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Analysis and generalization of fault diagnosis methods for process monitoring

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Fault diagnosis

ABSTRACT

In process monitoring, several diagnosis methods have been used for fault diagnosis. These methods have been developed from different backgrounds and considerations. In this paper, five existing diagnosis methods are analyzed and generalized. It is shown that they can be unified into three general methods, making the original diagnosis methods special cases of the general ones. Also, a new form of relative contributions is proposed. An analysis of the diagnosability shows that some diagnosis methods do not guarantee correct diagnosis even for simple sensor faults with large magnitudes. For faults with modest fault magnitudes, Monte Carlo simulation is applied to compare the performance of the diagnosis methods.

1. Introduction

Process monitoring is used in industry to detect and diagnose abnormal behavior of processes. Multivariate statistical methods and model-based methods are employed in process monitoring. Among the statistical methods, a popular method used in industry is principal component analysis (PCA) [11,18,19]. PCA partitions the measurement space into a principal component subspace (PCS) and a residual subspace (RS). Fault detection makes use of fault detection indices. A fault is detected when one of the fault detection indices is beyond its control limit. After a fault is detected, it is necessary to diagnose its cause. There exist several methods to perform fault diagnosis. Some of these methods examine contributions of a variable to a fault detection index with the idea that the contributing variables will have high values. Contribution analysis methods that have been proposed include complete decomposition contributions (CDC), partial decomposition contributions (PDC), diagonal contribution (DC), reconstruction-based contributions (RBC), and angle-based methods (ABC). Table 1 shows the diagnosis methods, the authors who proposed them and the indices they were used with. As can be seen, some diagnosis methods have not been proposed for all fault detection indices. In addition, Dunia et al. [6] propose to use a reconstructed index for fault diagnosis which is related to RBC. It is not clear, however, whether these diagnosis methods are independent, and which methods would outperform for a specific detection index.

An essential requirement for fault diagnosis is to avoid misdiagnosis as much as possible. Although contribution plots have been popularly used as fault diagnosis methods, no rigorous analysis of diagnosability is given until recently [1,2]. Contribution plots basically calculate the contributions of variables under a fault situation and pick variables with large contribution as the likely cause of the fault. With this notion, a well-defined contribution analysis should have the following desirable properties:

1. When no faults are present, all variable contributions should have statistically the same mean. This will establish a level ground to compare the contributions when there is a fault; and
2. if a fault is mainly attributed to one variable, the contribution of that variable should be the largest.

One objective of this paper is to reveal which fault diagnosis methods possess the above properties. In order to do the analysis of the diagnosis methods, they are expressed in general forms so that they can be used with any fault detection index [3]. Then, it is shown that the diagnosis methods can be unified into general diagnosis methods, and control limits for these methods are provided. Furthermore, a new form of relative contribution is proposed. An analysis of the diagnosability of the unified methods and their relative contributions is performed, and the results are compared for the different diagnosis methods. Monte Carlo simulation is applied to compare the performance of the diagnosis methods when single sensor faults with modest fault magnitudes happen in a system. Finally, conclusions are given.

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Table 1
Diagnosis methods.

Method	Index		
	SPE	T^2	φ
CDC	Miller et al. [9]	Wise et al. (PLS-Toolbox)	N/A
PDC	N/A	Nomikos [10]	N/A
Diagonal	N/A	Qin et al. [13]	Cherry and Qin [5]
RBC	Alcala and Qin [1,2]		
Angle-based methods	Raich and Cinar [14] Yoon and MacGregor [20]		*N/A*

2. PCA for fault detection

2.1. PCA Model

In a process with n measured variables, a PCA model can be built using m measurements, $\mathbf{x} \in \Re^n$, taken under normal conditions. The measurements are arranged in a data matrix as

$$\mathbf{X} = [\mathbf{x}(1) \quad \mathbf{x}(2) \cdots \quad \mathbf{x}(m)]^T \tag{1}$$

where $\mathbf{X} \in \Re^{m \times n}$. Then, the data is scaled to zero mean and unit variance, and its covariance matrix is calculated as

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

The covariance matrix is eigen-decomposed to obtain the principal and residual loadings of the model as

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

where $\mathbf{P} \in \Re^{n \times l}$ and $\boldsymbol{\Lambda} \in \Re^{l \times l}$ are the principal loadings and eigenvalues of $\mathbf{S}$, respectively. The number of principal components (PCs) retained in the model is l. The projections to the principal and residual subspaces, $\hat{\mathbf{x}}$ and $\tilde{\mathbf{x}}$, are calculated as

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

where $\mathbf{C}$ and $\tilde{\mathbf{C}}$ are the projection matrices to the PCS and RS.

2.2. Fault detection indices

Fault detection indices are used to monitor the behavior of a process. There are several definitions of fault detection indices, among them, the most popular are the squared prediction error (SPE), which is also known as the Q statistic, the Hotelling's T^2 statistic and a combination of both indices. A summary of these fault detection indices is presented here. More details are given in Qin [12].

2.2.1. Squared prediction error, SPE

The SPE is defined as

$$SPE = \mathbf{x}^T\tilde{\mathbf{P}}\tilde{\mathbf{P}}^T\mathbf{x} = \mathbf{x}^T\tilde{\mathbf{C}}\mathbf{x} \tag{4}$$

Its control limit δ^2 is calculated as $\delta^2 = g^{SPE}\chi^2_\alpha(h^{SPE})$ with $(1-\alpha)\times 100\%$ confidence level, $g^{SPE} = \theta_2/\theta_1$, $h^{SPE} = \theta_1^2/\theta_2$, $\theta_1 = \sum_{i=l+1}^{n}\lambda_i$, $\theta_2 = \sum_{i=l+1}^{n}\lambda_i^2$, and λ_i is the ith eigenvalue of $\mathbf{S}$. Jackson and Mudholkar [7] proposed this index for fault detection and derived an alternative control limit using third order moment approximation.

2.2.2. Hotelling's T^2 statistic

The T^2 index is defined as

$$T^2 = \mathbf{x}^T\mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{P}^T\mathbf{x} = \mathbf{x}^T\mathbf{D}\mathbf{x} \tag{5}$$

where $\mathbf{D} = \mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{P}^T$, with a control limit $\tau^2 = \chi^2_\alpha(l)$ and confidence level of $(1-\alpha)\times 100\%$.

2.2.3. Combined index φ

The combined index, proposed by Yue and Qin [21], is defined as

$$\varphi = \mathbf{x}^T\boldsymbol{\Phi}\mathbf{x} \tag{6}$$

where

$$\boldsymbol{\Phi} = \frac{\tilde{\mathbf{C}}}{\delta^2} + \frac{\mathbf{D}}{\tau^2} \tag{7}$$

The control limit of this index is $\zeta^2 = g^{\varphi}\chi^2_\alpha(h^{\varphi})$, where

$$g^{\varphi} = \frac{l/\tau^4 + \theta_2/\delta^4}{l/\tau^2 + \theta_1/\delta^2} \tag{8}$$

$$h^{\varphi} = \frac{(l/\tau^2 + \theta_1/\delta^2)^2}{l/\tau^4 + \theta_2/\delta^4} \tag{9}$$

and it has a $(1-\alpha)\times 100\%$ confidence level.

