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Fault Diagnosis Using Concurrent Projection to Latent Structures

Yu C. Pan * **Yining Dong** ** **S. Joe Qin** **

* *Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, Los Angeles, CA 90089, USA (e-mail: yupan@usc.edu).*
** *Ming Hsieh Department of Electrical Engineering, University of Southern California, Los Angeles, CA 90089, USA (e-mail: sqin@usc.edu)*

Abstract: Recently, a concurrent projection to latent structures (CPLS) for multivariate statistical process was proposed. It has been proved to be a better monitoring method than the traditional PLS. However, its fault diagnosis methods have not been developed yet. In this paper, we discuss a new fault diagnosis approach based on CPLS. Five monitoring indices used in CPLS are unified into two general forms. Based on these general forms, we define their complete decomposition contributions (CDC) and reconstruction-based contributions (RBC). The diagnosability of these two contribution methods is further analyzed. Finally, simulation case studies are presented to demonstrate the results.

Keywords: Concurrent projection to latent structures (CPLS), process monitoring, quality monitoring, contribution plots, fault diagnosis, data-driven

1. INTRODUCTION

Over the last two decades, multivariate statistical methods such as principal component analysis (PCA) and projection to latent structures (PLS) have been successfully applied to the monitoring of industrial processes (Nomikos and MacGregor (1995), Wise et al. (1989) & Qin (2012)). These methods build statistical models from normal operation data, and they partition measurements into a number of subspaces. Each subspace is monitored by a statistical index. A fault is detected when a new measurement breaks the normal statistical correlation causing one of the monitoring indices to go beyond its control limit.

Both PCA and PLS partition the process measurements $\mathbf{X}$ into a principal subspace and a residual subspace, and use the T^2 and Q indices to monitor them, respectively. When quality measurements are expensive or difficult to obtain, PCA has been used to monitor abnormal variations in process variables. On the other hand, PLS has been used to build an input-output relation to infer the quality variables, and this input-output relation is used to monitor the input subspace that is relevant to the output quality. However, this monitoring method for PLS has two problems. First, the principal subspace in PLS, which is thought to reflect major variations related to the quality measurements $\mathbf{Y}$, still contains variation orthogonal to $\mathbf{Y}$. Second, PLS does not extract variations of the process measurements in a descending order, and therefore, the residual subspace can still contain large variations, making it inappropriate to be monitored by the Q index. To solve these problems, methods including orthogonal PLS (OPLS), total PLS (TPLS), concurrent PLS (CPLS), and their variants have been proposed by Trygg and Wold (2002), Zhou et al. (2010), Qin and Zheng (2013), & Zhao et al. (2014).

Once a fault is detected, it is desirable to diagnose its cause. Many methods have been proposed to solve this problem. One popular category among them consists of contribution analysis methods. Contribution methods determine the contribution of each variable to the fault detection indices calculated. The idea is that faulty variables have high contributions to the fault detection index. Several contributions have been defined and used for fault diagnosis (Cherry and Qin (2006) & Qin et al. (2001)). Alcala and Qin (2011) showed that they can be unified into three general categories: diagonal contribution, general decompositive contribution, and reconstruction-based contribution. Diagonal contribution was proposed by Qin et al. (2001), and is specialized in dealing with mulit-block process monitoring. Among the general decompositive contributions, the complete decomposition contribution is mostly widely used in industry. In this paper, the complete decomposition contributions (CDC) and reconstruction-based contributions (RBC) are defined for CPLS monitoring indices and compared for sensor faults.

The remaining part of this article is organized as follows. Fault detection based on PLS models is briefly reviewed in Section 2. The CPLS algorithm is presented and its properties derived in Section 3. The CPLS fault detection indices and their general forms are calculated in Section 4. The CDCs and RBCs are defined for CPLS in Section 5, and their diagnosability are analyzed in Section 6. Simulation case studies are presented in Section 7. Finally, we conclude the article in Section 8.

2. PLS FOR PROCESS AND QUALITY MONITORING

Given an input matrix $\mathbf{X} \in \mathbb{R}^{n\times m}$ consisting of n samples with m process variables, and an output matrix $\mathbf{Y} \in \mathbb{R}^{n\times p}$ with p quality variables, the PLS algorithm first scales, and then projects $\mathbf{X}$ and $\mathbf{Y}$ to a low-dimensional space, which is defined by a small number of latent variables $(\mathbf{t}_1, \ldots \mathbf{t}_l)$, where l is the PLS component number. The mean-centered and scaled $\mathbf{X}$ and $\mathbf{Y}$ are decomposed as:

$$\begin{cases} \mathbf{X} = \sum_{i=1}^{l} \mathbf{t}_i \mathbf{p}_i^T + \mathbf{E} = \mathbf{T}\mathbf{P}^T + \mathbf{E} \\ \mathbf{Y} = \sum_{i=1}^{l} \mathbf{t}_i \mathbf{q}_i^T + \mathbf{F} = \mathbf{T}\mathbf{Q}^T + \mathbf{F} \end{cases} \tag{1}$$

