitoring; fault diagnosis; reconstruction; contribution analysis; diagnosability.

1. INTRODUCTION

Multivariate statistical methods such as principal component analysis (PCA) have been successfully applied to the monitoring of industrial processes (Nomikos and MacGregor [1995]; Wise and Gallagher [1996]). While much work has been reported in fault detection using data-correlation based models, only a few methods are available for fault diagnosis. As an early and popular method, contribution plots are used to diagnose the cause of a fault by determining the contribution of each variable to the fault detection statistics calculated (Miller et al. [1993], Nomikos and MacGregor [1995], Westerhuis et al. [2000]). Several approaches have been made for defining variable contributions (Nomikos [1997]; Wise et al. [2006]; Qin et al. [2001]; Cherry and Qin [2006]; Westerhuis et al. [2000]). Some of the approaches are complete partitions of the indices, some others involve several forms through approximations. Although the contribution plot approach is popular and has been adopted by many authors as the "default" method, there has been no rigorous analysis of diagnosability or guarantee of correct diagnosis in the literature. There are, however, reports that contribution plots involve fault "smearing" that can lead to misdiagnosis (Westerhuis et al. [2000]; Qin [2003]). The objective of this work is to propose a new method for contribution analysis based on the reconstruction of the fault detection index along the direction of a variable. In addition, a diagnosability analysis of traditional contributions and reconstruction-based contributions is performed.

2. STATISTICAL PROCESS MONITORING

2.1 Notation

A sample vector of n variables is denoted as $\mathbf{x} \in \Re^n$. If we assume that there are m samples, we can construct a data matrix $\mathbf{X} \in \Re^{m \times n}$ in which each row represents a sample. The data matrix is constructed as follows,

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}^T(1) \\ \mathbf{x}^T(2) \\ \vdots \\ \mathbf{x}^T(m) \end{bmatrix} \tag{1}$$

The sample mean and covariance of the variables are calculated from the data matrix $\mathbf{X}$ and used to scale the data to zero mean and unit variance. The covariance of $\mathbf{x}$ is approximated by the sample covariance matrix

$$\mathbf{S} \simeq \frac{1}{m-1}\mathbf{X}^T\mathbf{X} \tag{2}$$

Principal component analysis (PCA) performs eigendecomposition of the covariance matrix to obtain the principal and residual loadings, $\mathbf{P} \in \Re^{n\times l}$ and $\tilde{\mathbf{P}} \in \Re^{n\times(n-l)}$, where l is the number of principal components (PCs) retained in the model.

$$\begin{aligned}\mathbf{S} &= \bar{\mathbf{P}}\bar{\mathbf{\Lambda}}\bar{\mathbf{P}}^T = \begin{bmatrix}\mathbf{P} & \tilde{\mathbf{P}}\end{bmatrix}\begin{bmatrix}\mathbf{\Lambda} & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{\Lambda}}\end{bmatrix}\begin{bmatrix}\mathbf{P} & \tilde{\mathbf{P}}\end{bmatrix}^T \\ &= \mathbf{P}\mathbf{\Lambda}\mathbf{P}^T + \tilde{\mathbf{P}}\tilde{\mathbf{\Lambda}}\tilde{\mathbf{P}}^T\end{aligned} \tag{3}$$

The diagonal matrix $\mathbf{\Lambda}$ contains the principal eigenvalues and the diagonal matrix $\tilde{\mathbf{\Lambda}}$ contains the residual eigenvalues. It should be noticed that $\mathbf{P}$ and $\tilde{\mathbf{P}}$ are orthonormal.

A measurement $\mathbf{x}$ can be decomposed as

$$\mathbf{x} = \hat{\mathbf{x}} + \tilde{\mathbf{x}} \tag{4}$$

where

$$\mathbf{t} = \mathbf{P}^T\mathbf{x} \in \Re^l \tag{5}$$

$$\hat{\mathbf{x}} = \mathbf{P}\mathbf{P}^T\mathbf{x} = \mathbf{P}\mathbf{t} \tag{6}$$

are the scores and the projection to the PCS, respectively. The matrix $\mathbf{PP}^T$ is the projection matrix of the PCS and will be denoted as $\mathbf{C}$. The RS projection matrix will be denoted as $\tilde{\mathbf{C}}$ and the projection of $\mathbf{x}$ to the RS is defined as

$$\tilde{\mathbf{x}} = \tilde{\mathbf{P}}\tilde{\mathbf{P}}^T\mathbf{x} = \tilde{\mathbf{C}}\mathbf{x} \tag{7}$$

2.2 Fault Detection Indices

Statistical process monitoring makes use of statistical indices for fault detection. Qin [2003] summarizes five fault detection indices; among them, the most popular are SPE, T^2 and a combination of the two.