2.2.4. General index

Since the fault detection indices are quadratic forms, the notation can be simplified by considering just one general index, $Index(\mathbf{x})$, as

$$Index(\mathbf{x}) = \mathbf{x}^T\mathbf{M}\mathbf{x} \tag{10}$$

where $\mathbf{M}$ is shown in Table 2 for each detection index. The control limit of $Index(\mathbf{x})$ can be calculated using the results of Box [4] as

$$\eta = g_{Index}\chi^2_\alpha(h_{Index}) \tag{11}$$

where

$$g_{Index} = \frac{tr\{\mathbf{SM}\}^2}{tr\{\mathbf{SM}\}} \tag{12}$$

and

$$h_{Index} = \frac{[tr\{\mathbf{SM}\}]^2}{tr\{\mathbf{SM}\}^2} \tag{13}$$

The expression $tr\{\mathbf{A}\}$ denotes the trace of matrix $\mathbf{A}$ and the confidence level of the control limit is $(1-\alpha)\times 100\%$.

3. Fault diagnosis methods

3.1. Complete decomposition contributions

The complete decomposition contribution (CDC) decomposes the fault detection index as the summation of the variable contributions. This is a widely used method in industry and is called

Table 2
Values of **M**.

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

contribution plots when applied with the SPE index [9]. Wise et al. [17] proposed the CDC for the T^2 index. In general, the CDC is defined as

$$Index(\mathbf{x}) = \mathbf{x}^T\mathbf{M}\mathbf{x} = \|\mathbf{M}^{(1/2)}\mathbf{x}\|^2 = \sum_{i=1}^{n}\left(\xi_i^T\mathbf{M}^{(1/2)}\mathbf{x}\right)^2 = \sum_{i=1}^{n} CDC_i^{Index}$$

where

$$CDC_i^{Index} = \mathbf{x}^T\mathbf{M}^{(1/2)}\xi_i\xi_i^T\mathbf{M}^{(1/2)}\mathbf{x} \tag{14}$$

Here, ξ_i is the i th column of the identity matrix

$$\xi_i = [0 \quad 0\cdots1\cdots0]^T \tag{15}$$

For SPE, $\mathbf{M} = \tilde{\mathbf{C}}$. Since $\tilde{\mathbf{C}}$ is idempotent, $\tilde{\mathbf{C}}^{(1/2)} = \tilde{\mathbf{C}}$. Therefore,

$$\mathbf{M}^{(1/2)}\mathbf{x} = \tilde{\mathbf{C}}^{(1/2)}\mathbf{x} = \tilde{\mathbf{C}}x = \tilde{\mathbf{x}} \tag{16}$$

and

$$CDC_i^{SPE} = \left(\xi_i^T\tilde{\mathbf{x}}\right)^2 = \tilde{x}_i^2 \tag{17}$$

For the T^2 index

$$CDC_i^{T^2} = \left(\xi_i^T\mathbf{P}\boldsymbol{\Lambda}^{-(1/2)}\mathbf{P}^T\mathbf{x}\right)^2 \tag{18}$$

Wise et al. [17] defined $CDC_i^{T^2}$ by rearranging

$$T^2 = \mathbf{x}^T\mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{P}^T\mathbf{x} = \|\mathbf{P}\boldsymbol{\Lambda}^{-(1/2)}\mathbf{P}^T\mathbf{x}\|^2 \tag{19}$$

By setting $\mathbf{M} = \boldsymbol{\Phi}$, the CDC_i^{φ} is defined, which has not been published in the past.

3.2. Partial decomposition contributions

As the name suggests, the partial decomposition contribution (PDC) partially decomposes a fault detection index as the summation of variable contributions. It was first proposed by Nomikos [10] for the T^2 index. The PDC for T^2 index was defined as

$$T^2(\mathbf{x}) = \mathbf{x}^T\mathbf{D}\mathbf{x} = \mathbf{x}^T\mathbf{D}\mathbf{I}\mathbf{x} = \mathbf{x}^T\mathbf{D}\left(\sum_{i=1}^{n}\xi_i\xi_i^T\right)\mathbf{x} = \sum_{i=1}^{n}\mathbf{x}^T\mathbf{D}\xi_i\xi_i^T\mathbf{x}$$

where

$$PDC_i^{T^2} = \mathbf{x}^T\mathbf{D}\xi_i\xi_i^T\mathbf{x} \tag{20}$$

The previous result is obtained using the relationship $\mathbf{I} = \sum_{i=1}^{n}\xi_i\xi_i^T$. In the general case, $\mathbf{D}$ is substituted by $\mathbf{M}$ to obtain

$$PDC_i^{Index} = \mathbf{x}^T\mathbf{M}\xi_i\xi_i^T\mathbf{x}. \tag{21}$$

Here, it should be noted that, even though $\mathbf{M}$ and $\xi_i\xi_i^T$ are positive semidefinite matrices, $\mathbf{M}\xi_i\xi_i^T$ might not be positive semidefinite [22]. A consequence of this fact is that the PDC could have negative values. This result was shown by Westerhuis et al. [16] for the T^2 index in a system with two variables.

3.3. Diagonal contributions

The block-diagonal contribution was proposed by Qin et al. [13] to define block contributions by keeping the block-diagonal terms only for the T^2 index for multi-block process monitoring. Cherry and Qin [5] used it with the φ index. In the limiting case that each block includes only one variable, variable diagonal contributions (DC) can be defined in a similar way as follows,

$$DC_i^{T^2} = \mathbf{x}^T\xi_i\xi_i^T\mathbf{D}\xi_i\xi_i^T\mathbf{x} == d_{ii}x_i^2 \tag{22}$$

It can been seen for this limiting case the diagonal contributions reduces to univariate monitoring of the i th variable. While this is not recommended for fault detection as it ignores variable correlation, it can serve as a contribution analysis method for fault diagnosis. For a general index, the DC is calculated as

$$DC_i^{Index} = \mathbf{x}^T\xi_i\xi_i^T\mathbf{M}\xi_i\xi_i^T\mathbf{x} \tag{23}$$

3.4. Reconstruction-based contributions

The reconstruction-based contribution (RBC) uses the amount of reconstruction of a fault detection index along a variable direction as the contribution of that variable. It was proposed by Alcala and Qin [1,2]. The index of a reconstruction along a variable direction ξ_i is

$$Index\left(\mathbf{x}_i^r\right) = \|\mathbf{M}^{(1/2)}\mathbf{x}_i^r\|^2 = \|\mathbf{M}^{(1/2)}\left(\mathbf{x} - \xi_i f\right)\|^2 \tag{24}$$

where f is the reconstructed portion to be determined. The best reconstruction by minimizing the above index gives the optimal value for f,

$$f = \left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}\left(\xi_i^T\mathbf{M}\mathbf{x}\right) \tag{25}$$

The RBC is defined as

$$\begin{aligned} RBC_i^{Index} &= \|\mathbf{M}^{(1/2)}\xi_i f\|^2 \\ &= \mathbf{x}^T\mathbf{M}\xi_i\left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}\xi_i^T\mathbf{M}\mathbf{x} \end{aligned} \tag{26}$$

$$= \frac{\left(\xi_i^T\mathbf{M}\mathbf{x}\right)^2}{\xi_i^T\mathbf{M}\xi_i}. \tag{27}$$