In (1), $\mathbf{T} = [\mathbf{t}_1, \ldots \mathbf{t}_l]$ are the latent score vectors, $\mathbf{P} = [\mathbf{p}_1, \ldots \mathbf{p}_l]$ and $\mathbf{Q} = [\mathbf{q}_1, \ldots \mathbf{q}_l]$ are the loading vectors for $\mathbf{X}$ and $\mathbf{Y}$, respectively. The matrices $\mathbf{E}$ and $\mathbf{F}$ are the corresponding residuals to $\mathbf{X}$ and $\mathbf{Y}$. In general, the PLS decomposition is carried out iteratively. The first latent vector $\mathbf{t}_1$ is extracted by maximizing the covariance between $\mathbf{X}$ and $\mathbf{Y}$, and then both matrices are deflated to form $\mathbf{X}_1$ and $\mathbf{Y}_1$. The second latent vector is then extracted by maximizing the covariance between $\mathbf{X}_1$ and $\mathbf{Y}_1$, and the process is repeated until enough latent components have been extracted. Intuitively, it is desired to have the number of PLS components, l, to give the maximum prediction power to the PLS model based on data that are excluded from training data, where l is usually determined by cross-validation. Although the PLS decomposition is an iterative process, once the model is built and parameters stored, all score vectors can be computed directly from original $\mathbf{X}$:

$$\mathbf{T} = \mathbf{X}\mathbf{R} \quad \text{and} \quad \mathbf{R} = \mathbf{W}(\mathbf{P}^T\mathbf{W})^{-1}$$

where the weight vectors $\mathbf{W} = [\mathbf{w}_1, \ldots \mathbf{w}_l]$ are also parameters in the PLS decomposition. They are used to calculate the scores $\mathbf{t}_i = \mathbf{X}_i\mathbf{w}_i$. Readers who are interested in detail of PLS algorithms can refer to Geladi and Kowalski (1986) and Höskuldsson (1988).

To perform process monitoring on a new data sample $\mathbf{x}$, the PLS model projects it onto a principal subspace $\hat{\mathbf{x}}$, which is thought to reflect major variations related to $\mathbf{Y}$, and a residual subspace $\tilde{\mathbf{x}}$, which is thought to contain variation unrelated to the output $\mathbf{Y}$. However, unlike orthogonal projections in the PCA, Li et al. (2010) showed that the PLS induces an oblique projection decomposition.

Early literature (e.g., MacGregor et al. (1994)) suggests to monitor principal subspace by T^2 index and residual subspace by Q index.

$$T^2 = \mathbf{t}^T\Lambda^{-1}\mathbf{t} \le \frac{l(n^2-1)}{n(n-1)}F_{l,n-l,\alpha}$$

$$Q = ||\tilde{\mathbf{x}}||^2 = \mathbf{x}^T(\mathbf{I} - \mathbf{P}\mathbf{R}^T)\mathbf{x} \le g\chi^2_{h,\alpha}$$

where $\mathbf{t} = \mathbf{R}^T\mathbf{x}$, $\Lambda^{-1} = \frac{1}{n-1}\mathbf{T}^T\mathbf{T}$, $F_{l,n-l,\alpha}$ is the F-distribution with l and $l-1$ degrees of freedom, α is the level of significance, and χ^2_h is the χ^2-distribution with h degrees of freedom. The calculation of g and h can be found in MacGregor et al. (1994).

3. CONCURRENT PROJECTION TO LATENT STRUCTURES

Unlike PLS, the CPLS algorithm projects the input and output data spaces concurrently to five subspaces. They consist of: a joint input-output covariance subspace, an output-principal subspace, an output-residual subspace, an input-principal subspace, and an input-residual subspace. Based on the CPLS algorithm the data matrices $\mathbf{X}$ and $\mathbf{Y}$ are decomposed as follows:

$$\begin{cases} \mathbf{X} = \mathbf{U}_c\mathbf{R}_c^\dagger + \mathbf{T}_x\mathbf{P}_x^T + \tilde{\mathbf{X}} \\ \mathbf{Y} = \mathbf{U}_c\mathbf{Q}_c^T + \mathbf{T}_y\mathbf{P}_y^T + \tilde{\mathbf{Y}} \end{cases} \tag{2}$$

The CPLS algorithm is shown in Table 1. Note that there is a small modification on the original algorithm proposed by Qin and Zheng (2013). In step 4, the ratio between the variance of $\tilde{\mathbf{Y}}_c$ and $\mathbf{Y}$ is computed. If this ratio is small, essentially all of $\mathbf{Y}$ is predictable, then $\tilde{\mathbf{Y}}_c = \tilde{\mathbf{Y}}$ is simply the output residuals, and there are no output-principal variations. A similar modification has been made in step 6 for input space. Readers can refer to Qin and Zheng (2013) for details of CPLS algorithm.

