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On the Application of PCA Technique to Fault Diagnosis

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Abstract: In this paper, we briefly address the application of the standard principal component analysis (PCA) technique to fault detection and identification. Based on an analysis of the existing test statistic, we propose a new test statistic, which is similar to the Hawkin's T_H^2 statistic but without the numerical drawback. In comparison with the SPE index, the threshold setting associated with the new statistic is computationally simpler. Our further study is dedicated to the analysis of fault sensitivity. We consider the off-set and scaling faults, and evaluate the test statistic by viewing its sensitivity to the faults. Our final study focuses on identifying off-set and scaling faults. To this end, two algorithms are proposed. This paper also includes some critical remarks on the application of the PCA technique to fault diagnosis.

Key words: process monitoring; fault diagnosis; principal component analysis (PCA); multivariate analysis

Introduction

Principal component analysis (PCA) is a basic method in the framework of the multivariate analysis techniques. It has been successfully used in numerous areas including data compression, feature extraction, image processing, pattern recognition, signal analysis, and process monitoring[1]. Thanks to its simplicity and efficiency in processing huge amount of process data, PCA is recognised as a powerful tool of statistical process monitoring and widely used in the process industry for fault detection and diagnosis[2-4]. Recent development in the PCA technique is focused on achieving adaptive process monitoring using, for instance, recursive implementation of PCA[5], fast moving window PCA[6] or kernel PCA[7].

In our recent project dealing with the application of the standard PCA technique to the process monitoring, we have noticed that slight modifications on the PCA methods might lead to a performance improvement in detecting and identifying process faults. This experience motivates us to review the standard PCA technique, which is the first objective of this paper. Some critical remarks on the application of the PCA technique to fault diagnosis and the introduction of new test statistics are the results of our review study. The further objective of our study is to analyze the fault sensitivity of the test statistic used in the PCA and to apply the PCA technique to the identification of two different types of faults.

The paper is organised as follows. In Section 1, the standard PCA technique will first be reviewed. The focus is on the two well known statistics, T^2 and SPE, and their statistical interpretation. This study motivates us to introduce an alternative test statistic. Section 2 is dedicated to the check of the fault sensitivity under different test statistics and with respect to the off-set and scaling faults. Section 3 deals with the PCA-based identification of those two types of faults. In the last section, some critical remarks on the application of the PCA methods to fault diagnosis are included.

Notation The notation adopted throughout this

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paper is fairly standard. $\mathbf{R}^n$ denotes the n-dimentional Euclidean space and $\mathbf{R}^{n\times m}$ the set of all $n\times m$ real matrices. The superscript "T" stands for the transpose of a matrix. "$\boldsymbol{I}$" and "$\mathbf{0}$" denote the identity and zero matrices with appropriate dimension, respectively, and $\mathrm{diag}(\bullet,\cdots,\bullet)$ a diagonal matrix. $E(\bullet)$ represents mean value. $\boldsymbol{x}\sim N(\mathbf{0},\boldsymbol{\Sigma})$ means that $\boldsymbol{x}$ is normal distributed with zero mean and covariance. $X^2(l)$ and $F(l,N)$ stand for X^2-distributed with l degrees of freedom and F-distributed with l,N degrees of freedom, respectively.

1 Reviewing PCA and an Alternative Test Statistic

1.1 A brief description of PCA

We first briefly review the standard PCA technique.

Consider a process with m sensors. A standard PCA approach for fault diagnosis consists of three steps and can be briefly formulated as follows:

- Data collection and normalization: In this step, N samples for each sensor are first collected and recorded in a data matrix $\boldsymbol{X}\in\mathbf{R}^{N\times m}$. Matrix $\boldsymbol{X}$ is then scaled to zero mean, and often in addition to unit variance. Let the scaled data be

$$\boldsymbol{X}=\begin{bmatrix}\boldsymbol{x}_1^{\mathrm{T}}\\ \vdots\\ \boldsymbol{x}_N^{\mathrm{T}}\end{bmatrix}\in\mathbf{R}^{N\times m}$$

with $\boldsymbol{x}_i\in\mathbf{R}^m, i=1,\ldots,N,$ denoting a (scaled) sample vector of the m sensors.

- Computation of singular values, corresponding singular vectors and thresholds: First, the covariance matrix is formed,

$$\boldsymbol{\Sigma}\approx\frac{1}{N-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X},$$

and then, by means of, for example, an SVD (singular value decomposition), the principal components and the associated singular vectors are computed as

$$\frac{1}{N-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}=\boldsymbol{P\Lambda P}^{\mathrm{T}},\ \boldsymbol{\Lambda}=\begin{bmatrix}\boldsymbol{\Lambda}_{\mathrm{pc}} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\Lambda}_{\mathrm{res}}\end{bmatrix} \tag{1}$$

$$\boldsymbol{\Lambda}_{\mathrm{pc}}=\mathrm{diag}(\sigma_1^2,\ldots,\sigma_l^2)\in\mathbf{R}^{l\times l},$$

$$\boldsymbol{\Lambda}_{\mathrm{res}}=\mathrm{diag}(\sigma_{l+1}^2,\ldots,\sigma_m^2)\in\mathbf{R}^{(m-l)\times(m-l)}$$