3.5. Angle-based contributions

Angle information has been used for diagnosis by Raich and Cinar [14], and by Yoon and MacGregor [20]. The angle-based contribution (ABC) is formally defined as follows. For a fault sample $\mathbf{x}$, the angled-based contribution of the i th variable is measured by the angle between $\mathbf{x}$ and ξ_i after they are projected or rotated by $\mathbf{M}^{(1/2)}$. The projected vectors are

$$\bar{\xi}_i = \mathbf{M}^{(1/2)}\xi_i \quad \bar{\mathbf{x}} = \mathbf{M}^{(1/2)}\mathbf{x}$$

The ABC of variable i is the squared cosine of the angle between $\bar{\mathbf{x}}$ and $\bar{\xi}_i$, which is

$$ABC_i^{Index} = \left(\frac{\bar{\xi}_i^T\bar{\mathbf{x}}}{\|\bar{\xi}_i\|\|\bar{\mathbf{x}}\|}\right)^2 = \frac{\left(\xi_i^T\mathbf{M}\mathbf{x}\right)^2}{\xi_i^T\mathbf{M}\xi_i\mathbf{x}^T\mathbf{M}\mathbf{x}} \tag{28}$$

$$= \frac{RBC_i^{Index}}{Index(\mathbf{x})} \tag{29}$$

As can be seen, ABC and RBC differ only by $Index(\mathbf{x})$, which is independent of the Variable i. Therefore, the diagnosis results will be the same for ABC and RBC. In the rest of the paper, only RBC will be used for fault diagnosis.

From the optimal reconstruction in Eqs. (24) and (25), it is easy to show that

$$\|\mathbf{M}^{(1/2)}\mathbf{x}\|^2 = \|\mathbf{M}^{(1/2)}\left(\mathbf{x} - \xi_i f\right)\|^2 + \|\mathbf{M}^{(1/2)}\xi_i f\|^2$$

that is

$$Index(\mathbf{x}) = Index(\mathbf{x}_i^r) + RBC_i^{Index}. \tag{30}$$

Therefore,

$$ABC_i^{Index} = \frac{RBC_i^{Index}}{Index(\mathbf{x})} = 1 - \frac{Index(\mathbf{x}_i^r)}{Index(\mathbf{x})} \tag{31}$$

Dunia et al. [6] propose to use the reconstructed index and the ratio $Index(\mathbf{x}_i^r)/Index(\mathbf{x})$ for fault diagnosis. It is therefore clear that the angle-based contribution and the reconstruction method by Dunia et al. [6] are complementary.

Table 3
Control limits of diagnosis methods.

Method	Control limit
CDC	$\xi_i^T \mathbf{SM}\xi_i \chi^2_\alpha(1)$
PDC	$\xi_i^T \mathbf{SM}\xi_i \pm 3\sqrt{\left(\xi_i^T \mathbf{SM}\xi_i\right)^2 + \xi_i^T \mathbf{SM}^2\xi_i\xi_i^T \mathbf{S}\xi_i}$
RBC	$\frac{\xi_i^T \mathbf{MSM}\xi_i}{\xi_i^T \mathbf{M}\xi_i}\chi^2_\alpha(1)$
DC	$\xi_i^T \mathbf{S}\xi_i\xi_i^T \mathbf{M}\xi_i \chi^2_\alpha(1)$

3.6. General decompositive contributions

The complete and partial decomposition contributions can be unified into a more general type of contribution, the general decompositive contribution (GDC), which is defined as

$$GDC_i^{Index} = \mathbf{x}^T \mathbf{M}^{1-\beta}\xi_i\xi_i^T \mathbf{M}^{\beta}\mathbf{x}, \quad 0 \le \beta \le 1 \tag{32}$$

The PDC is just a special case of GDC when $\beta = 0$ or $\beta = 1$. This can be seen from

$$GDC_i^{Index} = \mathbf{x}^T \mathbf{M}\xi_i\xi_i^T \mathbf{x} = PDC_i^{Index}$$

and, when $\beta = \frac{1}{2}$, the CDC is obtained. The latter comes from

$$GDC_i^{Index} = \mathbf{x}^T \mathbf{M}^{(1/2)}\xi_i\xi_i^T \mathbf{M}^{(1/2)}\mathbf{x} = CDC_i^{Index}$$

Since ABC is a scaled version of RBC, RBC will be used as a general case for both diagnosis methods. Therefore, the five diagnosis methods can be unified into three general diagnosis methods: general decompositive contributions, reconstruction-based contributions and diagonal contributions.

4. Control limits for fault-free contributions

We can see from Eqs. (14), (20), (26), (23) and (32) that the contributions have the form $\mathbf{x}^T\mathbf{A}\mathbf{x}$. Control limits of the fault-free contributions can be calculated using the results of Box [4] if $\mathbf{A} \geq 0$. This is the case of CDC, RBC and DC. However, for the case of PDC, and, in general for GDC with $\beta \neq 1/2$, $\mathbf{A}$ is not guaranteed to be positive semidefinite. In this case, the upper and lower limits are calculated as three times the standard deviation above and below the mean of the contributions. Table 3 shows these control limits and their calculation is shown in Appendix A. It should be noted that the control limits are to be used in the next section to define relative contributions. Some work in the literature suggests the use of control limits for determining significant contributing variables to a fault situation. This should be discouraged as fault free variables can show increased contributions due to smearing in general.

5. Relative contributions

A minimum requirement for fault diagnosis is that variable contributions should be statistically equal when there is no fault in the system. In order to have statistically equal contributions, each contribution can be divided by its expectation, which results in what will be called a relative contribution whose expectation is 1. In order to see this, the relative contribution, rC_i^{Index}, of a contribution C_i^{Index} can be defined as

$$rC_i^{Index} = \frac{C_i^{Index}}{E\{C_i^{Index}\}} \tag{33}$$

The expectation of rC_i^{Index} is

$$E[rC_i^{Index}] = E[\frac{C_i^{Index}}{E\{C_i^{Index}\}}] = \frac{E\{C_i^{Index}\}}{E\{C_i^{Index}\}} = 1$$

Table 4
Relative contributions based on expectation.

Method	Expectation of contributions	Rel. contributions	Expression
GDC	$\xi_i^T \mathbf{SM}\xi_i$	rGDC	$\frac{\mathbf{x}^T \mathbf{M}^{1-\beta}\xi_i\xi_i^T \mathbf{M}^{\beta}\mathbf{x}}{\xi_i^T \mathbf{SM}\xi_i}$
CDC		rCDC	$\frac{\left(\xi_i^T \mathbf{M}^{(1/2)}\mathbf{x}\right)^2}{\xi_i^T \mathbf{SM}\xi_i}$
PDC		rPDC	$\frac{\mathbf{x}^T \mathbf{M}\xi_i\xi_i^T \mathbf{x}}{\xi_i^T \mathbf{SM}\xi_i}$
RBC	$\frac{\xi_i^T \mathbf{MSM}\xi_i}{\xi_i^T \mathbf{M}\xi_i}$	rRDC	$\frac{\left(\xi_i^T \mathbf{Mx}\right)^2}{\xi_i^T \mathbf{MSM}\xi_i}$
DC	$\xi_i^T \mathbf{S}\xi_i\xi_i^T \mathbf{M}\xi_i$	rDC	$\frac{\mathbf{x}^T \xi_i\xi_i^T \mathbf{x}}{\xi_i^T \mathbf{S}\xi_i}$

Relative contributions have been suggested by authors like Westerhuis et al. [16]. They use the control limits of the contributions as scaling factors. This is based on the idea that, when a fault happens in a variable with a normally small contribution, another variable, with a normally large contribution, might be identified as the faulty one. The expectations of the contributions and their relative contributions are shown in Table 4. The calculation of the contribution expectations are shown in Appendix C.