Squared prediction error, SPE The SPE index is defined as the squared norm of the residual vector $\tilde{\mathbf{x}}$.

$$SPE \equiv \|\tilde{\mathbf{x}}\|^2 = \mathbf{x}^T\tilde{\mathbf{P}}\tilde{\mathbf{P}}^T\mathbf{x} = \mathbf{x}^T\tilde{\mathbf{C}}\mathbf{x} \tag{8}$$

with a control limit δ^2 as

$$\delta^2 = g^{SPE}\chi^2_\alpha\left(h^{SPE}\right) \tag{9}$$

with $(1-\alpha)\times 100\%$ confidence level and

$$g^{SPE} = \frac{\theta_2}{\theta_1} \tag{10}$$

$$h^{SPE} = \frac{\theta_1^2}{\theta_2} \tag{11}$$

where $\theta_1 = \sum_{i=l+1}^{n}\lambda_i$, $\theta_2 = \sum_{i=l+1}^{n}\lambda_i^2$, and λ_i is the i^{th} eigenvalue of the covariance $\mathbf{S}$.

Hotelling's T^2 statistic The variation of a process in the PCS is measured by the T^2 index and it is defined as

$$T^2 = \mathbf{t}^T\mathbf{\Lambda}^{-1}\mathbf{t} = \mathbf{x}^T\mathbf{P}\mathbf{\Lambda}^{-1}\mathbf{P}^T\mathbf{x} = \mathbf{x}^T\mathbf{D}\mathbf{x} \tag{12}$$

where $\mathbf{D} = \mathbf{P}\mathbf{\Lambda}^{-1}\mathbf{P}^T$ is positive semidefinite. The process is normal if

$$T^2 \le \tau^2 \tag{13}$$

and the control limit τ^2 is

$$\tau^2 = \chi^2_\alpha\left(l\right) \tag{14}$$

with confidence level $(1-\alpha)\times 100\%$.

Combined index φ The combined index by Yue and Qin [2001] combines the SPE and T^2 indices into one single index as follows

$$\varphi = \frac{SPE}{\delta^2} + \frac{T^2}{\tau^2} = \mathbf{x}^T\mathbf{\Phi}\mathbf{x} \tag{15}$$

where

$$\mathbf{\Phi} = \frac{\tilde{\mathbf{C}}}{\delta^2} + \frac{\mathbf{D}}{\tau^2} \tag{16}$$

The process is considered normal if $\varphi \le \zeta^2$, where the control limit ζ^2 is

$$\zeta^2 = g^\varphi\chi^2_\alpha\left(h^\varphi\right) \tag{17}$$

where

$$g^\varphi = \left(\frac{l}{\tau^4} + \frac{\theta_2}{\delta^4}\right) / \left(\frac{l}{\tau^2} + \frac{\theta_1}{\delta^2}\right) \tag{18}$$

$$h^\varphi = \left(\frac{l}{\tau^2} + \frac{\theta_1}{\delta^2}\right)^2 / \left(\frac{l}{\tau^4} + \frac{\theta_2}{\delta^4}\right) \tag{19}$$

with $(1-\alpha)\times 100\%$ confidence level.

2.3 Fault diagnosis by contribution plots

A fault is detected after one or more fault detection indices exceed the control limits. Contribution plots are based on the idea that the variables with the largest contributions to the fault detection index are most likely the faulty variables. The contributions plots are constructed by determining the contribution of each variable to the fault detection index calculated. In order to calculate these contributions, first we have to notice that the expressions of the fault detection indices given by Equations 8, 12 and 15 have the general quadratic form

$$Index(\mathbf{x}) = \mathbf{x}^T\mathbf{M}\mathbf{x} = \|\mathbf{x}\|^2_M \tag{20}$$

where $\mathbf{M}$ is given in Table 1 for each index.

Table 1. Values of $\mathbf{M}$

Index	$\mathbf{M}$
SPE	$\tilde{\mathbf{C}}$
T^2	$\mathbf{D}$
φ	$\mathbf{\Phi}$

$Index(\mathbf{x})$ can be expressed as

$$\begin{aligned} Index(\mathbf{x}) &= \mathbf{x}^T\mathbf{M}\mathbf{x} = \|\mathbf{M}^{\frac{1}{2}}\mathbf{x}\|^2 \\ &= \sum_{i=1}^{n}\left(\xi_i^T\mathbf{M}^{\frac{1}{2}}\mathbf{x}\right)^2 = \sum_{i=1}^{n} c_i^{Index} \end{aligned} \tag{21}$$