$$\boldsymbol{P}=[P_{\mathrm{pc}}\quad P_{\mathrm{res}}]\in\mathbf{R}^{m\times m},$$

$$\boldsymbol{P}_{\mathrm{pc}}\in\mathbf{R}^{m\times l},\ \boldsymbol{P}_{\mathrm{res}}\in\mathbf{R}^{m\times(m-l)},$$

$$\boldsymbol{PP}^{\mathrm{T}}=\boldsymbol{P}_{\mathrm{pc}}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}+\boldsymbol{P}_{\mathrm{res}}\boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}=\boldsymbol{I}_{m\times m},$$

$$\begin{bmatrix}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\\ \boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}\end{bmatrix}[\boldsymbol{P}_{\mathrm{pc}}\quad \boldsymbol{P}_{\mathrm{res}}]=\begin{bmatrix}\boldsymbol{I}_{l\times l} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{I}_{(m-l)\times(m-l)}\end{bmatrix},$$

where $\sigma_1\geqslant\cdots\geqslant\sigma_l$ are the l largest (principal) singular values and

$$\sigma_l>>\sigma_{l+1}\geqslant\cdots\geqslant\sigma_m.$$

For the fault detection purpose, the so-called SPE (squared prediction error) statistic and Hotelling's T^2 statistic are often used. For a significance level α, the corresponding thresholds are respectively set to be

$$\mathrm{SPE}:J_{\mathrm{th,SPE}}=\theta_1\left(\frac{c_\alpha\sqrt{2\theta_2h_0^2}}{\theta_1}+1+\frac{\theta_2h_0(h_0-1)}{\theta_1^2}\right)^{1/h_0} \tag{2}$$

$$T^2:J_{\mathrm{th},T^2}=\frac{l(N^2-1)}{N(N-l)}F_\alpha(l,N-l) \tag{3}$$

where c_α is the normal deviate corresponding to the upper $1-\alpha$ percentile and

$$\theta_i=\sum_{j=l+1}^{m}(\sigma_j^2)^i,\ i=1,2,3,\ h_0=1-\frac{2\theta_1\theta_3}{3\theta_2^2}.$$

- On-line computation of SPE statistic and Hotelling's T^2 statistic and fault detection: For a new scaled measurement $x\in\mathbf{R}^m$ the SPE statistic and Hotelling's T^2 statistic are respectively (on-line) computed as

$$\mathrm{SPE}=\|(I-\boldsymbol{P}_{\mathrm{pc}}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}})x\|^2=\boldsymbol{x}^{\mathrm{T}}(I-\boldsymbol{P}_{\mathrm{pc}}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}})^2\boldsymbol{x},$$

$$T^2=\boldsymbol{x}^{\mathrm{T}}\boldsymbol{P}_{\mathrm{pc}}\boldsymbol{\Lambda}_{\mathrm{pc}}^{-1}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\boldsymbol{x}.$$

The fault detection logic is

$\mathrm{SPE}\leqslant J_{\mathrm{th,SPE}}$ or $T^2\leqslant J_{\mathrm{th},T^2}\Rightarrow$ fault-free, otherwise faulty.

Remark In order to simplify our study and notation, it is assumed, throughout the paper, that the sample number N is large enough so that X^2-distribution instead of F-distribution can be adopted.

1.2 On the test statistic and an alternative test statistic

Assume that the process is normal and

$$\boldsymbol{x}\sim N(\mathbf{0},\boldsymbol{\Sigma}) \tag{4}$$

It holds

$$\boldsymbol{z}_{\mathrm{pc}}=\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\boldsymbol{x}\in\mathbf{R}^l,\ \boldsymbol{z}_{\mathrm{pc}}\sim N(\mathbf{0},\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\boldsymbol{\Sigma}\boldsymbol{P}_{\mathrm{pc}})=N(\mathbf{0},\boldsymbol{\Lambda}_{\mathrm{pc}}).$$

Thus, the T^2 statistic satisfies X^2-distribution with l degrees of freedom. It is interesting to notice that

$$\mathrm{SPE}=\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{I}-\boldsymbol{P}_{\mathrm{pc}}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}})^2x=\boldsymbol{x}^{\mathrm{T}}\boldsymbol{P}_{\mathrm{res}}\boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}\boldsymbol{P}_{\mathrm{res}}\boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}\boldsymbol{x}=\boldsymbol{x}^{\mathrm{T}}\boldsymbol{P}_{\mathrm{res}}\boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}x.$$

Moreover, on the assumption Eq. (4),

$$\boldsymbol{z}_{\rm res}=\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}\in\mathbf{R}^{(m-l)},\ \boldsymbol{z}_{\rm res}\sim N(\boldsymbol{0},\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{\Sigma}\boldsymbol{P}_{\rm res})=N(\boldsymbol{0},\boldsymbol{\Lambda}_{\rm res})\quad(5)$$

As a result,

$$\boldsymbol{x}^{\rm T}\boldsymbol{P}_{\rm res}\boldsymbol{\Lambda}_{\rm res}^{-1}\boldsymbol{P}_{\rm res}^{\rm T}x\quad(6)$$

satisfies X^2-distribution with $m-l$ degrees of freedom and would be a reasonable statistic for the fault detection purpose. In fact, the statistic defined by Eq. (6) is called Hawkin's T_H^2 statistic, which is, however, less used in practice due to the drawback with the possible ill-conditioning $\boldsymbol{\Lambda}_{\rm res}$ when some of the singular values of $\sigma_{l+1},\cdots,\sigma_m$ are too close to zero. To avoid this difficulty on the one hand and to make use of the easy/available computation of the X^2-distribution on the other hand, we propose below an alternative test statistic.