As shown in Tables 3 and 4, the control limits and expectations of the contributions differ by a factor $\chi^2_\alpha(1)$ in most cases; this makes both relative contributions approaches to have essentially the same diagnosis results. Despite of this, an advantage of using the expectation for the relative contributions is that the expectation is easier to calculate than the control limits.

It is interesting to note that the value of the relative diagonal contribution is independent of the fault detection index used to calculate it. Also, it is clear that the methods in the first column of Table 4 do not have, statistically, the same contributions when there are no faults. The relative contribution methods in column 3 possess this property.

6. Analysis of diagnosability

A fault in Sensor j is represented as $\mathbf{x} = \mathbf{x}^* + \xi_j f$; here, $\mathbf{x}^*$ is the fault-free part of the measurement, ξ_j is the direction of the fault and f its magnitude. If the fault is very large, compared to the fault-free measurement, the faulty measurement can be expressed as

$$\mathbf{x} = \xi_j f. \tag{34}$$

This sensor fault is the simplest kind of fault that can happen in a process. A basic requirement for a diagnosis method is that the diagnosis of this fault should point to the right variable or fault. If the diagnosis method is not able to do so, then there is no guarantee that such method will diagnose correctly more complex faults.

6.1. Diagnosis using general decompositive contributions

Substituting the fault in Eq. (34) into Eq. (32) we get

$$GDC_i^{Index} = \begin{cases} [\mathbf{M}^{1-\beta}]_{ij}[\mathbf{M}^{\beta}]_{ij} f^2 & \text{for} \quad i \neq j \\ [\mathbf{M}^{1-\beta}]_{jj}[\mathbf{M}^{\beta}]_{jj} f^2 & \text{for} \quad i = j \end{cases}$$

In this equation, we use the notation $[\mathbf{M}^{1-\beta}]_{ij} = \xi_i^T \mathbf{M}^{1-\beta}\xi_j$ and $[\mathbf{M}^{\beta}]_{ij} = \xi_i^T \mathbf{M}^{\beta}\xi_j$. Correct diagnosis is guaranteed if the GDC of the non faulty variable is less than or equal to the GDC of the faulty variable, this is, if

$$[\mathbf{M}^{1-\beta}]_{ij}\left[\mathbf{M}^{\beta}\right]_{ij} \le [\mathbf{M}^{1-\beta}]_{jj}[\mathbf{M}^{\beta}]_{jj} \tag{35}$$

Here, we consider two cases. One is for $\beta = 0$, where $\mathbf{M}^{\beta}$ is the identity matrix, in which case $[\mathbf{M}^{\beta}]_{ij} = 0$ for $i \neq j$. Therefore, from

Eq. (35), correct diagnosis is guaranteed if

$$0 \leq [\mathbf{M}]_{jj} \tag{36}$$

Since this inequality always holds for positive semidefinite matrices, correct diagnosis is guaranteed for $\beta = 0$, and this corresponds to the case of PDC.

The other case is for $\beta = (1/2)$, which is the case of CDC, and guarantees correct diagnosis if

$$[\mathbf{M}^{(1/2)}]_{ij}^2 \leq [\mathbf{M}^{(1/2)}]_{jj}^2 \tag{37}$$

However, in general, the relationship in Eq. (37) does not hold; therefore, correct diagnosis is not guaranteed for CDC.

6.1.1. Diagnosis-ability of Relative GDC

Substitution of the fault in Eq. (34) in the expression for rGDC in Table 4 leads to

$$rGDC_i^{Index} = \begin{cases} \dfrac{[\mathbf{M}^{1-\beta}]_{ij}[\mathbf{M}^{\beta}]_{ij}}{\xi_i^T \mathbf{S}\mathbf{M}\xi_i} f^2 & \text{for} \quad i \neq j \\ \dfrac{[\mathbf{M}^{1-\beta}]_{jj}[\mathbf{M}^{\beta}]_{jj}}{\xi_j^T \mathbf{S}\mathbf{M}\xi_j} f^2 & \text{for} \quad i = j \end{cases}$$

Correct diagnosis is guaranteed if

$$\frac{[\mathbf{M}^{1-\beta}]_{ij}[\mathbf{M}^{\beta}]_{ij}}{\xi_i^T \mathbf{S}\mathbf{M}\xi_i} \leq \frac{[\mathbf{M}^{1-\beta}]_{jj}[\mathbf{M}^{\beta}]_{jj}}{\xi_j^T \mathbf{S}\mathbf{M}\xi_j} \tag{38}$$

Again, for $\beta = 0$, rGDC = rPDC, we have

$$0 \leq \frac{m_{jj}}{\xi_j^T \mathbf{S}\mathbf{M}\xi_j} \tag{39}$$

This inequality is always true; therefore, correct diagnosis is guaranteed with rPDC.

For $\beta = (1/2)$, rGDC = rCDC, we have

$$\frac{[\mathbf{M}^{(1/2)}]_{ij}^2}{\xi_i^T \mathbf{S}\mathbf{M}\xi_i} \leq \frac{[\mathbf{M}^{(1/2)}]_{jj}^2}{\xi_j^T \mathbf{S}\mathbf{M}\xi_j} \tag{40}$$

Since this inequality does not always hold, correct diagnosis is not guaranteed with rCDC.

6.2. Diagnosis using reconstruction-based contributions

Substitution of the fault in Eq. (34) into Eq. (27) leads to

$$RBC_i^{Index} = \begin{cases} \dfrac{\left(m_{ij}\right)^2}{m_{ii}} f^2 & \text{for} \quad i \neq j \\ m_{jj} f^2 & \text{for} \quad i = j \end{cases}$$

In this case, $m_{ij} = \xi_i^T \mathbf{M}\xi_j$ and $m_{jj} = \xi_j^T \mathbf{M}\xi_j$. Correct diagnosis is guaranteed if the RBC value of the non-faulty variable is less than or equal to the RBC value of the faulty one. Thus, the following inequality has to hold

$$\frac{(m_{ij})^2}{m_{ii}} \leq m_{jj}$$

Using the Cauchy–Schwarz inequality

$$(m_{ij})^2 \leq m_{ii} m_{jj} \tag{41}$$

The RBC value of the non-faulty variable is

$$\frac{\left(m_{ij}\right)^2}{m_{ii}} \leq \frac{m_{ii} m_{jj}}{m_{ii}} = m_{jj} \tag{42}$$

The resulting expression is just the inequality needed to guarantee correct diagnosis. Therefore, correct diagnosis is guaranteed with RBC. Furthermore, it should be noted that, if $\mathbf{M}$ is positive definite, $\mathbf{M} > 0$, Eq. (42) becomes

$$\frac{(m_{ij})^2}{m_{ii}} < m_{jj} \tag{43}$$

which implies a stronger diagnosability power of the RBC. This is the case when the φ index is used for fault diagnosis since $\mathbf{M} = \mathbf{\Phi} > 0$.