where

$$c_i^{Index} = \left(\xi_i^T\mathbf{M}^{\frac{1}{2}}\mathbf{x}\right)^2 \tag{22}$$

is the contribution of variable x_i to $Index(\mathbf{x})$. Here ξ_i is the i^{th} column of the identity matrix and the direction of x_i; for example, in a system with five sensors, the direction of sensor x_3 is

$$\xi_3 = [0 \quad 0 \quad 1 \quad 0 \quad 0]^T \tag{23}$$

SPE contribution The variable contributions for the SPE index are obtained by substitution of $\mathbf{M} = \tilde{\mathbf{C}}$ into Equation 22

$$c_i^{SPE} = \left(\xi_i^T\tilde{\mathbf{C}}\mathbf{x}\right)^2 = \tilde{x}_i^2 \tag{24}$$

which is the definition given by Miller et al. [1993].

T^2 contribution The variable contributions for the T^2 index are obtained by substitution of $\mathbf{M} = \mathbf{D}$ into Equation 22

$$c_i^{T^2} = \left(\xi_i^T\mathbf{D}^{\frac{1}{2}}\mathbf{x}\right)^2 \tag{25}$$

which is the definition proposed by Wise et al. [2006].

φ contribution The variable contributions for the φ index are obtained by substitution of $\mathbf{M} = \mathbf{\Phi}$ into Equation 22

$$c_i^{\varphi} = \left(\xi_i^T \mathbf{\Phi}^{\frac{1}{2}} \mathbf{x}\right)^2 \tag{26}$$

Although there are other definitions for the variable contributions of the T^2 and φ indices, such definitions involve several forms through approximations (Nomikos [1997]; Qin et al. [2001]; Cherry and Qin [2006]). However, for all fault detection indices there are two common problems with the contribution plots.

i. When there is no fault, these contributions in Equations 24, 25 and 26 are uneven across variables. Therefore, a fault in a normally small-contributing variable may not have the largest contribution than other variables unless the fault magnitude is very large. This can be a source of misdiagnosis.
ii. As will be analyzed in Section 4 of this paper, these definitions of contributions can lead to misdiagnosis regardless of the fault magnitude even if a fault happens only to a single variable.

These defective characteristics of the existing contribution plots lead us to explore alternative methods for contribution analysis, which will be given in the next section.

3. CONTRIBUTION BY RECONSTRUCTION

The reconstruction of a fault detection index along a variable direction minimizes the effect of such variable over the detection index (Dunia and Qin [1998]). We can use the amount of reconstruction along a variable direction as an amount of contribution of the variable to the fault detection index that is reconstructed. Hence, this amount of reconstruction will be designated as the reconstruction-based contribution (RBC) of this variable to the fault detection index.

3.1 Reconstruction-based contribution

The reconstructed vector along direction ξ_i is

$$\mathbf{z}_i = \mathbf{x} - \xi_i f_i \tag{27}$$

and the fault detection index of the reconstructed measurement is

$$Index(\mathbf{z}_i) = \mathbf{z}_i^T \mathbf{M} \mathbf{z}_i = \|\mathbf{z}_i\|_M^2 \tag{28}$$

$$= \|\mathbf{x} - \xi_i f_i\|_M^2 \tag{29}$$

The task of reconstruction is to find a value of f_i such that $Index(\mathbf{z}_i)$ is minimized. This value of f_i is found to be

$$f_i = \left(\xi_i^T \mathbf{M} \xi_i\right)^{-1} \xi_i^T \mathbf{M} \mathbf{x} \tag{30}$$

The reconstruction-based contribution of variable x_i to the fault detection index, RBC_i^{Index}, can be calculated from Equations 29 and 30 as

$$\begin{aligned} RBC_i^{Index} &= \|\xi_i f_i\|_M^2 = \|\xi_i \left(\xi_i^T \mathbf{M} \xi_i\right)^{-1} \xi_i^T \mathbf{M} \mathbf{x}\|_M^2 \\ &= \mathbf{x}^T \mathbf{M} \xi_i \left(\xi_i^T \mathbf{M} \xi_i\right)^{-1} \xi_i^T \mathbf{M} \mathbf{x} \end{aligned} \tag{31}$$

Although the RBC approach is defined by reconstruction along each variable, the diagnosis power of RBC is not limited to single-variable faults. It is to be used exactly like the traditional contributions in Equations 24, 25 and 26. Furthermore, ξ_i direction in the above derivation does not have to be a sensor direction as in Equation 23; it can be an arbitrary process fault direction. In addition, ξ_i does not have to be a vector; it can be a column-like matrix representing a multi-dimensional fault or multiple sensor faults. Therefore, RBC is more general than the conventional contribution plots.