Once the CPLS model is built, it can decompose a single sample as follows:

$$\mathbf{u}_c = \mathbf{R}_c^T\mathbf{x}$$

$$\tilde{\mathbf{x}}_c = (\mathbf{x} - \mathbf{R}_c^{\dagger T}\mathbf{u}_c)$$

$$\tilde{\mathbf{y}}_c = (\mathbf{y} - \mathbf{Q}_c\mathbf{u}_c)$$

$$\mathbf{t}_x = \mathbf{P}_x^T\tilde{\mathbf{x}}_c = \mathbf{P}_x^T\mathbf{x} \tag{5}$$

$$\mathbf{t}_y = \mathbf{P}_y^T\tilde{\mathbf{y}}_c = \mathbf{P}_y^T(\mathbf{y} - \mathbf{Q}_c\mathbf{u}_c)$$

$$\tilde{\mathbf{x}} = (\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T)\tilde{\mathbf{x}}_c = (\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T)\mathbf{x} \tag{6}$$

$$\tilde{\mathbf{y}} = (\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^T)\tilde{\mathbf{y}}_c = (\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^T)(\mathbf{y} - \mathbf{Q}_c\mathbf{u}_c)$$

The second equalities in (5) and (6) are not obvious. To prove them, we derive some properties of CPLS here.

Lemma 1. $\tilde{\mathbf{X}}_c\mathbf{R}_c = \mathbf{0}$.

Proof. In step 6 of the CPLS algorithm in Table 1,

$$\begin{aligned} \tilde{\mathbf{X}}_c\mathbf{R}_c &= (\mathbf{X} - \mathbf{U}_c\mathbf{R}_c^\dagger)\mathbf{R}_c \\ &= \mathbf{X}\mathbf{R}_c - \mathbf{U}_c(\mathbf{R}_c^T\mathbf{R}_c)^{-1}\mathbf{R}_c^T\mathbf{R}_c \\ &= \mathbf{U}_c - \mathbf{U}_c \\ &= \mathbf{0} \end{aligned}$$

Lemma 2. $\mathbf{P}_x^T\mathbf{R}_c^{\dagger T} = \mathbf{0}$ and $\mathbf{P}_{\tilde{x}}^T\mathbf{R}_c^{\dagger T} = \mathbf{0}$.

Table 1. Concurrent PLS algorithm

1. Scale $\mathbf{X}$ and $\mathbf{Y}$ to zero-mean and unit-variance. Perform PLS on $\mathbf{X}$ and $\mathbf{Y}$ using (1) to give $\mathbf{T}$, $\mathbf{Q}$, and $\mathbf{R}$. The number of PLS components l is determined by cross-validation.
2. Perform singular value decomposition (SVD) on the *"predictable output"* $\hat{\mathbf{Y}} = \mathbf{T}\mathbf{Q}^T$.
$$\hat{\mathbf{Y}} = \mathbf{U}_c\mathbf{D}_c\mathbf{V}_c^T = \mathbf{U}_c\mathbf{Q}_c^T$$
where $\mathbf{Q}_c = \mathbf{V}_c\mathbf{D}_c$ includes all l_c nonzero singular values in descending order and the corresponding right singular vectors.
3. Set $\mathbf{U}_c = \mathbf{X}\mathbf{R}_c$ where $\mathbf{R}_c = \mathbf{R}\mathbf{Q}^T\mathbf{V}_c\mathbf{D}_c^{-1}$
4. Form the *"unpredictable output"* $\tilde{\mathbf{Y}}_c = \mathbf{Y} - \mathbf{U}_c\mathbf{Q}_c^T$ and compare the variance between $\tilde{\mathbf{Y}}_c$ and $\mathbf{Y}$.
$$R_y = \frac{var(\tilde{\mathbf{Y}}_c)}{var(\mathbf{Y})} \tag{3}$$
where $var(\mathbf{A})$ is simply the sum of squared singular values of $\mathbf{A}$. If $R_y < 0.05$, there is no output-principal subspace, and $\tilde{\mathbf{Y}}_c = \tilde{\mathbf{Y}}$ is simply the output residuals. Skip step 5 and go to step 6. Otherwise if $R_y \geq 0.05$, go to step 5.
5. Perform PCA on $\tilde{\mathbf{Y}}_c$ with l_y principal components
$$\tilde{\mathbf{Y}}_c = \mathbf{T}_y\mathbf{P}_y^T + \mathbf{T}_{\tilde{y}}\mathbf{P}_{\tilde{y}}^T = \mathbf{T}_y\mathbf{P}_y^T + \tilde{\mathbf{Y}}$$
to yield the output-principal scores $\mathbf{T}_y$ and output residuals $\tilde{\mathbf{Y}}$.
6. Form the *"output-irrelevant input"* $\tilde{\mathbf{X}}_c = \mathbf{X} - \mathbf{U}_c\mathbf{R}_c^\dagger$, where $\mathbf{R}_c^\dagger = (\mathbf{R}_c^T\mathbf{R}_c)^{-1}\mathbf{R}_c^T$ and compare the variance between $\tilde{\mathbf{X}}_c$ and $\mathbf{X}$.
$$R_x = \frac{var(\tilde{\mathbf{X}}_c)}{var(\mathbf{X})}$$
If $R_x < 0.05$, there is no input-principal subspace, and $\tilde{\mathbf{X}}_c = \tilde{\mathbf{X}}$ is simply the input residuals. Skip step 7 and stop. Otherwise if $R_x \geq 0.05$, go to step 7.
7. Perform PCA on on $\tilde{\mathbf{X}}_c$ with l_x principal components
$$\tilde{\mathbf{X}}_c = \mathbf{T}_x\mathbf{P}_x^T + \mathbf{T}_{\tilde{x}}\mathbf{P}_{\tilde{x}}^T = \mathbf{T}_x\mathbf{P}_x^T + \tilde{\mathbf{X}} \tag{4}$$
to yield the input-principal scores $\mathbf{T}_x$ and input residuals $\tilde{\mathbf{X}}$.

