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Evaluation of PCA methods with improved fault isolation capabilities on a paper machine simulator

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ABSTRACT

The work presented in this paper addresses the issues of fault detection and isolation properties of the partial PCA method and the isolation-enhanced PCA method. In order to increase the sensitivity of the residuals with respect to various faults, the structured residuals generated from both partial PCA and isolation-enhanced PCA are optimized. For the residual evaluation, the bootstrap technique is combined with the CUSUM method to achieve fast and robust detection. Three sensor faults and three actuator faults were studied using simulations employing a rigorous, first principles based, paper machine simulator. All the faults were correctly detected and isolated with both studied methods, and the results are compared with the classical T^2 and SPE contribution plot methods.

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Keywords:

PCA, Fault detection, Fault isolation, Paper machine simulator

1. Introduction

The handling of abnormal situations, such as equipment failures and process disturbances, has received increasing attention from industry and academia alike. The potential benefits, even those resulting from modest improvements in abnormal situation handling, are enormous. An important group of equipment failures in process industries are obviously the faults in actuators and sensors, and this paper focuses on faults of this type. The paper industry is an industrial sector with a high level of automation and, considering that a modern paper mill has hundreds of sensors and actuators connected to its automation systems, it is evident that some systematic methods are needed to process the data.

On-line process monitoring with fault detection can provide stability and efficiency for a wide range of processes. Early detection and isolation of abnormal and undesired process states and equipment failures are essential requirements for safe and reliable processes. Process analysis based on statistical methods promotes understanding of the process phenomena, and ultimately improves plant performance. In recent years there has been increasing interest among researchers in applying different process monitoring and fault diagnosis methods. A large number of applications have been reviewed, e.g. by Isermann and Ballé [1] and Patton et al. [2]. Venkatasubramanian et al. [3–5] published an article series reviewing monitoring methods, especially those applied in the field of chemical process industries. They classified the methods according to the form of process knowledge used. One category is based on process models, and includes both qualitative causal models and quantitative

methods. The other category is based on process history, and includes both qualitative (e.g. rule-based) and quantitative methods (neural networks and multivariate statistical methods).

Common features of the statistical methods used are their ability to reduce correlations between variables and reduce the dimensionality of the data. These characteristics enable efficient extraction of the relevant information and analysis of the data. The most important statistical monitoring methods are based on principal component analysis (PCA) and partial least squares regression (PLS). Dynamic variants of PCA and PLS consider the dynamic nature of the monitored process and analyze both cross-correlation and auto-correlation of the variables [6–8]. Recursive methods for PCA and PLS have been proposed in [9,10]. The recursive methods are especially suitable for time-dependent processes with slow changes. Multi-scale principal component analysis (MSPCA), a combination of PCA and wavelet analysis, removes the autocorrelations of variables by means of wavelet analysis, and eliminates cross-correlations between variables with PCA [11]. The method is suitable for processes with auto-correlated measurements and time-varying characteristics. Nonlinear principal component analysis (NLPCA) is a combination of neural networks and PCA. Dong and McAvoy [12] proposed an NLPCA method, which integrates a principal curve algorithm and neural networks.

Principal component analysis and its variations, as presented above have some inherent problems related to their fault isolation capabilities. The normally used T^2 and SPE indices do not offer any probable location for the detected faults. So-called contribution plots can give some assistance when locating the faults, but these plots do not however always provide reliable and unambiguous results especially with control loops. Improved fault isolation can be achieved with the recently introduced partial PCA method [13], and the related isolation-enhanced PCA method [14].

The aim of this paper is to assess the fault isolation capabilities of the partial PCA method and the isolation-enhanced PCA method on the basis of a paper machine case study in which six different faults are introduced into the system. The paper is organized as follows. In the next section the system description, as well as the partial PCA method and the associated residual limits, are introduced. The isolation-enhanced PCA method is also introduced. In Section 3 the case study is presented. The studied process is first described, followed by a description of the studied faults. The fault diagnosis results obtained using Partial PCA and isolation-enhanced PCA are given in Section 4. These results are also compared with those given by standard PCA with contribution plots. The conclusions are drawn and summarized in Section 5.

2. Partial PCA and isolation-enhanced PCA

Partial PCA was first introduced by Gertler and McAvoy [16], and was further described and extended to nonlinear cases by Huang et al. [13]. The related isolation-enhanced PCA method [14] relies on algebraic transformations of the residuals represented by the last principal components, assuming that the eigenvalues have been sorted decreasingly and that the eigenvectors have been sorted accordingly. However, the basic idea behind these two methods is the same as utilizing the similarity between the PCA residual model and the explicit system model, used to generate the structured residuals by the parity space method. As a further improvement, a method for designing optimal structured residuals for the partial PCA method was proposed by Gertler and Cao [19].