3.2 RBC of SPE index

RBC_i^{SPE} is obtained from Equation 31 using $\mathbf{M} = \tilde{\mathbf{C}}$

$$RBC_i^{SPE} = \mathbf{x}^T \tilde{\mathbf{C}} \xi_i \left(\xi_i^T \tilde{\mathbf{C}} \xi_i\right)^{-1} \xi_i^T \tilde{\mathbf{C}} \mathbf{x} = \frac{\left(\xi_i^T \tilde{\mathbf{C}} \mathbf{x}\right)^2}{\tilde{c}_{ii}} \tag{32}$$

where $\tilde{c}_{ii} = \xi_i^T \tilde{\mathbf{C}} \xi_i$ is the i^{th} diagonal element of $\tilde{\mathbf{C}}$.

3.3 RBC for the T^2 and φ indices

$RBC_i^{T^2}$ can be found by substitution of $\mathbf{M} = \mathbf{D}$ in Equation 31,

$$RBC_i^{T^2} = \mathbf{x}^T \mathbf{D} \xi_i d_{ii}^{-1} \xi_i^T \mathbf{D} \mathbf{x} = \frac{\left(\xi_i^T \mathbf{D} \mathbf{x}\right)^2}{d_{ii}} \tag{33}$$

where d_{ii} is the i^{th} diagonal element of $\mathbf{D}$.

Regarding the φ index, RBC_i^{φ} is calculated by substitution of $\mathbf{M} = \mathbf{\Phi}$ into Equation 31, which leads to

$$RBC_i^{\varphi} = \mathbf{x}^T \mathbf{\Phi} \xi_i \left(\xi_i^T \mathbf{\Phi} \xi_i\right)^{-1} \xi_i^T \mathbf{\Phi} \mathbf{x} = \frac{\left(\xi_i^T \mathbf{\Phi} \mathbf{x}\right)^2}{\phi_{ii}} \tag{34}$$

where ϕ_{ii} is the i^{th} diagonal element of $\mathbf{\Phi}$.

3.4 Control limits of reconstruction-based contributions

If there are no faults, the control limits for the RBC's of the three indices can be derived from Equation 31 applying the results of Box [1954]. These control limits, with $(1-\alpha) \times 100\%$ confidence level, are

$$\gamma^2_{(Index,i)} = g_i^{Index} \chi^2_{\alpha}\left(h_i^{Index}\right) \tag{35}$$

where

$$g_i^{Index} = \frac{\xi_i^T \mathbf{M} \mathbf{S} \mathbf{M} \xi_i}{\xi_i^T \mathbf{M} \xi_i} \tag{36}$$

and

$$h_i^{Index} = 1 \tag{37}$$

Unfortunately, these control limits cannot be used to identify which variable is the cause of the fault due to the effect of smearing in these contributions. In the next section we show that the effect of smearing exists even if the fault sample is only in a single sensor direction. Therefore, fault diagnosis can only be based on the magnitude of contributions.

4. DIAGNOSABILITY OF TRADITIONAL AND RBC CONTRIBUTIONS

Contribution analysis has been used for fault diagnosis for years, but there is no fundamental analysis on the conditions of correct fault identification using contributions. Westerhuis et al. [2000], for example, discuss that a fault in one variable smears to contributions of other variables in traditional contribution plots. In this section we show that RBC's also have smearing. However, we show that RBC's can always give correct fault diagnosis, while the traditional contributions cannot guarantee correct diagnosis even if the fault measurement is only in a single variable direction.
When there is a fault in a variable direction, the fault measurement can be represented as $\mathbf{x} = \mathbf{x}^* + \xi_j f$, where $\mathbf{x}^*$ is the fault-free part of the measurement and $\xi_j f$ is the faulty part, which is composed of the fault direction ξ_j, and the magnitude of the fault f. In the simple case where $\mathbf{x}$ is exactly in the ξ_j direction we have

$$\mathbf{x} = \xi_j f \tag{38}$$

We are concerned about whether or not the effect of a fault in Variable j is smeared into the contribution of Variable i and, if there is smearing, we want to know if c_j^{SPE} has the largest of the contributions.