Let

$$\boldsymbol{\Xi}=\mathrm{diag}\left(\frac{\sigma_m^2}{\sigma_{l+1}^2},\ldots,\frac{\sigma_m^2}{\sigma_{m-1}^2},1\right)\in\mathbf{R}^{(m-l)\times(m-l)}.$$

It turns out that

$$\bar{\boldsymbol{z}}_{\rm res}=\boldsymbol{\Xi}^{1/2}\boldsymbol{z}_{\rm res}=\boldsymbol{\Xi}^{1/2}\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}\sim N(\boldsymbol{0},\sigma_m^2\boldsymbol{I}_{(m-l)\times(m-l)})$$

and moreover

$$\bar{\boldsymbol{z}}_{\rm res}^{\rm T}\bar{\boldsymbol{z}}_{\rm res}=\boldsymbol{z}_{\rm res}^{\rm T}\boldsymbol{\Xi}\boldsymbol{z}_{\rm res}=\sigma_m^2\boldsymbol{x}^{\rm T}\boldsymbol{P}_{\rm res}\boldsymbol{\Lambda}_{\rm res}^{-1}\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}.$$

Since $\boldsymbol{x}^{\rm T}\boldsymbol{P}_{\rm res}\boldsymbol{\Lambda}_{\rm res}^{-1}\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}$ is X^2-distributed with $m-l$ degrees of freedom, define

$$T_{\rm new}^2=\bar{\boldsymbol{z}}_{\rm res}^{\rm T}\bar{\boldsymbol{z}}_{\rm res}=\boldsymbol{z}_{\rm res}^{\rm T}\boldsymbol{\Xi}\boldsymbol{z}_{\rm res}=\boldsymbol{x}^{\rm T}\boldsymbol{P}_{\rm res}\boldsymbol{\Xi}\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}\quad(7)$$

as the test statistic results in a threshold setting, for a given significance level, α, equal to

$$J_{\rm th,new}=\sigma_m^2X_\alpha^2(m-l)\quad(8)$$

1.3 Some remarks

$\boldsymbol{P}_{\rm pc},\boldsymbol{P}_{\rm res}$ define two subspaces, which are called, known in the PCA relevant literatures, principal component subspace and residual subspace respectively. In the standard PCA technique, the projections

$$\hat{\boldsymbol{x}}=\boldsymbol{P}_{\rm pc}\boldsymbol{P}_{\rm pc}^{\rm T}\boldsymbol{x},\ \tilde{\boldsymbol{x}}=\boldsymbol{P}_{\rm res}\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}\Rightarrow\boldsymbol{x}=\hat{\boldsymbol{x}}+\tilde{\boldsymbol{x}}$$

are introduced for the study on fault detection. It is interesting to notice that

- both $\boldsymbol{P}_{\rm pc}\boldsymbol{P}_{\rm pc}^{\rm T}\in\mathbf{R}^{m\times m}$ and $\boldsymbol{P}_{\rm res}\boldsymbol{P}_{\rm res}^{\rm T}\in\mathbf{R}^{m\times m}$ are singular matrices, since $\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{P}_{\rm pc}\boldsymbol{P}_{\rm pc}^{\rm T}=\boldsymbol{0},\ \boldsymbol{P}_{\rm pc}^{\rm T}\boldsymbol{P}_{\rm res}\boldsymbol{P}_{\rm res}^{\rm T}=\boldsymbol{0}.$
- the test statistics used in the PCA are the quadratic forms associated with $\boldsymbol{z}_{\rm pc}=\boldsymbol{P}_{\rm pc}^{\rm T}\boldsymbol{x}$ and $\boldsymbol{z}_{\rm res}=\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}.$

The introduction of the new statistic Eq. (7) is motivated by this observation. Also in our subsequent study, we shall focus on $\boldsymbol{z}_{\rm pc},\boldsymbol{z}_{\rm res}$ instead of $\hat{\boldsymbol{x}},\tilde{\boldsymbol{x}}$.

We would like to point out that

- the new statistic $\boldsymbol{T}_{\rm new}^2$ is X^2-distributed, and
- different from the SPE, for which the associated threshold has been derived by an approximation[8], the corresponding threshold can be exactly determined using the available X^2 data table as shown in Eq. (8), and
- the associated computation is (considerably) less complicated than the computation of $J_{\rm th,SPE}$ given in Eq. (2).

2 Fault Sensitivity Analysis

In this section, we analyze the fault sensitivity of the test statistic introduced in the last section.