Proof. By using (4) and *Lemma* 1.

$$\tilde{\mathbf{X}}_c\mathbf{R}_c = [\mathbf{T}_x \ \mathbf{T}_{\tilde{x}}] \begin{bmatrix} \mathbf{P}_x^T \\ \mathbf{P}_{\tilde{x}}^T \end{bmatrix} \mathbf{R}_c = \mathbf{0}$$

Since $[\mathbf{T}_x \ \mathbf{T}_{\tilde{x}}]$ is full rank, $\mathbf{P}_x^T\mathbf{R}_c = \mathbf{0}$ and $\mathbf{P}_{\tilde{x}}^T\mathbf{R}_c = \mathbf{0}$. Therefore $\mathbf{P}_x^T\mathbf{R}_c^{\dagger T} = \mathbf{P}_x^T\mathbf{R}_c(\mathbf{R}_c^T\mathbf{R}_c)^{-1} = \mathbf{0}$ and $\mathbf{P}_{\tilde{x}}^T\mathbf{R}_c^{\dagger T} = \mathbf{P}_{\tilde{x}}^T\mathbf{R}_c(\mathbf{R}_c^T\mathbf{R}_c)^{-1} = \mathbf{0}$.

We are now ready to prove the second equalities in (5) and (6).

Lemma 3. $\mathbf{t}_x = \mathbf{P}_x^T\mathbf{x}$ and $\tilde{\mathbf{x}} = (\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T)\mathbf{x}$

Proof. This can be easily proved by using *Lemma* 2.

$$\begin{aligned}
\mathbf{t_x} &= \mathbf{P}_x^T\tilde{\mathbf{x}}_c \\
&= \mathbf{P}_x^T(\mathbf{x} - \mathbf{R}_c^{\dagger T}\mathbf{u}_c) \\
&= \mathbf{P}_x^T\mathbf{x} - \mathbf{P}_x^T\mathbf{R}_c^{\dagger T}\mathbf{u}_c \\
&= \mathbf{P}_x^T\mathbf{x}
\end{aligned}$$

Table 2. Values for $\mathbf{M}$

Index	$\mathbf{T}_c^2$	$\mathbf{T}_x^2$	$\mathbf{Q}_c$
$\mathbf{M}$	$(n-1)\mathbf{R}_c\mathbf{R}_c^T$	$\mathbf{P}_x\mathbf{\Lambda}_x^{-1}\mathbf{P}_x^T$	$\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T$

$$\begin{aligned}
\tilde{\mathbf{x}} &= (\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T)\tilde{\mathbf{x}}_c \\
&= (\mathbf{P}_{\tilde{x}}\mathbf{P}_{\tilde{x}}^T)(\mathbf{x} - \mathbf{R}_c^{\dagger T}\mathbf{u}_c) \\
&= \mathbf{P}_{\tilde{x}}\mathbf{P}_{\tilde{x}}^T\mathbf{x} - \mathbf{P}_{\tilde{x}}\mathbf{P}_{\tilde{x}}^T\mathbf{R}_c^{\dagger T}\mathbf{u}_c \\
&= \mathbf{P}_{\tilde{x}}\mathbf{P}_{\tilde{x}}^T\mathbf{x} \\
&= (\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T)\mathbf{x}
\end{aligned}$$

4. CPLS BASED FAULT DETECTION

Each of the five subspaces can be monitored with the following T^2 and Q indices.