4.1 Fault smearing and diagnosability of SPE contributions

The SPE contributions of a fault sample of the form in Equation 38 are

$$\begin{aligned} c_i^{SPE} &= \left(\xi_i^T \tilde{\mathbf{C}} \mathbf{x}\right)^2 = \left[\xi_i^T \tilde{\mathbf{C}} \left(\xi_j f\right)\right]^2 = \left(\tilde{c}_{ij} f\right)^2 \\ &= \begin{cases} \tilde{c}_{ij}^2 f^2 & \text{for } i \neq j \\ \tilde{c}_{jj}^2 f^2 & \text{for } i = j \end{cases} \end{aligned} \tag{39}$$

Similarly, the RBC_i^{SPE} values of this fault are

$$\begin{aligned} RBC_i^{SPE} &= \tilde{c}_{ii}^{-1} \left(\xi_i^T \tilde{\mathbf{C}} \mathbf{x}\right)^2 = \tilde{c}_{ii}^{-1} \left[\xi_i^T \tilde{\mathbf{C}} \left(\xi_j f\right)\right]^2 \\ &= \left(\tilde{c}_{ii}^{-\frac{1}{2}} \tilde{c}_{ij} f\right)^2 \\ &= \begin{cases} \tilde{c}_{ii}^{-1} \tilde{c}_{ij}^2 f^2 & \text{for } i \neq j \\ \tilde{c}_{jj} f^2 & \text{for } i = j \end{cases} \end{aligned} \tag{40}$$

Therefore, the effect of a fault in Variable j is smeared into the traditional contributions and RBC values of Variable i. A natural question is whether or not the smearing leads to misdiagnosis by c_i^{SPE} or RBC_i^{SPE}. This is, we want to know if the contribution plots will make c_j^{SPE} the largest. Correct diagnosis using c_i^{SPE} is guaranteed only if

$$\tilde{c}_{jj}^2 \geq \tilde{c}_{ij}^2 \tag{41}$$

and that using RBC_i^{SPE} is guaranteed only if

$$\tilde{c}_{jj} \geq \tilde{c}_{ii}^{-1} \tilde{c}_{ij}^2 \tag{42}$$

The next theorem gives the answers.

Theorem 1. Even if a fault sample $\mathbf{x}$ coincides with the j^{th} variable direction ξ_j, there is no guarantee that $c_j^{SPE} \geq c_i^{SPE}$ for $i \neq j$, but we always have $RBC_j^{SPE} \geq RBC_i^{SPE}$ for $i \neq j$.

The proof of this theorem is given in Appendix A. This theorem raises a serious question about the possibility of misdiagnosis using traditional contribution plots.

To give an example of misdiagnosis using c_i^{SPE} consider the case of three variables and the residual loadings $\tilde{\mathbf{p}} = [\tilde{p}_1 \quad \tilde{p}_2 \quad \tilde{p}_3]^T$. Since $\tilde{\mathbf{C}} = \tilde{\mathbf{p}}\tilde{\mathbf{p}}^T$ we have $\tilde{c}_{ij}^2 = \tilde{p}_i^2 \tilde{p}_j^2$. Assume $|\tilde{p}_1|$ is larger than $|\tilde{p}_2|$ and $|\tilde{p}_3|$ without loss of generality. If the fault is in Variable $j = 3$, the contributions to SPE are

$$\left[c_1^{SPE} \quad c_2^{SPE} \quad c_3^{SPE}\right] = \left[\tilde{p}_1^2 \tilde{p}_3^2 \quad \tilde{p}_2^2 \tilde{p}_3^2 \quad \tilde{p}_3^2 \tilde{p}_3^2\right] f^2 \tag{43}$$

The contribution of Variable 1, c_1^{SPE}, is the largest even though the fault is in Variable 3 direction.

4.2 Fault smearing and diagnosability of T^2 contributions

The T^2 contributions of a fault sample of the form in Equation 38 are

$$\begin{aligned} c_i^{T^2} &= \left(\xi_i^T \mathbf{D}^{\frac{1}{2}} \mathbf{x}\right)^2 = \left[\xi_i^T \mathbf{D}^{\frac{1}{2}} \left(\xi_j f\right)\right]^2 = \left([\mathbf{D}^{\frac{1}{2}}]_{ij} f\right)^2 \\ &= \begin{cases} [\mathbf{D}^{\frac{1}{2}}]_{ij}^2 f^2 & \text{for } i \neq j \\ \left[\mathbf{D}^{\frac{1}{2}}\right]_{jj}^2 f^2 & \text{for } i = j \end{cases} \end{aligned} \tag{44}$$

where $[\mathbf{D}^{\frac{1}{2}}]_{ij}$ is the ij^{th} element of the square root of $\mathbf{D}$.