6.2.1. Diagnosis-ability of relative RBC

Substituting the fault in Eq. (34) into the rRBC equation in Table 4 we obtain

$$RBC_i^{Index} = \begin{cases} \dfrac{\left(\xi_i^T \mathbf{M}\xi_j\right)^2}{\xi_i^T \mathbf{M}\mathbf{S}\mathbf{M}\xi_i} f^2 & \text{for} \quad i \neq j \\ \dfrac{\left(\xi_j^T \mathbf{M}\xi_j\right)^2}{\xi_j^T \mathbf{M}\mathbf{S}\mathbf{M}\xi_j} f^2 & \text{for} \quad i = j \end{cases}$$

Correct diagnosis is guaranteed if

$$\frac{\left(\xi_i^T \mathbf{M}\xi_j\right)^2}{\xi_i^T \mathbf{M}\mathbf{S}\mathbf{M}\xi_i} \leq \frac{\left(\xi_j^T \mathbf{M}\xi_j\right)^2}{\xi_j^T \mathbf{M}\mathbf{S}\mathbf{M}\xi_j} \tag{44}$$

In general, this inequality does not always hold and correct diagnosis is not guaranteed. However, when

$$\mathbf{M}\mathbf{S}\mathbf{M} = \mathbf{M} \tag{45}$$

the original RBC expression is obtained; thus, correct diagnosis is guaranteed. Eq. (45) implies that, if $\mathbf{M}$ is a pseudo inverse of $\mathbf{S}$, correct diagnosis is guaranteed with rRBC. This is the case of T^2.

6.3. Diagnosis using diagonal contributions

The substitution of the fault in Eq. (34) into Eq. (23) leads to

$$DC_i^{Index} = \begin{cases} 0 & \text{for} \quad i \neq j \\ m_{jj} f^2 & \text{for} \quad i = j \end{cases}$$

These results are obtained knowing that $\xi_i^T \xi_j = 0$ for $i \neq j$, $\xi_i^T \xi_i = 1$ and $m_{jj} = \xi_j^T \mathbf{M}\xi_j$.

Again, correct diagnosis is guaranteed if the contribution of the non-faulty variable is less than or equal to the contribution of the faulty variable, this is, if the following inequality holds,

$$0 \leq m_{jj} \tag{46}$$

Since $\mathbf{M} \geq 0$, its diagonal elements are greater than or equal to zero, then the inequality always holds and correct diagnosis is guaranteed. However, a drawback of the diagonal contribution is that it does not consider the correlation between variables, which makes it similar to univariate monitoring.

6.3.1. Diagnosis-ability of relative DC

The rDC values of the fault in Eq. (34) are substituted in the rDC expression in Table 4 to obtain

$$DC_i^{Index} = \begin{cases} 0 & \text{for} \quad i \neq j \\ \dfrac{1}{\xi_j^T \mathbf{S}\xi_j} f^2 & \text{for} \quad i = j \end{cases}$$

Since $0 \leq \frac{1}{\xi_j^T \mathbf{S}\xi_j}$, correct diagnosis is guaranteed with rDC.

The diagnosis results shown in this section are summarized in Table 5. It can be seen that, for single sensor faults with large magnitudes, correct diagnosis is guaranteed for PDC, rPDC, RBC, rRBC with $\mathbf{M} = \mathbf{D}$, DC, and rDC. However, CDC, rCDC, and rRBC with $\mathbf{M} \neq \mathbf{D}$ do not guarantee correct diagnosis. This result is interesting, but it

Table 5
Guarantee of correct fault diagnosis for simple sensor faults.

Method	*SPE*	T^2	φ
CDC	No	No	No
rCDC	No	No	No
PDC	Yes	Yes	Yes
rPDC	Yes	Yes	Yes
RBC	Yes	Yes	Yes
rRBC	No	Yes	No
DC	Yes	Yes	Yes
rDC	Yes	Yes	Yes

should not be overstated for general process faults. It is arguable that diagonal contributions reduce to a single variable monitoring schedule and, therefore, yield clear diagnosis results for single sensor faults. For process faults that affect multiple sensors in a correlated manner, or faults with small to medium sizes, this result is not applicable. Even for single sensor faults with modest fault magnitudes, noise has an impact. In order to assess the diagnosability of faults with arbitrary magnitudes, a Monte Carlo simulation will be carried out in the next section.

7. Simulation study

The purpose of this example is to compare the rates of correct diagnosis given by the diagnosis methods when single sensor faults with modest sizes happen in a process. The rates of diagnosis of GDC and rGDC are determined for different values of β. Relative contributions using the control limits, given in Table 3, as scaling factors are also calculated and are denoted as $\text{rGDC}_{\text{limit}}$. This is done to compare the performance of relative contributions using the means and control limits as scaling factors. Moreover, the rates of correct diagnosis for CDC, PDC, DC, RBC and their relative contributions are calculated and compared. The relative contributions are denoted with a notation similar to the one used with rGDC. All the comparisons are made for the cases when faults are detected by one of the SPE, T^2 and φ indices. The process model is

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} = \begin{bmatrix} -0.3441 & 0.4815 & 0.6637 \\ -0.2313 & -0.5936 & 0.3545 \\ -0.5060 & 0.2495 & 0.0739 \\ -0.5552 & -0.2405 & -0.1123 \\ -0.3371 & 0.3822 & -0.6115 \\ -0.3877 & -0.3868 & -0.2045 \end{bmatrix} \begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix} + noise$$

The random variables t_1, t_2 and t_3 are uniformly distributed in the ranges [0, 2], [0, 1.6] and [0, 1.2], respectively. The noise in the process is normally distributed, has zero-mean and a standard deviation of 0.2. The PCA model is built with 3000 samples that are scaled to zero-mean and unit variance. The simulated faults are of the form

$$\mathbf{x}_{faulty} = \mathbf{x}^* + \xi_i f \qquad (47)$$

The fault-free measurements, $\mathbf{x}^*$, are generated with the process model; the fault magnitude f is uniformly distributed between 0 and 5; the direction ξ_i is uniformly random among the six variable directions. Overall, 2000 fault samples are generated.