Off-set and scaling (multiplicative) faults are the two types of faults which are mostly considered both in the theoretic study and practical application. Given a measurement sample $\boldsymbol{x}$, the off-set and scaling faults can be modelled as follows.

$$\boldsymbol{x}=\boldsymbol{x}_{\rm o}+\boldsymbol{f},\boldsymbol{f}\neq\boldsymbol{0}\Rightarrow\text{off-set fault},$$

$$\boldsymbol{x}=\boldsymbol{F}\boldsymbol{x}_{\rm o},\boldsymbol{F}\neq\boldsymbol{I}\Rightarrow\text{scaling fault},$$

where $\boldsymbol{x}_{\rm o}$ represents the sample in the fault-free case and $\boldsymbol{f}\in\mathbf{R}^m$ a (non-zero) constant fault vector. Next, we shall study the test statistic introduced in the last section in detecting off-set and scaling faults.

Note that the SPE, $T_{\rm H}^2$ and $T_{\rm new}^2$ statistic consist of (different) quadratic forms of vector $\boldsymbol{z}_{\rm res}=\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}$, while the T^2 statistic is based on $\boldsymbol{z}_{\rm pc}=\boldsymbol{P}_{\rm pc}^{\rm T}\boldsymbol{x}$. To simplify the notation, use $T_{\rm res}^2$ to represent the statistic associated with $\boldsymbol{z}_{\rm res}=\boldsymbol{P}_{\rm res}^{\rm T}\boldsymbol{x}$, i.e., the SPE, $T_{\rm H}^2$ and $T_{\rm new}^2$ statistics.

2.1 Sensitivity to the off-set faults

Recall that the covariance matrices of $\boldsymbol{z}_{\rm pc},\boldsymbol{z}_{\rm res}$ are respectively $\boldsymbol{\Lambda}_{\rm pc}$ and $\boldsymbol{\Lambda}_{\rm res}$, furthermore

$$\sigma_{\min}(\boldsymbol{\Lambda}_{\rm pc})=\sigma_l>>\sigma_{\max}(\boldsymbol{\Lambda}_{\rm res})=\sigma_{l+1}.$$

As a result, the $T_{\rm res}^2$ statistic can be (significantly) more sensitive to the off-set fault than the T^2 statistic. To demonstrate it, consider the Hawkin's $T_{\rm H}^2$ statistic and Hotelling's T^2 statistic. It holds, for a significance level α,

$$\max_{x_o \in N(\mathbf{0},\boldsymbol{\Sigma})}(\boldsymbol{x}_o^T \boldsymbol{P}_{res}\boldsymbol{\Lambda}_{res}^{-1}\boldsymbol{P}_{res}^T \boldsymbol{x}_o) \leqslant J_{th,T_H^2} = X_\alpha^2(m-l),$$

$$\max_{x_o \in N(\mathbf{0},\boldsymbol{\Sigma})}(\boldsymbol{x}_o^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x}_o) \leqslant J_{th,T^2} = X_\alpha^2(l).$$

Thus, if a fault $\boldsymbol{f}$ causes

$$(\boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f})^{1/2} > 2\sigma_{l+1} J_{th,T_H^2}^{1/2} = 2\sigma_{l+1}(X_\alpha^2(m-l))^{1/2} \quad (9)$$

we have

$$(\boldsymbol{x}^T \boldsymbol{P}_{res}\boldsymbol{\Lambda}_{res}^{-1}\boldsymbol{P}_{res}^T \boldsymbol{x})^{1/2} \geqslant$$
$$(\boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{\Lambda}_{res}^{-1}\boldsymbol{P}_{res}^T \boldsymbol{f})^{1/2} - (\boldsymbol{x}_o^T \boldsymbol{P}_{res}\boldsymbol{\Lambda}_{res}^{-1}\boldsymbol{P}_{res}^T \boldsymbol{x}_o)^{1/2} \geqslant$$
$$\sigma_{l+1}^{-1}(\boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f})^{1/2} - J_{th,T_H^2}^{1/2} > J_{th,T_H^2}^{1/2} \Rightarrow \text{faulty},$$

i.e., this fault can be, with the significance level α, detected. Note that Eq. (9) is a sufficient condition that a fault can be detected. On the other hand, we have

$$E(T^2) = E(\boldsymbol{x}^T P_{pc}\Lambda_{pc}^{-1}\boldsymbol{P}_{pc}^T x) =$$
$$E(\boldsymbol{x}_o^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x}_o) + \boldsymbol{f}^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{f} \leqslant$$
$$E(\boldsymbol{x}_o^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x}_o) + \sigma_l^{-2}\boldsymbol{f}^T \boldsymbol{P}_{pc}\boldsymbol{P}_{pc}^T \boldsymbol{f} =$$
$$l + \frac{\sigma_{l+1}^2 \boldsymbol{f}^T \boldsymbol{P}_{pc}\boldsymbol{P}_{pc}^T \boldsymbol{f} \cdot \sigma_{l+1}^{-2}\boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f}}{\sigma_l^2 \boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f}}.$$