The $RBC_i^{T^2}$ values of the fault sample are

$$\begin{aligned} RBC_i^{T^2} &= d_{ii}^{-1} \left(\xi_i^T \mathbf{D} \mathbf{x}\right)^2 = \left[d_{ii}^{-\frac{1}{2}} \xi_i^T \mathbf{D} \left(\xi_j f\right)\right]^2 \\ &= \left[d_{ii}^{-\frac{1}{2}} d_{ij} f\right]^2 \\ &= \begin{cases} d_{ii}^{-1} d_{ij}^2 f^2 & \text{for } i \neq j \\ d_{jj} f^2 & \text{for } i = j \end{cases} \end{aligned} \tag{45}$$

Similar to the SPE index, there is smearing of a fault in Variable j into Variable i and it is desirable to know whether or not the smearing effect may lead to misdiagnosis. Correct diagnosis for $c_i^{T^2}$ is guaranteed only if

$$[\mathbf{D}^{\frac{1}{2}}]_{jj}^2 \geq [\mathbf{D}^{\frac{1}{2}}]_{ij}^2 \tag{46}$$

and that for $RBC_i^{T^2}$ is guaranteed only if

$$d_{jj} \geq d_{ii}^{-1} d_{ij}^2 \tag{47}$$

The following theorem guarantees correct diagnosis using $RBC_i^{T^2}$ but not the traditional contribution $c_i^{T^2}$.

Theorem 2. Even if a fault sample $\mathbf{x}$ coincides with the j^{th} variable direction ξ_j, there is no guarantee that $c_j^{T^2} \geq c_i^{T^2}$ for $i \neq j$, but we always have $RBC_j^{T^2} \geq RBC_i^{T^2}$ for $i \neq j$.

The proof of this theorem is given in Appendix B.

4.3 Fault smearing and diagnosability of φ contributions

For the case of φ , the variable contributions of a fault sample of the form in Equation 38 are

$$c_i^{\varphi} = \left(\xi_i^T \mathbf{\Phi}^{\frac{1}{2}} \mathbf{x}\right)^2 = \left(\xi_i^T \mathbf{\Phi}^{\frac{1}{2}} \xi_j f\right)^2 = \left([\mathbf{\Phi}^{\frac{1}{2}}]_{ij} f\right)^2$$
$$= \begin{cases} [\mathbf{\Phi}^{\frac{1}{2}}]_{ij}^2 f^2 & \text{for } i \neq j \\ \left[\mathbf{\Phi}^{\frac{1}{2}}\right]_{jj}^2 f^2 & \text{for } i = j \end{cases} \quad (48)$$

The term $[\mathbf{\Phi}^{\frac{1}{2}}]_{ij}$ is the ij^{th} element of the squared root of matrix $\mathbf{\Phi}$.

The RBC_i^{φ} values of the fault measurement can be found in Equation 34 as

$$RBC_i^{\varphi} = \phi_{ii}^{-1} \left(\xi_i^T \mathbf{\Phi} \mathbf{x}\right)^2 = \left[\phi_{ii}^{-\frac{1}{2}} \xi_i^T \mathbf{\Phi} \left(\xi_j f\right)\right]^2$$
$$= \left[\phi_{ii}^{-\frac{1}{2}} \phi_{ij} f\right]^2$$
$$= \begin{cases} \phi_{ii}^{-1} \phi_{ij}^2 f^2 & \text{for } i \neq j \\ \phi_{jj} f^2 & \text{for } i = j \end{cases} \quad (49)$$

Similar to the SPE and T^2 indices, there is a smearing effect of a fault in Variable j into the values of c_i^{φ} and RBC_i^{φ}. We can guarantee correct diagnosis for c_j^{φ} only if

$$[\mathbf{\Phi}^{\frac{1}{2}}]_{jj}^2 \geq [\mathbf{\Phi}^{\frac{1}{2}}]_{ij}^2 \quad (50)$$

and for RBC_j^{φ} only if

$$\phi_{jj} \geq \phi_{ii}^{-1} \phi_{ij}^2 \quad (51)$$

The following theorem guarantees correct diagnosis using RBC_i^{φ} but not the traditional contributions c_i^{φ}.

Theorem 3. Even if a fault sample $\mathbf{x}$ coincides with the j^{th} variable direction ξ_j, there is no guarantee that $c_j^{\varphi} \geq c_i^{\varphi}$ for $i \neq j$, but we always have $RBC_j^{\varphi} > RBC_i^{\varphi}$ for $i \neq j$.

The proof of this theorem is given in Appendix C.

In summary, for the simple case of a sensor fault, RBC methods guarantee correct fault diagnosis, but the traditional contribution approaches do not guarantee it. The case depicted in Equation 38 is also the case of a very large fault magnitude which makes the normal portion $\mathbf{x}^*$ negligible. For modest fault magnitude the randomness in $\mathbf{x}^*$ will likely affect the diagnosis results, which will be studied next by simulation.