$$T_c^2 = (n-1)\mathbf{u}_c^T\mathbf{u}_c = (n-1)\mathbf{x}^T\mathbf{R}_c\mathbf{R}_c^T\mathbf{x} \leq \chi^2_{l_c,\alpha}$$

$$T_x^2 = \mathbf{t}_x^T\mathbf{\Lambda}_x^{-1}\mathbf{t}_x = \mathbf{x^T P_x \Lambda_x^{-1} P_x^T x} \leq \chi^2_{l_x,\alpha}$$

$$\begin{aligned}
Q_x &= ||\tilde{\mathbf{x}}||^2 = \mathbf{x}^T(\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T)^T(\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T)\mathbf{x} \\
&= \mathbf{x}^T(\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^T)\mathbf{x} \\
&\leq g_x\chi^2_{h_x,\alpha}
\end{aligned}$$

$$\begin{aligned}
T_y^2 &= \mathbf{t}_y^T\mathbf{\Lambda}_y^{-1}\mathbf{t}_y = \tilde{\mathbf{y}}_c^T\mathbf{P}_y\mathbf{\Lambda}_y^{-1}\mathbf{P}_y^T\tilde{\mathbf{y}}_c \\
&= (\mathbf{y} - \mathbf{Q}_c\mathbf{u}_c)^T\mathbf{P}_y\mathbf{\Lambda}_y^{-1}\mathbf{P}_y^T(\mathbf{y} - \mathbf{Q}_c\mathbf{u}_c) \\
&\leq \chi^2_{l_y,\alpha}
\end{aligned} \tag{7}$$

$$\begin{aligned}
Q_y &= ||\tilde{\mathbf{y}}||^2 = \tilde{\mathbf{y}}_c^T(\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^T)^T(\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^T)\tilde{\mathbf{y}}_c \\
&= \tilde{\mathbf{y}}_c^T(\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^T)\tilde{\mathbf{y}}_c \\
&= (\mathbf{y} - \mathbf{Q}_c\mathbf{u}_c)^T(\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^T)(\mathbf{y} - \mathbf{Q}_c\mathbf{u}_c) \\
&\leq g_y\chi^2_{h_y,\alpha}
\end{aligned} \tag{8}$$

where T_c^2, T_x^2, Q_x, T_y^2, and Q_y are the monitoring indices for the variations in input-output covariance subspace, input-principal subspace, input residual subspace, output-principal subspace, and output residual subspace, respectively. The symbol α is the level of significance, and χ^2_a is the χ^2-distribution with a degrees of freedom. The calculation for the parameters g_x, h_x, g_y, and h_y is given in Qin and Zheng (2013). The above control limits are valid only when n is large (Box et al. (1954)).

The indices T_c^2, T_x^2, and Q_x that monitor the input space can be written in quadratic forms in terms of $\mathbf{x}$. To simplify the notation, we can expressed them in a general form

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

where $\mathbf{M}$ is shown in Table 2 for each detection index.

The indices T_y^2 and Q_y that monitor the output space can be written in quadratic forms only in terms of $\tilde{\mathbf{y}}_c$ and not in terms of $\mathbf{y}$. Expanding (7) and (8) will result in quadratic polynomials in terms of $\mathbf{y}$. Again, to simplify the notation, we can express them in a general form:

$$\text{Index}(\mathbf{y}) = \mathbf{y}^T\mathbf{N}\mathbf{y} - 2\mathbf{y}^T\mathbf{a} + c(\mathbf{x})$$

where $\mathbf{N}$, $\mathbf{a}$ and $c(\mathbf{x})$ are shown in Table 3 for each detection index. These two general forms will be used to define contributions and analyze their diagnosabilities.

Table 3. Values for $\mathbf{N}$, $\mathbf{a}$ and $c(\mathbf{x})$

Index	$\mathbf{T}_y^2$	$\mathbf{Q}_y$
$\mathbf{N}$	$\mathbf{P}_y\mathbf{\Lambda}_y^{-1}\mathbf{P}_y^T$	$\mathbf{I}-\mathbf{P}_y\mathbf{P}_y^T$
$\mathbf{a}$	$\mathbf{N}\mathbf{Q}_c\mathbf{R}_c^T\mathbf{x}$	$\mathbf{N}\mathbf{Q}_c\mathbf{R}_c^T\mathbf{x}$
$c(\mathbf{x})$	$\mathbf{x}^T\mathbf{R}_c\mathbf{Q}_c^T\mathbf{N}\mathbf{Q}_c\mathbf{R}_c\mathbf{x}$	$\mathbf{x}^T\mathbf{R}_c\mathbf{Q}_c^T\mathbf{N}\mathbf{Q}_c\mathbf{R}_c\mathbf{x}$

5. FAULT DIAGNOSIS BY CONTRIBUTIONS

In this section, we define the complete decomposition contributions (CDC) and reconstruction-based contributions (RBC) from the general forms.