Assume that

$$\boldsymbol{f}^T \boldsymbol{P}_{pc}\boldsymbol{P}_{pc}^T \boldsymbol{f} \approx \boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f},$$
$$\sigma_{l+1}^{-2}\boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f} = 4J_{th,T_H^2} + \delta, \quad \delta > 0 \quad (10)$$
$$\Rightarrow (\boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f})^{1/2} > 2\sigma_{l+1} J_{th,T_H^2}^{1/2} \quad (11)$$

It turns out

$$E(\boldsymbol{x}^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x}) \leqslant l + \frac{\sigma_{l+1}^2(4X_\alpha^2(m-l)+\delta)}{\sigma_l^2}.$$

For

$$\frac{\sigma_{l+1}^2}{\sigma_l^2} \leqslant \frac{X_\alpha^2(l) - l}{4X_\alpha^2(m-l)+\delta} \quad (12)$$

we finally have

$$E(\boldsymbol{x}^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x}) \leqslant X_\alpha^2(l) = J_{th,T^2} \quad (13)$$

It follows from Eq. (13) that f is expectably undetected under condition Eq. (12), although it is detectable using the Hawkin's T_H^2 (see Eq. (10)) and for $\boldsymbol{f}^T \boldsymbol{P}_{pc}\boldsymbol{P}_{pc}^T \boldsymbol{f} \approx \boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f}$.

The previous analysis reveals that a statistic associated with $\boldsymbol{P}_{res}^T \boldsymbol{x}$ is more sensitive to an off-set fault than the T^2 statistic when the fault has the same influence on both statistics, i.e., $\boldsymbol{f}^T \boldsymbol{P}_{pc}\boldsymbol{P}_{pc}^T \boldsymbol{f} \approx \boldsymbol{f}^T \boldsymbol{P}_{res}\boldsymbol{P}_{res}^T \boldsymbol{f}$.

2.2 Sensitivity to the scaling faults

For our purpose, we now compare the Hawkin's T_H^2 statistic and Hotelling's T^2 statistic in detecting scaling faults. To simplify the study, it is assumed that the scaling fault is modelled by

$$\boldsymbol{F} = \alpha_f \boldsymbol{I}, \alpha_f \geqslant 1, \text{ and } \alpha_f > 1 \Rightarrow \text{faulty}.$$

It turns out that

$$T^2 = \boldsymbol{x}^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x} = \alpha_f^2 \boldsymbol{x}_o^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x}_o,$$
$$T_H^2 = \boldsymbol{x}^T \boldsymbol{P}_{res}\boldsymbol{\Lambda}_{res}^{-1}\boldsymbol{P}_{res}^T \boldsymbol{x} = \alpha_f^2 \boldsymbol{x}_o^T \boldsymbol{P}_{res}\boldsymbol{\Lambda}_{res}^{-1}\boldsymbol{P}_{res}^T \boldsymbol{x}_o.$$

Remember that for the same significance level α,

$$\max_{x_o \in N(\mathbf{0},\boldsymbol{\Sigma})}(\boldsymbol{x}_o^T \boldsymbol{P}_{res}\boldsymbol{\Lambda}_{res}^{-1}\boldsymbol{P}_{res}^T \boldsymbol{x}_o) \leqslant J_{th,T_H^2} = X_\alpha^2(m-l),$$
$$\max_{x_o \in N(\mathbf{0},\boldsymbol{\Sigma})}(\boldsymbol{x}_o^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x}_o) \leqslant J_{th,T^2} = X_\alpha^2(l).$$

Replacing $\max_{x_o \in N(\mathbf{0},\boldsymbol{\Sigma})}(\boldsymbol{x}_o^T \boldsymbol{P}_{res}\boldsymbol{\Lambda}_{res}^{-1}\boldsymbol{P}_{res}^T \boldsymbol{x}_o)$, $\max_{x_o \in N(\mathbf{0},\boldsymbol{\Sigma})}(\boldsymbol{x}_o^T \boldsymbol{P}_{pc}\boldsymbol{\Lambda}_{pc}^{-1}\boldsymbol{P}_{pc}^T \boldsymbol{x}_o)$, respectively, by J_{th,T_H^2}, J_{th,T^2} and defining the fault sensitivity by

$$S_H = \frac{\max T_H^2\big|_{\text{faulty}}}{\max T_H^2\big|_{\text{fault-free}}}, \quad S = \frac{\max T^2\big|_{\text{faulty}}}{\max T^2\big|_{\text{fault-free}}},$$

we have

$$S_H = \frac{\alpha_f^2 J_{th,T_H^2}}{J_{th,T_H^2}} = \alpha_f^2, \quad S = \frac{\alpha_f^2 J_{th,T^2}}{J_{th,T^2}} = \alpha_f^2.$$

This analysis demonstrates that the Hawkin's T_H^2 statistic and Hotelling's T^2 statistic may offer the similar performance in detecting scaling faults.