5. SIMULATION STUDY

The purpose of this example is to compare the rate of detection given by each fault detection index by Monte-Carlo simulation. In addition, the rate of correct fault diagnosis by the contribution approaches c_i^{Index} and RBC_i^{Index} will be determined given that a fault is detected using one of the fault detection indices. The process model to be used is

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} = \begin{bmatrix} -0.2310 & -0.0816 & -0.2662 \\ -0.3241 & 0.7055 & -0.2158 \\ -0.217 & -0.3056 & -0.5207 \\ -0.4089 & -0.3442 & -0.4501 \\ -0.6408 & 0.3102 & 0.2372 \\ -0.4655 & -0.433 & 0.5938 \end{bmatrix} \begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix} + noise \quad (52)$$

where t_1, t_2 and t_3 are zero-mean random variables with standard deviations of 1, 0.8 and 0.6, respectively. The noise included in the process is zero-mean with standard deviation of 0.2 and is normally distributed. In order to build the model, 1000 samples are generated. The data is scaled to zero-mean and unit variance. After generating and scaling the data, PCA is applied to make the model. The simulated faults are of the form

$$\mathbf{x}_{faulty} = \mathbf{x}^* + \xi_i f \quad (53)$$

where $\mathbf{x}^*$ is generated according to the model given above and the fault magnitude f is a random number uniformly distributed between 0 and 5. Also, the direction ξ_i is uniformly random out of the six possible variable directions. The number of simulated faults is 2000.

The rate of successful fault detection is given in Table 2 in three categories: faults detected by SPE, faults detected by T^2 and faults detected by φ. As we can see from Table 2, for single sensor faults the SPE index has a higher fault detection rate than the T^2 and φ indices. However, the difference between the SPE and φ rates is negligible compared to the difference between the SPE and T^2 rates.

Table 3 shows the rates of correct diagnosis given by the traditional contribution and RBC methods when a fault is detected by the SPE index (column 1), the T^2 index (column 2) and the φ index (column 3). For the first column, the first row shows the rate of correct diagnosis obtained when c_i^{SPE} and RBC_i^{SPE} are used, the second row shows rates of correct diagnosis given by $c_i^{T^2}$ and $RBC_i^{T^2}$, and the third row shows the diagnosis results of c_i^{φ} and RBC_i^{φ}. The second and third columns are similar to the first column except that, in these cases, the faults are detected using the T^2 and φ indices. In all cases in Table 3 the rate of correct diagnosis by RBC is larger than that of the traditional contribution methods. Also, the largest rates are given when the contribution approaches that involve the combined index are used.

Table 2. Percent of faults successfully detected by SPE, T^2, φ.

Index	SPE	T^2	φ
Rate(%)	78.4	25.7	76.5

Table 3. Rate of correct diagnosis given by c_i^{Index} and RBC_i^{Index} for faults detected by *Index*.

%	SPE		T^2		φ	
Index	Cont	RBC	Cont	RBC	Cont	RBC
SPE	78.3	90.9	60.7	91.1	78.0	91.2
T^2	46.8	57.6	93.8	95.8	48.0	58.3
φ	95.3	97.9	100	100	97.0	99.0

6. CONCLUSION

A new reconstruction-based contribution method is proposed for fault diagnosis as an alternative to the traditional contribution plots. This RBC method has a larger rate of correct fault diagnosis compared to the traditional contribution methods. Although the contribution plot method has been popular and adopted by many researchers and practitioners, it is surprising that, even for the simple case of sensor faults and large fault magnitudes, the traditional contribution plots fail to guarantee correct diagnosis results. On the other hand, the proposed reconstruction-based contribution method guarantees that the faulty variable has the largest contribution. For the case of modest fault magnitudes where the noise plays a role, Monte Carlo simulation results show that the proposed RBC method has a higher rate of correct diagnosis for SPE, T^2 and the combined index. To our knowledge this is the first work that provides rigorous analysis of the contribution plots, although evidence of misdiagnosis has been reported in the literature.

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Appendix A. PROOF OF THEOREM 1

Since $\tilde{\mathbf{C}} \geq 0$, we have

$$[\xi_i \quad \xi_j]^T \tilde{\mathbf{C}} [\xi_i \quad \xi_j] = \begin{bmatrix} \tilde{c}_{ii} & \tilde{c}_{ij} \\ \tilde{c}_{ij} & \tilde{c}_{jj} \end{bmatrix} \geq 0 \tag{A.1}$$