5.1 Complete decomposition contributions

In general, the CDC for monitoring indices with a quadratic form is defined as

$$\begin{aligned}\text{Index}(\mathbf{x}) &= \mathbf{x}^T\mathbf{M}\mathbf{x} = ||\mathbf{M}^{(1/2)}\mathbf{x}||^2\\ &= \sum_{i=1}^{n}\left(\xi_i^T\mathbf{M}^{(1/2)}\mathbf{x}\right)^2\\ &= \sum_{i=1}^{n}\text{CDC}_i^{\text{Index}(\mathbf{x})}\end{aligned}$$

where ξ_i is the i th column of the identity matrix and

$$\text{CDC}_i^{\text{Index}(\mathbf{x})} = \left(\xi_i^T\mathbf{M}^{(1/2)}\mathbf{x}\right)^2. \tag{9}$$

There is no general way to define the CDC for monitoring indices with a quadratic polynomial. However, from the expression of the Index($\mathbf{y}$)

$$\begin{aligned}\text{Index}(\mathbf{y}) &= \mathbf{y}^T\mathbf{N}\mathbf{y} - 2\mathbf{y}^T\mathbf{a} + c(\mathbf{x})\\ &= ||\mathbf{N}^{(1/2)}\mathbf{y}||^2 - 2\mathbf{y}^T\mathbf{a} + c(\mathbf{x})\\ &= \sum_{i=1}^{n}\left(\xi_i^T\mathbf{N}^{(1/2)}\mathbf{y}\right)^2 - 2\mathbf{y}^T\mathbf{a} + c(\mathbf{x})\end{aligned}$$

We propose the CDC to be

$$\text{CDC}_i^{\text{Index}(\mathbf{y})} = \left(\xi_i^T\mathbf{N}^{(1/2)}\mathbf{y}\right)^2 - 2y_ia_i + c(\mathbf{x})/n \tag{10}$$

where y_i and a_i are the i th component of vectors $\mathbf{y}$ and $\mathbf{a}$, respectively. This definition allows the sum of all CDCs to be equal to Index($\mathbf{y}$) while eliminating the "*smearing*" effect on the linear and constant terms of the quadratic polynomials. Smearing is when a fault in the i th variable affects the contribution of other variables (Westerhuis et al. (2000)). Smearing is unavoidable in both CDCs and RBCs, and can lead to misdiagnosis. The smearing effect will be further studied in section 6.

5.2 Reconstruction-based contributions

The RBC was proposed by Alcala and Qin (2009) & Alcala and Qin (2010). It uses the amount of reconstruction of a fault detection index along a variable direction as the contribution of that variable. The reconstructed index with a quadratic form along a variable direction ξ_i is

$$\text{Index}\left(\mathbf{x}_i^r\right) = ||\mathbf{M}^{(1/2)}\mathbf{x}_i^r||^2 = ||\mathbf{M}^{(1/2)}(\mathbf{x}-\xi_i f)||^2 \tag{11}$$

where f is the reconstructed portion to be determined. The best reconstruction by minimizing (11) gives the optimal value of f. If we take the derivative of Index($\mathbf{x}_i^r$) with respect to f and set it equals to zero, the expression of f can be solved as

$$f = \left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}\left(\xi_i^T\mathbf{M}\mathbf{x}\right) \tag{12}$$

The RBC is defined as

$$\begin{aligned}\text{RBC}_i^{\text{Index}(\mathbf{x})} &= \text{Index}(\mathbf{x}) - \text{Index}(\mathbf{x}_i^r)\\ &= \mathbf{x}^T\mathbf{M}\mathbf{x} - (\mathbf{x}-\xi_i f)^T\mathbf{M}(\mathbf{x}-\xi_i f)\\ &= 2\mathbf{x}^T\mathbf{M}\xi_i f - f^T\xi_i^T\mathbf{M}\xi f\\ &= \frac{(\xi_i^T\mathbf{M}\mathbf{x})^2}{\xi_i^T\mathbf{M}\xi_i}\end{aligned} \tag{13}$$

Note that $\left(\xi_i^T\mathbf{M}\xi_i\right)^{-1}$ can be zero. In that case, this fault is not reconstructible and the RBC does not exist. The symbol f is a scalar, and therefore its transpose is equal to itself. The forth equality in (13) is the result of applying (12).

Similarly the reconstructed index with a quadratic polynomial along a variable direction ξ_i is

$$\begin{aligned}\text{Index}\left(\mathbf{y}_i^r\right) &= \mathbf{y}_i^{rT}\mathbf{N}\mathbf{y}_i^T - 2\mathbf{y}_i^{rT}\mathbf{a} + c(\mathbf{x})\\ &= (\mathbf{y}-\xi_i f)^T\mathbf{N}(\mathbf{y}-\xi_i f)\\ &\qquad -2(\mathbf{y}-\xi_i f)^T\mathbf{a} + c(\mathbf{x}).\end{aligned} \tag{14}$$