The rates of detected faults achieved by the fault detection indices are 83.9% for SPE, 58.5% for T^2, and 83.3% for φ. Once the faults are detected, fault diagnosis is performed on the detected faults. These results can be seen in Fig. 1. Fig. 1(a) and (b) shows the rates of correct diagnosis when the faults are detected with the SPE and T^2 indices, respectively. Fault diagnosis is performed with GDC, rGDC and $\text{rGDC}_{\text{limit}}$ with the values of β ranging from 0 to 1. For SPE and T^2, the best rates are obtained when β is near 0 or 1, and the worst rates are obtained when β is near 0.5. These results agree with the diagnosis results for sensor faults with very large

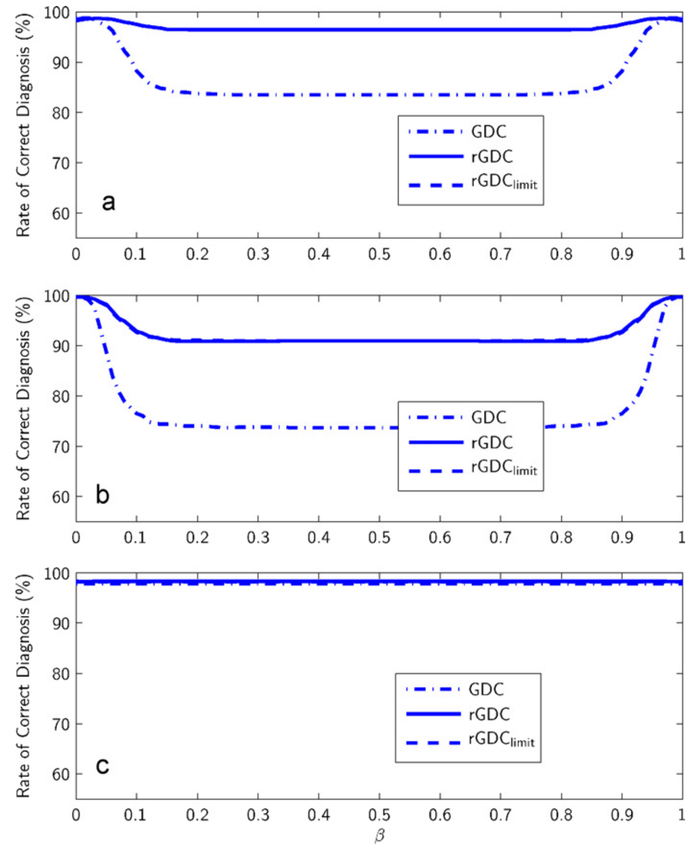

Fig. 1. Rates of correct diagnosis using GDC for faults detected with different indices. (a) Faults detected with SPE. (b) Faults detected with T^2. (c) Faults detected with φ.

magnitudes, where correct diagnosis is guaranteed with GDC and rGDC for $\beta = 0, 1$; but not for $\beta = 0.5$. Also, it can be seen that, for *SPE* and T^2, the rates of correct diagnosis of the relative contributions are larger than the ones of GDC. However, there is almost no difference among the results of the relative contributions when the mean and control limits are used as scaling factors. Therefore, the use of either of the relative contribution approaches makes a substantial improvement on the diagnosis of the faults.

Fig. 1(c) shows the diagnosis results for the faults detected with the φ index, which amounts to 83.3% of all fault samples. In this case, the correct diagnosis rates are large, around 97–98%, and there is a small improvement on the diagnosis results when relative contributions are used.

Table 6 shows the rates of correct diagnosis for all contribution analysis methods and their relative contributions. Since the relative contributions based on contribution means are essentially the same as those based on the contribution control limits, only relative contributions based on means are compared in Table 6. The first column shows the methods used for fault diagnosis, the sec-

Table 6
Percent rates of correct diagnosis for detected faulty samples.

Diagnosis	Index		
Method	*SPE*	T^2	φ
CDC	83.51	73.74	97.82
rCDC	96.45	90.96	98.32
PDC	98.75	99.83	97.82
rPDC	98.26	99.74	98.32
DC	97.82	99.91	98.00
rDC	98.01	99.91	98.75
RBC	96.83	93.35	97.32
rRBC	96.45	93.35	97.44

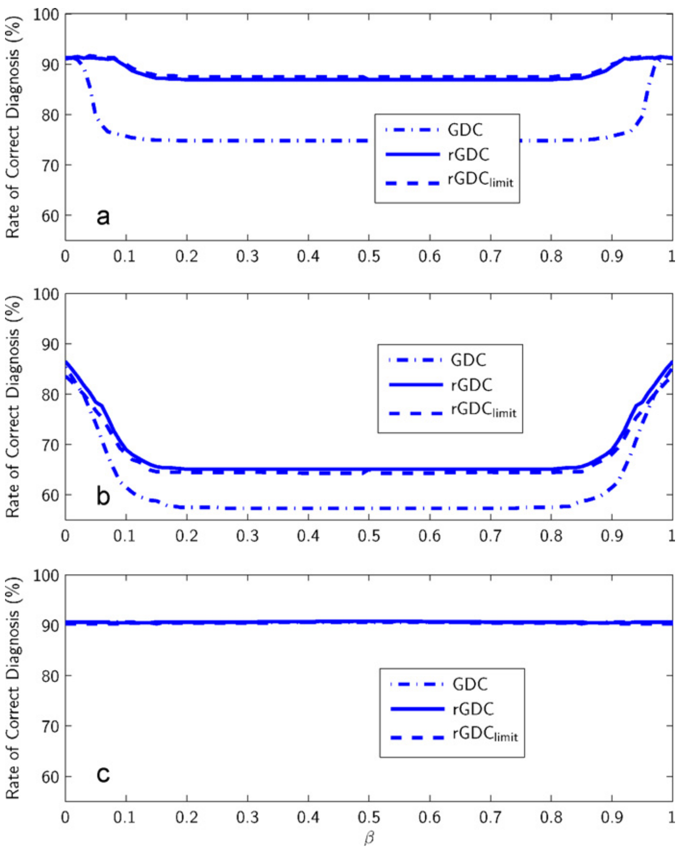

Fig. 2. Rates of correct diagnosis for all simulated faults, using GDC with different indices. (a) Diagnosis results using SPE. (b) Diagnosis results using T^2. (c) Diagnosis results using φ.

ond column shows the diagnosis results when faults are detected and diagnosed with the SPE index, the third one does the same for the T^2 index and the fourth one does it for the φ index. Similar to the diagnosis results of GDC, the rates of correct diagnosis given by CDC improve when relative contributions are used. However, for PDC, the diagnosis rates with SPE and T^2 are slightly lower when relative contributions are used. For DC, the diagnosis rates given by relative contributions increase for the SPE index, and stay the same for the T^2 index. In the RBC case, the diagnosis rates with SPE are slightly lower when the relative contributions are employed; however, with T^2, the use of relative contributions does not make a change on the diagnosis results. On the other hand, when the index ϕ is used, the relative contributions produce a small improvement in the diagnosis rates given by the four methods. For the combined index, the rates of correct diagnosis fluctuate around 97–98%; for the SPE index, around 96–98%, except for one case; and for the T2, between 90% and 99%, except for one case. As observed earlier, the fault detection rates based on the three detection indices are very different. In general only faults with relatively large magnitudes can be detected by the T^2 index. Therefore, it is unfair to compare successful diagnosis rates for faulty samples being detected by a specific fault detection index. Next we compare the fault diagnosis results for all 2000 samples with various magnitudes and random faulty variables.

Fig. 2 shows the rates of correct diagnosis for all simulated faults analyzed with GDC and different values of β. These rates are very similar to the ones where only detected faults are analyzed, the only difference is that the rates of correct diagnosis have decreased in this case. Yet, the combined index achieves a rate of correct diagnosis near 91%.