2.3 Combined indices and a detection scheme

Notice that in the previous study, it has been assumed that both the off-set and scaling faults have a similar influence on $\boldsymbol{z}_{pc} = \boldsymbol{P}_{pc}^T \boldsymbol{x}$ and $\boldsymbol{z}_{res} = \boldsymbol{P}_{res}^T \boldsymbol{x}$. Removing this assumption, it is clear that matrices $\boldsymbol{P}_{pc}^T, \boldsymbol{P}_{res}^T$ may also considerably affect the fault sensitivity. For instance, those faults that belong to the (left) null-subspace of $\boldsymbol{P}_{pc}^T, \boldsymbol{P}_{res}^T$ can not be, independent of the "size" of the faults, detected by the T^2 statistic and T_{res}^2 statistic, respectively. In order to reduce or eliminate the influence of the mapping matrices $\boldsymbol{P}_{pc}^T, \boldsymbol{P}_{res}^T$ on the fault sensitivity, the so-called combined indices can be used[2,3], which are generally formulated as

$$T_c^2 = \beta_1 T^2 + \beta_2 T_{res}^2 \quad (14)$$

with known constants $\beta_1, \beta_2 > 0$. Rewriting Eq. (14) into

$$T_c^2 = \boldsymbol{x}^T \boldsymbol{P\Phi P}^T \boldsymbol{x}, \boldsymbol{\Phi} = \begin{bmatrix} \beta_1 \boldsymbol{\Lambda}_{pc}^{-1} & \mathbf{0} \\ \mathbf{0} & \beta_2 \boldsymbol{Q} \end{bmatrix},$$

makes it clear that a combined index is a quadratic statistic of signal $\boldsymbol{P}^{\mathrm{T}}\boldsymbol{x}$, where

$$\boldsymbol{Q}=\begin{cases}\boldsymbol{\Lambda}_{\mathrm{res}}^{-1}, T_{\mathrm{res}}^2=T_{\mathrm{H}}^2,\\ \boldsymbol{I}, T_{\mathrm{res}}^2=\mathrm{SPE},\\ \boldsymbol{\Xi}, T_{\mathrm{res}}^2=T_{\mathrm{new}}^2.\end{cases}$$

Since $\boldsymbol{P}^{\mathrm{T}}\boldsymbol{x}\sim N(\boldsymbol{0},\boldsymbol{\Lambda})$, $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{\Lambda}^{-1}\boldsymbol{P}^{\mathrm{T}}\boldsymbol{x}$ is X^2-distributed with m degrees of freedom. This fact motivates us to introduce the following (combined) statistic.

Considering the possible numerical difficulty with the computation of $\boldsymbol{\Lambda}^{-1}$, we propose

$$T_{\mathrm{c,new}}^2=\boldsymbol{x}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{\Xi}\boldsymbol{P}^{\mathrm{T}}\boldsymbol{x},\ \boldsymbol{\Xi}=\mathrm{diag}\left(\frac{\sigma_m^2}{\sigma_1^2},\ldots,\frac{\sigma_m^2}{\sigma_{m-1}^2},1\right) \tag{15}$$

which is a combined index given by

$$T_{\mathrm{c,new}}^2=\boldsymbol{x}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{\Xi}\boldsymbol{P}^{\mathrm{T}}\boldsymbol{x}=\sigma_m^2T^2+T_{\mathrm{new}}^2=\sigma_m^2(T^2+T_{\mathrm{H}}^2) \tag{16}$$

It is clear that the corresponding threshold is

$$J_{\mathrm{th,c,new}}=\sigma_m^2X_\alpha^2(m)$$

for a given significance level α.

Next, we would like to analyze the combined test statistic briefly. To simplify our study but without loss of generality, we use $T_{\mathrm{c,new}}^2$ representing the combined index T_{c}^2 for our study. Since

$$X_\alpha^2(m)>X_\alpha^2(l),\quad X_\alpha^2(m)>X_\alpha^2(m-l),$$

the combined index may be of a lower fault sensitivity than the separate use of T_{H}^2, T^2. To illustrate this, we consider those faults satisfying $\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\boldsymbol{f}=\boldsymbol{0}$. In this case, f will cause the same change in T_{H}^2 and T_{c}^2. Recall that the threshold corresponding to T_{c}^2 is considerably higher than the one associated with T_{H}^2. Thus, T_{H}^2 is much more sensitive to these faults than the T_{c}^2 index.

On the other hand, considering that it often holds

$$X_\alpha^2(m)<X_\alpha^2(l)+X_\alpha^2(m-l),$$

there do exist faults which result in

$$T_{\mathrm{c}}^2(x)=\boldsymbol{x}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{\Lambda}^{-1}\boldsymbol{P}^{\mathrm{T}}\boldsymbol{x}>X_\alpha^2(m)$$

but

$$T^2(x)<X_\alpha^2(l)\ \text{and}\ T_{\mathrm{H}}^2(x)<X_\alpha^2(m-l).$$

That means, in this case a combined index is more sensitive to the faults than using

$$(J_{\mathrm{th,H}}-T_{\mathrm{H}}^2(x)<0)\cup(J_{\mathrm{th},T^2}-T^2(x)<0)>0$$
$$\Rightarrow \text{faulty, otherwise fault-free} \tag{17}$$