Minimizing (14) gives the optimal value of f. Once again, take the derivative of Index($\mathbf{y}_i^r$) with respect to f and set it to zero. The expression of f can be solved as

$$f = (\mathbf{y}^T\mathbf{N}\xi_i - a_i)(\xi_i^T\mathbf{N}\xi)^{-1} \tag{15}$$

The RBC for a quadratic polynomial is defined as

$$\begin{aligned}\text{RBC}_i^{\text{Index}(\mathbf{y})} &= \text{Index}(\mathbf{y}) - \text{Index}(\mathbf{y}_i^r)\\ &= \mathbf{y}^T\mathbf{N}\mathbf{y} - 2\mathbf{y}^T\mathbf{a} + c(\mathbf{x})\\ &\qquad -(\mathbf{y}-\xi_i f)^T\mathbf{N}(\mathbf{y}-\xi_i f)\\ &\qquad +2(\mathbf{y}-\xi_i f)^T\mathbf{a} - c(\mathbf{x})\\ &= 2\mathbf{y}^T\mathbf{N}\xi_i f - f^2\xi_i^T\mathbf{N}\xi_i - 2f\xi_i^T\mathbf{a}\\ &= \frac{(\mathbf{y}^T\mathbf{N}\xi_i - a_i)^2}{\xi_i^T\mathbf{N}\xi_i}\end{aligned} \tag{16}$$

The last equality in (16) is the result of applying (15).

6. ANALYSIS OF DIAGNOSABILITY

Contribution methods have been used in practice, but not much fundamental analysis on their diagnosabilities has been developed. Alcala and Qin (2009) proposed to approach this by examining the case where a sensor fault happened in the ξ_j direction with a sufficiently large fault magnitude f. A fault in sensor j is represented as $\mathbf{x} = \mathbf{x}^* + \xi_j f$ where $\mathbf{x}^*$ is the fault-free part of the measurement. When f is sufficiently large, $\mathbf{x}^*$ is negligible compared to $\xi_j f$, and therefore

$$\mathbf{x} \approx \xi_j f. \tag{17}$$

Similarly for fault sample $\mathbf{y}$

$$\mathbf{y} \approx \xi_j f. \tag{18}$$

This case will be utilized to examine the diagnosability of the above defined contributions.

6.1 Diagnosis using complete decomposition contributions

Substituting the fault in (17) into (9), and (18) into (10) we get

$$\mathrm{CDC}_i^{\mathrm{Index}(\mathbf{x})} = \begin{cases} [\mathbf{M}^{(1/2)}]_{ij}^2 f^2 & \text{for } i \neq j \\ [\mathbf{M}^{(1/2)}]_{jj}^2 f^2 & \text{for } i = j \end{cases}$$

and

$$\mathrm{CDC}_i^{\mathrm{Index}(\mathbf{y})} = \begin{cases} [\mathbf{N}^{(1/2)}]_{ij}^2 f^2 + c(\mathbf{x})/n & \text{for } i \neq j \\ [\mathbf{N}^{(1/2)}]_{jj}^2 f^2 - 2fa_j + c(\mathbf{x})/n & \text{for } i = j \end{cases}$$

where $[\mathbf{A}]_{ij} = \xi_i^T \mathbf{A} \xi_j$ is the ij th element of the matrix $\mathbf{A}$. Correct diagnosis using CDC is guaranteed only if

$$[\mathbf{M}^{(1/2)}]_{jj}^2 \geq [\mathbf{M}^{(1/2)}]_{ij}^2 \tag{19}$$

and

$$[\mathbf{N}^{(1/2)}]_{jj}^2 f^2 - 2fa_j \geq [\mathbf{N}^{(1/2)}]_{ij}^2 f^2. \tag{20}$$

The inequalities (19) and (20) however, are not always true. It is worth noting that if we assume the data are stationary, the model is fixed, and so is $\mathbf{M}$. Therefore, when (19) does not hold, the CDC method completely fails, and the correct diagnosing rate is zero.

6.2 Diagnosis using reconstruction-based contributions

Substituting the fault in (17) into (13) and (18) into (16) we get

$$\mathrm{RBC}_i^{\mathrm{Index}(\mathbf{x})} = \begin{cases} [\mathbf{M}]_{ij}^2 [\mathbf{M}]_{ii}^{-1} f^2 & \text{for } i \neq j \\ [\mathbf{M}]_{jj} f^2 & \text{for } i = j \end{cases}$$

and

$$\begin{aligned} \mathrm{RBC}_i^{\mathrm{Index}(\mathbf{y})} &= \begin{cases} \{[\mathbf{N}]_{ij} f - a_i\}^2 [\mathbf{N}]_{ii}^{-1} & \text{for } i \neq j \\ \{[\mathbf{N}]_{jj} f - a_j\}^2 [\mathbf{N}]_{jj}^{-1} & \text{for } i = j \end{cases} \\ &\approx \begin{cases} [\mathbf{N}]_{ij}^2 [\mathbf{N}]_{ii}^{-1} f^2 & \text{for } i \neq j \\ [\mathbf{N}]_{jj} f^2 & \text{for } i = j \end{cases} \end{aligned} \tag{21}$$

The approximation in (21) assumes f is sufficiently large and therefore a_i and a_j are negligible compared to $[\mathbf{N}]_{ij} f$ and $[\mathbf{N}]_{jj} f$. Correct diagnosis using RBC is guaranteed only if

$$[\mathbf{M}]_{jj} \geq [\mathbf{M}]_{ij}^2 [\mathbf{M}]_{ii}^{-1} \tag{22}$$

and

$$[\mathbf{N}]_{jj} \geq [\mathbf{N}]_{ij}^2 [\mathbf{N}]_{ii}^{-1}. \tag{23}$$

Since both $\mathbf{M}$ and $\mathbf{N}$ are positive semi-definite matrices, (22) and (23) always hold. The proof is given in the appendix of Alcala and Qin (2009).