Since $\tilde{c}_{jj}^2 \geq \tilde{c}_{ij}^2$ does not always hold, $c_j^{SPE} \geq c_i^{SPE}$ is not guaranteed. However,

$$det \begin{bmatrix} \tilde{c}_{ii} & \tilde{c}_{ij} \\ \tilde{c}_{ij} & \tilde{c}_{jj} \end{bmatrix} = \tilde{c}_{ii}\tilde{c}_{jj} - \tilde{c}_{ij}^2 \geq 0 \tag{A.2}$$

$$\begin{aligned} \tilde{c}_{ii}\tilde{c}_{jj} &\geq \tilde{c}_{ij}^2 \\ \tilde{c}_{jj} &\geq \tilde{c}_{ii}^{-1}\tilde{c}_{ij}^2 \\ \tilde{c}_{jj}f^2 &\geq \tilde{c}_{ii}^{-1}\tilde{c}_{ij}^2 f^2 \\ RBC_j^{SPE} &\geq RBC_i^{SPE} \end{aligned} \tag{A.3}$$

Appendix B. PROOF OF THEOREM 2

Since $\mathbf{D} \geq 0$, we have $\mathbf{D}^{\frac{1}{2}} \geq 0$. Therefore

$$[\xi_i \quad \xi_j]^T \mathbf{D}^{\frac{1}{2}} [\xi_i \quad \xi_j] = \begin{bmatrix} \left[\mathbf{D}^{\frac{1}{2}}\right]_{ii} & \left[\mathbf{D}^{\frac{1}{2}}\right]_{ij} \\ \left[\mathbf{D}^{\frac{1}{2}}\right]_{ij} & \left[\mathbf{D}^{\frac{1}{2}}\right]_{jj} \end{bmatrix} \geq 0 \tag{B.1}$$

Since $[\mathbf{D}^{\frac{1}{2}}]_{jj}^2 \geq [\mathbf{D}^{\frac{1}{2}}]_{ij}^2$ does not always hold, $c_j^{T^2} \geq c_i^{T^2}$ is not guaranteed. However, from $\mathbf{D} \geq 0$ we have

$$[\xi_i \quad \xi_j]^T \mathbf{D} [\xi_i \quad \xi_j] = \begin{bmatrix} d_{ii} & d_{ij} \\ d_{ij} & d_{jj} \end{bmatrix} \geq 0 \tag{B.2}$$

$$det \begin{bmatrix} d_{ii} & d_{ij} \\ d_{ij} & d_{jj} \end{bmatrix} = d_{ii}d_{jj} - d_{ij}^2 \geq 0 \tag{B.3}$$

$$\begin{aligned} d_{ii}d_{jj} &\geq d_{ij}^2 \\ d_{jj} &\geq d_{ii}^{-1}d_{ij}^2 \\ d_{jj}f^2 &\geq d_{ii}^{-1}d_{ij}^2 f^2 \\ RBC_j^{T^2} &\geq RBC_i^{T^2} \end{aligned} \tag{B.4}$$

Appendix C. PROOF OF THEOREM 3

Since $\mathbf{\Phi} > 0$, we have $\mathbf{\Phi}^{\frac{1}{2}} > 0$. Therefore

$$[\xi_i \quad \xi_j]^T \mathbf{\Phi}^{\frac{1}{2}} [\xi_i \quad \xi_j] = \begin{bmatrix} \left[\mathbf{\Phi}^{\frac{1}{2}}\right]_{ii} & \left[\mathbf{\Phi}^{\frac{1}{2}}\right]_{ij} \\ \left[\mathbf{\Phi}^{\frac{1}{2}}\right]_{ij} & \left[\mathbf{\Phi}^{\frac{1}{2}}\right]_{jj} \end{bmatrix} > 0 \tag{C.1}$$

Since $\left[\mathbf{\Phi}^{\frac{1}{2}}\right]_{jj}^2 \geq \left[\mathbf{\Phi}^{\frac{1}{2}}\right]_{ij}^2$ does not always hold, $c_j^{\varphi} \geq c_i^{\varphi}$ is not guaranteed. On the other hand, from $\mathbf{\Phi} > 0$ we have

$$[\xi_i \quad \xi_j]^T \mathbf{\Phi} [\xi_i \quad \xi_j] = \begin{bmatrix} \phi_{ii} & \phi_{ij} \\ \phi_{ij} & \phi_{jj} \end{bmatrix} > 0 \tag{C.2}$$

$$det \begin{bmatrix} \phi_{ii} & \phi_{ij} \\ \phi_{ij} & \phi_{jj} \end{bmatrix} = \phi_{ii}\phi_{jj} - \phi_{ij}^2 > 0 \tag{C.3}$$

$$\begin{aligned} \phi_{ii}\phi_{jj} &> \phi_{ij}^2 \\ \phi_{jj} &> \phi_{ii}^{-1}\phi_{ij}^2 \\ \phi_{jj}f^2 &> \phi_{ii}^{-1}\phi_{ij}^2 f^2 \\ RBC_j^{\varphi} &> RBC_i^{\varphi} \end{aligned} \tag{C.4}$$