The previous discussion reveals that

- the use of a combined index is of advantage when the distribution of $\boldsymbol{\Lambda}^{-1}\boldsymbol{f}$ is nearly uniform in the measurement subspace and
- the separate use of two test statistics, as described in Eq. (17), will improve the fault sensitivity if it can be assumed that $\boldsymbol{f}^{\mathrm{T}}\boldsymbol{P}_{\mathrm{pc}}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\boldsymbol{f}>>\boldsymbol{f}^{\mathrm{T}}\boldsymbol{P}_{\mathrm{res}}\boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}\boldsymbol{f}$ or $\boldsymbol{f}^{\mathrm{T}}\boldsymbol{P}_{\mathrm{res}}\boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}\boldsymbol{f}>>\boldsymbol{f}^{\mathrm{T}}\boldsymbol{P}_{\mathrm{pc}}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\boldsymbol{f}$.

3 Fault Identification

In this section, we shall first study the problems of identifying off-set and scaling faults respectively, and then present a procedure for the fault identification.

3.1 Identification of off-set faults

Given

$$\boldsymbol{x}=\boldsymbol{x}_{\mathrm{o}}+\boldsymbol{f}\in\mathbf{R}^m,\ \boldsymbol{x}_{\mathrm{o}}\sim\boldsymbol{N}(\boldsymbol{0},\boldsymbol{\Sigma})$$

with known $\boldsymbol{\Sigma}$ and unknown constant vector $\boldsymbol{f}$, it is well known that

$$\bar{x}=\frac{1}{M}\sum_{i=1}^{M}x_i$$

delivers a GLR (generalized likelihood ratio) estimate for $\boldsymbol{f}$ [9], where $x_i, i=1,\ldots,M$, are the M samples of $\boldsymbol{x}$. It is interesting to note that for $M=1$ the test statistic adopted by the GLR is the X^2-distribution analog to the one used in the PCA approaches.

Suppose that using the standard PCA method a fault is detected with sample x_k. We propose to use the following algorithm for identifying the detected fault $\boldsymbol{f}$:

- Collecting further M samples and scaling the samples by
$$x_k=\tilde{x}_k-\bar{x}, x_{k+1}=\tilde{x}_{k+1}-\bar{x},\ldots,x_{k+M}=\tilde{x}_{k+M}-\bar{x} \tag{18}$$
where $\tilde{x}_k,\ldots,\tilde{x}_{k+M}$ denote the (original) measurements and $\bar{x}$ the mean value achieved using the training data, as described in Subsection II-A.
- Computing the estimate of $\boldsymbol{f}$, denoted by $\hat{f}$
$$\hat{f}=\frac{1}{M+1}\sum_{i=k}^{k+M}x_i \tag{19}$$

It is worth mentioning that the above algorithm can also be realized in a recursive manner.

3.2 Identification of scaling faults

Consider

$$\boldsymbol{x}=\boldsymbol{F}\boldsymbol{x}_{\mathrm{o}},\ \boldsymbol{F}\neq\boldsymbol{I}\Rightarrow\text{scaling fault}$$

and suppose that a fault has been detected using a standard PCA method. Let $x_k,\ldots,x_{k+M}$ be $M+1$ scaled samples collected after the fault has been detected. We then have

$$\frac{1}{M}[x_k \quad \cdots \quad x_{k+M}]\begin{bmatrix} x_k \\ \vdots \\ x_{k+M} \end{bmatrix} \approx \boldsymbol{F\Sigma F}^{\mathrm{T}} = \boldsymbol{FP\Lambda P}^{\mathrm{T}}\boldsymbol{F}^{\mathrm{T}}.$$

An SVD of

$$\frac{1}{M}[x_k \quad \cdots \quad x_{k+M}]\begin{bmatrix} x_k \\ \vdots \\ x_{k+M} \end{bmatrix} = \boldsymbol{V\Pi V}^{\mathrm{T}},$$

$$\boldsymbol{\Pi} = \mathrm{diag}(\bar{\sigma}_1^2,\ldots,\bar{\sigma}_m^2), \boldsymbol{VV}^{\mathrm{T}} = \boldsymbol{I},$$

leads to

$$\boldsymbol{V\Pi}^{1/2} = \boldsymbol{FP\Lambda}^{1/2}.$$

On the assumption that $\boldsymbol{\Lambda}_{\mathrm{res}} \approx \mathbf{0}$, the pseudo inverse of $\boldsymbol{P\Lambda}^{1/2}$ is given by

$$(\boldsymbol{P\Lambda}^{1/2})^{+} \approx \begin{bmatrix} \boldsymbol{\Lambda}_{\mathrm{pc}}^{-1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\begin{bmatrix} \boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}} \\ \boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}} \end{bmatrix}.$$

Therefore,

$$\hat{\boldsymbol{F}} = \boldsymbol{V}_1\boldsymbol{\Pi}_{\mathrm{pc}}^{1/2}\boldsymbol{\Lambda}_{\mathrm{pc}}^{-1/2}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}} \tag{20}$$

with

$$\boldsymbol{\Pi}_{\mathrm{pc}}^{1/2} = \mathrm{diag}(\bar{\sigma}_1,\ldots,\bar{\sigma}_l),\ \boldsymbol{V} = [\boldsymbol{V}_1 \quad \boldsymbol{V}_2],\ \boldsymbol{V}_1 \in \mathbf{R}^{m\times l}$$

delivering a reasonable estimate for $\boldsymbol{F}$.