In summary, for the simplest case of a sufficiently large sensor fault, RBC methods guarantee correct fault diagnosis, but the CDC methods do not. However, for modest fault magnitudes the randomness in the fault-free portion $\mathbf{x}^*$ will likely affect the diagnosis results, which will be studied next by simulation.

7. SIMULATION CASE STUDIES

In this section, we use synthetic simulations to create a number of representing sensor fault scenarios to demonstrate and compare the effectiveness of the above defined contributions for fault diagnosis.

The simulated numerical example without faults is as follows.

$$\begin{cases} \mathbf{x}_k = \mathbf{A}\mathbf{z}_k + \mathbf{e}_k \\ \mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{v}_k \end{cases} \tag{24}$$

where $\mathbf{A} = \begin{pmatrix} 1 & 3 & 4 & 0 & 0 \\ 3 & 0 & 4 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}^T$, $\mathbf{C} = \begin{pmatrix} 2 & 2 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$, $\mathbf{z}_k \in \mathbb{R}^4 \sim \mathbf{U}([0,1])$, $\mathbf{e}_k \in \mathbb{R}^5 \sim N(0, 0.1^2)$, and $\mathbf{v}_k \in \mathbb{R}^2 \sim N(0, 0.08^2)$. $\mathbf{U}([0,1])$ is the uniform distribution in the interval $[0,1]$.

All of the parameters are more or less randomly chosen, except that $\mathbf{x}_4$ is independent of other input variables, and it is the only input variable that contributes to $\mathbf{y}_2$. This will make sure that $\mathbf{x}_4$ is in the input-output covariance subspace.

Equation (24) is used to generate normal operation data, and the number of PLS components $l = 3$ is determined by 10-fold cross-validation. In this model, R_y in (3) is less than 0.05, and therefore there is no output principal subspace.

A sensor fault is added in the following form in the input space or in the output space.

Table 4. Percent rates of correct diagnosis for scenario 1 & 2

	Scenario 1			Scenario 2		
		Q_y			T_c^2	
f	FDR	CDC	RBC	FDR	CDC	RBC
0.5	5.8	37.93	0.00	33.8	98.82	94.08
1	7.8	38.46	0.00	86.6	100.00	99.31
2	31.6	51.90	60.13	100.0	100.00	100.00
3	100.0	66.40	98.60	100.0	100.00	100.00
10	100.0	99.20	100.00	100.0	100.00	100.00

Table 5. Percent rates of correct diagnosis for scenario 3

	Scenario 3					
		T_x^2			Q_x	
f	FDR	CDC	RBC	FDR	CDC	RBC
0.5	1.8	0.00	22.22	26.0	30.77	34.62
1	8.2	0.00	31.71	75.8	43.01	45.91
2	28.8	0.00	30.56	100.0	63.20	62.80
3	53.6	0.00	35.45	100.0	79.20	73.60
10	100.0	0.00	65.60	100.0	100.00	100.00

$$\mathbf{x}_k = \mathbf{x}_k^* + \xi_x f_x \quad , \quad \mathbf{y}_k = \mathbf{y}_k^* + \xi_y f_y$$

where $\mathbf{x}_k^*$ and $\mathbf{y}_k^*$ are the fault-free values, ξ_x and ξ_y are the fault directions, and f_x and f_y are the respective fault magnitudes.

Three scenarios are being studied.

(1) A sensor fault was added to $\mathbf{y}_1$, which was detected only by Q_y;
(2) A sensor fault was added to $\mathbf{x}_4$, which was detected only by T_c^2; and
(3) A sensor fault was added to $\mathbf{x}_2$, which was detected by both T_x^2 and Q_x.

Due to the page limitation, their fault detection indices are not plotted here. The percent rates of correct diagnosis and the fault detection rates (FDR) with various fault magnitudes are given in Table 4 and 5. From the result, we can see that although RBC can guarantee correct diagnosis when the fault magnitude is sufficiently large, it is very hard to tell which method is better with a modest fault magnitude. However, it is interesting to note that the CDC method completely failed on T_x^2 index in scenario 3.

8. CONCLUSIONS

In this article, CPLS based contributions for fault diagnosis are proposed and studied. We unified the five CPLS monitoring indices into two general forms, and based on these general forms, we defined their complete decomposition contributions (CDC) and reconstruction-based contributions (RBC). Diagnosability of the CDCs and RBCs are also analyzed. At the end, synthetic case studies on sensor faults are presented. A future step is to test this fault diagnosis framework on process faults.

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