Table 7
Percent rates of correct diagnosis for all simulated faulty samples.

Diagnosis	Index		
Method	*SPE*	T^2	φ
CDC	74.80	57.30	90.60
rCDC	86.90	65.10	90.80
PDC	91.10	85.30	90.60
rPDC	91.30	86.50	90.60
DC	88.90	89.00	89.00
rDC	89.00	89.00	89.00
RBC	87.00	66.50	91.40
rRBC	86.90	66.50	91.30

The rates of correct diagnosis for all the simulated faults, obtained with all contribution analysis methods and their relative contributions, are shown in Table 7. Similar to the changes observed in the figures, the rates of correct diagnosis shown in Table 7 are lower than the ones shown in Table 6.

In Table 7, the rates of correct diagnosis for SPE and T^2 using CDC show a significant increment when relative contributions are used; for φ, the increment is minimal. The PDC method shows an small increment of 1.2 percentage points for T^2 when relative contributions are used. The rest of methods do not show a significant change when relative contributions are applied.

It is interesting to note from the results in Tables 6 and 7 that the complete decomposition contributions for SPE and T^2, although most popularly used in the literature and practice, give significantly worse results than other methods. In particular, diagonal contributions, which are essentially univariate calculations, give favorable results. This, however, should not lead one to favor univariate statistical monitoring. For this simulation example, the average variance of the simulated variables is 0.3845, and if univariate monitoring was developed for each of them, their control limits would be ±0.8945 for 99% confidence. This would make only about 82% of the simulated faults detectable by univariate monitoring, while the multivariate detection rate is as high as 84%.

It should be noted that these rates are by themselves random quantities, therefore, they should not be strictly compared by magnitude. Nor general conclusions can be drawn from these simulation studies. For a comparative study on more complex process faults we refer to Li et al. [8].

8. Conclusions

In this paper it is shown that most of the fault diagnosis methods can be unified into three general diagnosis methods. A new form of relative contribution is proposed, which uses the mean value of the contribution as the scaling factor. This relative contribution ensures that all variable contributions are statistically equal when no fault is present in a process. It is shown that some methods do not guarantee correct diagnosis even for single sensor faults with small magnitudes, while others do. A simulation is performed for the special case of simple sensor faults with modest magnitudes; the results show that the most popular contribution plots methods (CDC) give significantly worse results than others for the SPE and T^2 indices. An effective remedy is to use relative contributions. Also, it is shown that the contribution methods that use the SPE and φ indices show a higher sensitivity to faults than the T^2 index. The rates of correct diagnosis given by the relative contributions when the mean and control limits are used as scaling factors are nearly identical for all methods and indices. This means that either approach can be used for relative contributions; however, expressions based on the mean of the contributions are easier to determine and analyze.

The unification and derivation of relative contributions are major contributions of this work. The rigorous analysis results are performed to show that some methods can fail even for simple sensor faults with large magnitudes. While this result is interesting, it should not be overstated for general process faults. For process faults that affect multiple sensors in a correlated manner, or faults with small to medium sizes, this result is not applicable. Further research is needed for diagnosis analysis of these methods for general process faults.

Acknowledgements

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Appendix A. Control limits for diagnosis methods

The results of Box [4] show that a quadratic form $J = \mathbf{x}^T\mathbf{A}\mathbf{x}$ is distributed approximately as $g\chi^2_\alpha(h)$ if $\mathbf{A} \geq 0$, $\mathbf{x}$ is zero mean and is normally distributed. The confidence level is $(1-\alpha)\times 100$ and the parameters g and h are calculated as

$$g = \frac{tr\{\mathbf{SA}\}^2}{tr\{\mathbf{SA}\}} \tag{A.1}$$

$$h = \frac{[tr\{\mathbf{SA}\}]^2}{tr\{\mathbf{SA}\}^2} \tag{A.2}$$

and $tr\{\mathbf{A}\}$ is the trace of matrix $\mathbf{A}$.

A.1. Control limits for GDC = CDC

GDC equals CDC when $\beta = (1/2)$. In this case the control limits are calculated similarly for RBC and DC. Using Eq. (14) we can calculate the parameters of the control limits of this contribution as

$$g_i = \frac{tr\{\mathbf{SM}^{(1/2)}\xi_i\xi_i^T\mathbf{M}^{(1/2)}\}^2}{tr\{\mathbf{SM}^{(1/2)}\xi_i\xi_i^T\mathbf{M}^{(1/2)}\}} = \frac{tr\{(\xi_i^T\mathbf{M}^{(1/2)}\mathbf{SM}^{(1/2)}\xi_i)^2\}}{tr\{\xi_i^T\mathbf{M}^{(1/2)}\mathbf{SM}^{(1/2)}\xi_i\}} = \xi_i^T\mathbf{SM}\xi_i \tag{A.3}$$

$$h_i = \frac{\left[tr\{\mathbf{SM}^{(1/2)}\xi_i\xi_i^T\mathbf{M}^{(1/2)}\}\right]^2}{tr\{\mathbf{SM}^{(1/2)}\xi_i\xi_i^T\mathbf{M}^{(1/2)}\}^2} = 1. \tag{A.4}$$

The result of g_i comes from the relationship $\mathbf{SM}^a = \mathbf{M}^a\mathbf{S}$ in Eq. (B.1).

A.2. Control limits for GDC when $\beta \neq (1/2)$

The variance of a quadratic form can be calculated [15] with the following equation

$$Var\{\mathbf{x}^T\mathbf{A}\,\mathbf{x}\} = 2tr\{\mathbf{A}\,\mathbf{S}\}^2 + 4\bar{\mathbf{x}}^T\mathbf{A}\,\mathbf{S}\,\mathbf{A}\bar{\mathbf{x}} \tag{A.5}$$

where $\bar{\mathbf{x}} = E\{\mathbf{x}\}$, which in this case is $\bar{\mathbf{x}} = 0$.

It is required that $\mathbf{A}$ be symmetric; but, from Eq. (32), when $\beta \neq 1/2$ in GDC, $\mathbf{A} = \mathbf{M}^{1-\beta}\xi_i\xi_i^T\mathbf{M}^\beta$ and is not symmetric. However, we can make the GDC to have a symmetric matrix in the following way

$$GDC_i^{Index} = \frac{1}{2}\mathbf{x}^T\left(\mathbf{M}^{1-\beta}\xi_i\xi_i^T\mathbf{M}^\beta + \mathbf{M}^\beta\xi_i\xi_i^T\mathbf{M}^{1-\beta}\right)\mathbf{x} \tag{A.6}$$

If we substitute the new matrix $\mathbf{A}$ in Eq. (A.5) we obtain the variance, σ_i^2, of GDC as

$$\sigma_i^2 = Var\{GDC_i^{Index}\} = \frac{1}{2}tr\{(\mathbf{M}^{1-\beta}\xi_i\xi_i^T\mathbf{M}^\beta + \mathbf{M}^\beta\xi_i\xi_i^T\mathbf{M}^{1-\beta})\mathbf{S}\}^2 = \left(\xi_i^T\mathbf{SM}\xi_i\right)^2 + \xi_i^T\mathbf{SM}^{2(1-\beta)}\xi_i\xi_i^T\mathbf{SM}^{2\beta}\xi_i \tag{A.7}$$

and the standard deviation, σ_i, as

$$\sigma_i = \sqrt{\left(\xi_i^T\mathbf{SM}\xi_i\right)^2 + \xi_i^T\mathbf{SM}^{2(1-\beta)}\xi_i\xi_i^T\mathbf{SM}^{2\beta}\xi_i} \tag{A.8}$$