3.3 A fault identification procedure

In this subsection, we summarize the major results achieved in the previous subsections into the following algorithm aiming at identifying the faults. We assume that a fault has been detected using T^2, T_{res}^2 test statistics.

- Collect $M+1$ samples and scale the samples according to Eq. (18),
- Estimate the off-set fault using Eq. (19) and denote it by $\hat{f}$,
- Re-scale the samples by
  $\bar{x}_k = x_k - \hat{f},\ \bar{x}_{k+1} = x_{k+1} - \hat{f},\ldots,\bar{x}_{k+M} = x_{k+M} - \hat{f},$
- Form
  $$\frac{1}{M}[\bar{x}_k \quad \cdots \quad \bar{x}_{k+M}]\begin{bmatrix} \bar{x}_k \\ \vdots \\ \bar{x}_{k+M} \end{bmatrix},$$
- and compute the following SVD,
  $$\frac{1}{M}[\bar{x}_k \quad \cdots \quad \bar{x}_{k+M}]\begin{bmatrix} \bar{x}_k \\ \vdots \\ \bar{x}_{k+M} \end{bmatrix} = \boldsymbol{V\Pi V}^{\mathrm{T}},$$
- Compute $\hat{\boldsymbol{F}}$ using Eq. (20).

4 Conclusions

In this paper, we have briefly studied the application of the standard PCA technique to fault detection and identification. In the standard PCA technique, $\boldsymbol{z}_{\mathrm{pc}} = \boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\boldsymbol{x}$ and $\boldsymbol{z}_{\mathrm{res}} = \boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}\boldsymbol{x}$ instead of $\hat{\boldsymbol{x}} = \boldsymbol{P}_{\mathrm{pc}}\boldsymbol{P}_{\mathrm{pc}}^{\mathrm{T}}\boldsymbol{x}$ and $\tilde{\boldsymbol{x}} = \boldsymbol{P}_{\mathrm{res}}\boldsymbol{P}_{\mathrm{res}}^{\mathrm{T}}\boldsymbol{x}$ are essential for building the test statistic used in the standard PCA. Based on this fact, we have proposed a new test statistic, which is similar to the Hawkin's T_H^2 statistic but without the numerical drawback. In comparison with the SPE statistic, the threshold setting associated with the new statistic proposed in this paper is computationally (remarkably) simpler and statistically without approximation.

In our study on the fault sensitivity, it has been demonstrated that the test statistic associated with $\boldsymbol{z}_{\mathrm{res}}$ can be more sensitive to the off-set faults. In comparison, the test statistic associated with $\boldsymbol{z}_{\mathrm{pc}}$ and $\boldsymbol{z}_{\mathrm{res}}$ may be similarly sensitive to the scaling faults. We have further revealed the advantages and disadvantages of using a combined statistic, and proposed a modified one.

The final study has been dedicated to identifying off-set and scaling faults. To this end, two algorithms have been proposed.

It is worth mentioning that the new statistic proposed in this paper and the modifications on the standard PCA have been successfully tested using the data collected from real industrial processes.

In conclusion, we would like to make a critical remark on the application of the PCA technique to the fault diagnosis. It is well-known that the basic idea behind the PCA is to reduce the dimension of a data set, while retaining as much as possible the variation present in the data set[1]. Viewing the standard PCA-based fault diagnosis methods, we can only identify the consistence between the PCA-based fault diagnosis methods and the original idea of the PCA technique in detecting and identifying the scaling faults under certain conditions, as shown by the discussion in Subsections 2.2 and 3.2. In general, the facts are:

- In the PCA-based fault diagnosis methods both projections onto the principal component subspace and residual subspace, $\boldsymbol{z}_{\mathrm{pc}}$ and $\boldsymbol{z}_{\mathrm{res}}$, are used for diagnosis purposes. From the computational viewpoint, no reduction in the computation amount is realised.
- In dealing with fault detection in practice, the

projection onto the residual subspace is often preferred, which is reasonable as demonstrated in Subsection 2.1 and considering that off-set faults are the most typical faults in practice. In fact, from the viewpoint of fault diagnosis, an earlier and more reliable fault detection can be achieved if the uncertainty, which is expressed in terms of the covariance in a random process, is less dominant. This is exactly the case for $\boldsymbol{z}_{\mathrm{res}}$ in comparison with $\boldsymbol{z}_{\mathrm{pc}}$. However, the application of the PCA technique to data compression, for example, is based on the use of the projection onto the principal component subspace, which contains the most information saved in the original data set.

These observations motivate us to review the PCA-based fault diagnosis methods. Based on our study in this paper, we understand that the core of the PCA-based fault diagnosis methods consists of a numerically reliable implementation of the X^2 statistic (F statistic when the sample number is not large enough) for fault detection, which is mainly achieved based on the SVD.

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