The expectation of GDC is given in Appendix C as $\xi_i^T\mathbf{SM}\xi_i$. Defining its upper and lower limits as three times the standard deviation above and below the expectation we get

$$\xi_i^T\mathbf{SM}\xi_i \pm 3\sqrt{\left(\xi_i^T\mathbf{SM}\xi_i\right)^2 + \xi_i^T\mathbf{SM}^{2(1-\beta)}\xi_i\xi_i^T\mathbf{SM}^{2\beta}\xi_i} \tag{A.9}$$

For the case of PDC, $\beta = 0$, the control limits are

$$\xi_i^T\mathbf{SM}\xi_i \pm 3\sqrt{\left(\xi_i^T\mathbf{SM}\xi_i\right)^2 + \xi_i^T\mathbf{SM}^2\xi_i\xi_i^T\mathbf{S}\xi_i} \tag{A.10}$$

A.3. Control limits for RBC

Using Eqs. (26), (A.1) and (A.2), the parameters of the control limits for RBC are calculated as

$$g_i = \frac{tr\{\mathbf{SM}\xi_i\left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}\xi_i^T\mathbf{M}\}^2}{tr\{\mathbf{SM}\xi_i\left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}\xi_i^T\mathbf{M}\}} = \frac{\xi_i^T\mathbf{SM}^2\xi_i}{\xi_i^T\mathbf{M}\xi_i} \tag{A.11}$$

$$h_i = \frac{[tr\{\mathbf{SM}\xi_i\left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}\xi_i^T\mathbf{M}\}]^2}{tr\{\mathbf{SM}\xi_i\left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}\xi_i^T\mathbf{M}\}^2} = 1 \tag{A.12}$$

A.4. Control limits for DC

The parameters of the control limits for DC are calculated using Eqs. (23), (A.1) and (A.2)

$$g_i = \frac{tr\{\mathbf{S}\xi_i\xi_i^T\mathbf{M}\xi_i\xi_i^T\}^2}{tr\{\mathbf{S}\xi_i\xi_i^T\mathbf{M}\xi_i\xi_i^T\}} = \xi_i^T\mathbf{S}\xi_i\xi_i^T\mathbf{M}\xi_i \tag{A.13}$$

$$h_i = \frac{\left[tr\{\mathbf{S}\xi_i\xi_i^T\mathbf{M}\xi_i\xi_i^T\}\right]^2}{tr\{\mathbf{S}\xi_i\xi_i^T\mathbf{M}\xi_i\xi_i^T\}^2} = 1 \tag{A.14}$$

Appendix B. Symmetry of $\mathbf{SM}^a$

The symmetric positive semidefinite matrices $\mathbf{M}$ and $\mathbf{S}$ are of the form $\mathbf{P}\boldsymbol{\Lambda}_M\mathbf{P}^T$ and $\mathbf{P}\boldsymbol{\Lambda}_S\mathbf{P}^T$, respectively. $\mathbf{P}$ is the eigenvector matrix of $\mathbf{S}$, and $\boldsymbol{\Lambda}_M$ and $\boldsymbol{\Lambda}_S$ are the diagonal matrices with the eigenvalues of $\mathbf{M}$ and $\mathbf{S}$, respectively. Since $\mathbf{S}$ and $\mathbf{M}$ share the same eigenvectors, we can write

$$\mathbf{SM}^a = \mathbf{P}\boldsymbol{\Lambda}_S\mathbf{P}^T\left(\mathbf{P}\boldsymbol{\Lambda}_M\mathbf{P}^T\right)^a = \mathbf{P}\boldsymbol{\Lambda}_S\mathbf{P}^T\mathbf{P}\boldsymbol{\Lambda}_M^a\mathbf{P}^T = \mathbf{P}\boldsymbol{\Lambda}_S\boldsymbol{\Lambda}_M^a\mathbf{P}^T$$

Since $\boldsymbol{\Lambda}_S$ and $\boldsymbol{\Lambda}_M^a$ are diagonal, $\boldsymbol{\Lambda}_S\boldsymbol{\Lambda}_M^a = \boldsymbol{\Lambda}_M^a\boldsymbol{\Lambda}_S$; thus, we have

$$\mathbf{SM}^a = \mathbf{P}\boldsymbol{\Lambda}_M^a\boldsymbol{\Lambda}_S\mathbf{P}^T = \mathbf{P}\boldsymbol{\Lambda}_M^a\mathbf{P}^T\mathbf{P}\boldsymbol{\Lambda}_S\mathbf{P}^T$$

and

$$\mathbf{SM}^a = \mathbf{M}^a\mathbf{S}. \tag{B.1}$$

Appendix C. Expectation of fault contributions

The expectation of a quadratic form $\mathbf{x}^T\mathbf{A}\mathbf{x}$ is calculated [15] as

$$E\{\mathbf{x}^T\mathbf{A}\mathbf{x}\} = E\{tr(\mathbf{x}^T\mathbf{A}\mathbf{x})\} = E\{tr(\mathbf{A}\mathbf{x}^T\mathbf{x})\} = tr(E\{\mathbf{A}\mathbf{x}^T\mathbf{x}\}) = tr\{\mathbf{AS}\} \tag{C.1}$$

The expectation of GDC is calculated using Eq. (32)

$$E\{GDC_i^{Index}\} = tr\{\mathbf{M}^{1-\beta}\xi_i\xi_i^T\mathbf{M}^\beta\mathbf{S}\} = tr\{\xi_i^T\mathbf{M}^\beta\mathbf{SM}^{1-\beta}\xi_i\} = \xi_i^T\mathbf{SM}\xi_i \tag{C.2}$$

This last equation comes from Eq. (B.1), $\mathbf{SM}^a = \mathbf{M}^a\mathbf{S}$. As we can see, the expectation of the GDC is the same for any value of β.

The expectation of RBC is calculated from Eq. (26)

$$E\{RBC_i^{Index}\} = tr\{\mathbf{M}\xi_i\left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}\xi_i^T\mathbf{MS}\} = \frac{tr\{\xi_i^T\mathbf{MSM}\xi_i\}}{\xi_i^T\mathbf{M}\xi_i} = \frac{\xi_i^T\mathbf{MSM}\xi_i}{\xi_i^T\mathbf{M}\xi_i} \tag{C.3}$$

The expectation of DC is calculated from Eq. (23) as

$$E\{DC_i^{Index}\} = tr\{\xi_i\xi_i^T\mathbf{M}\xi_i\xi_i^T\mathbf{S}\} = tr\{\xi_i^T\mathbf{M}\xi_i\xi_i^T\mathbf{S}\xi_i\} = \xi_i^T\mathbf{M}\xi_i\xi_i^T\mathbf{S}\xi_i \tag{C.4}$$

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