2.1. Standard PCA

Assume that the system being studied is described by m linear static relationship equations with n observed variables $\mathbf{x}^0(t) = [x_1^0(t) \dots x_n^0(t)]^T$ and k unobserved disturbances $\mathbf{d}(t) = [d_1(t) \dots d_k(t)]^T$

$$\mathbf{B}\mathbf{x}^0(t) + \mathbf{D}\mathbf{d}(t) = 0 \quad (1)$$

where the observation $\mathbf{x}^0(t)$ is fault free but with noise, and $\mathbf{B}$ and $\mathbf{D}$ are $m \times n$ and $m \times k$ matrices, respectively. With the assumption that the number of disturbances is smaller than the number of linear equations ($k < m$), the disturbances can be eliminated from the above equations and thus only $m-k$ relationship equations exist among n variables $\mathbf{x}^0(t)$, as shown below.

$$\mathbf{B}^* \mathbf{x}^0(t) = 0 \quad (2)$$

where $\mathbf{B}^*$ is the $(m-k) \times n$ matrix.

Following implementation of the standard PCA algorithm to the N observations (assuming that the training data are well activated and that all disturbances are active) of $\mathbf{x}^0(t)$, the principal component model can be obtained with first $n-m+k$ principal components. The reason for this is that the $m-k$ linear relationship equations among the data make the last $m-k$ eigenvalues relatively smaller than the first $n-m+k$ eigenvalues [19]. Also note that k more principal components have to be selected in the PCA model due to the existence of k disturbances in the training data set.

Using the obtained PCA model, the new observation of $\mathbf{x}^0(t)$ can be projected into the representation space (spanned by the first $n-m+k$ principal components) and its orthogonal complement space, the residual space (spanned by the last $m-k$ principal components) as shown below.

$$\mathbf{p}^0(t) = \mathbf{Q}'_M \mathbf{x}^0(t) \quad (3)$$

$$\mathbf{e}^0(t) = \mathbf{Q}'_R \mathbf{x}^0(t) = 0 \quad (4)$$

with $\mathbf{Q}'_M = [\mathbf{q}_1 \dots \mathbf{q}_{n-m+k}]$ and $\mathbf{Q}'_R = [\mathbf{q}_{n-m+k+1} \dots \mathbf{q}_n]$, where $\mathbf{q}_i$ is the eigenvector of the covariance matrix of the training data set. $\mathbf{p}^0(t)$ and $\mathbf{e}^0(t)$ are the projections of the observation $\mathbf{x}^0(t)$ in the representation

space and the residual space, respectively, which are called scores and primary residuals in the PCA framework.

Similarity can be found between Eqs. (2) and (4). It has been reported that, even though the matrix $\mathbf{B}^*$ and $\mathbf{Q}'_R$ are not exactly the same, they span the same residual subspace which is orthogonal to the fault-free data [14]. Based on this similarity, the parity space fault isolation method is applied to the primary residuals in Eq. (4), to generate the structured residuals. Two methods were proposed by Gertler et al. [14,16] for obtaining the structured residuals: partial PCA and isolation-enhanced PCA.

2.2. Partial PCA

The main idea in partial PCA is that a set of PCA models are constructed using only subsets of the original variables in the training data set, which make the residuals of each partial PCA model insensitive to specific fault(s), and sensitive to the others.

The system described by Eq. (2) is again considered here. If h variables ($h \leq m-k-1$) in $\mathbf{x}^0(t)$ are eliminated from Eq. (2), the only $m-k-h$ relationship equations exist among $n-h$ variables. Thus the PCA representation space constructed from the reduced training data with $n-h$ variables is $n-m+k$ dimensional, while the dimension of the residual space is only $m-k-h$.

Furthermore, if the additive faults $\Delta\mathbf{x}_{n-h}(t)$ are considered for the $n-h$ variables as:

$$\mathbf{x}_{n-h}(t) = \mathbf{x}_{n-h}^0(t) + \Delta\mathbf{x}_{n-h}(t) \quad (5)$$

where $\mathbf{x}_{n-h}^0(t)$ is the fault-free observation, then Eq. (4) can be modified for this PCA model, as shown below

$$\begin{aligned} \mathbf{e}(t) &= \mathbf{Q}'_{R,n-h} \mathbf{x}_{n-h}(t) = \mathbf{Q}'_{R,n-h} \mathbf{x}_{n-h}^0(t) + \mathbf{Q}'_{R,n-h} \Delta\mathbf{x}_{n-h}(t) = \\ &\mathbf{e}^0(t) + \mathbf{Q}'_{R,n-h} \Delta\mathbf{x}_{n-h}(t) = \mathbf{Q}'_{R,n-h} \Delta\mathbf{x}_{n-h}(t) \end{aligned} \quad (6)$$

where $\mathbf{Q}'_{R,n-h} = [\mathbf{q}_{n-m+k+1} \dots \mathbf{q}_{n-h}]^T$, is the residual loading matrix of this PCA model. The above equation implies that the primary residuals of the partial PCA model are only sensitive to these faults in the $n-h$ variables. Based on this property, the structured residuals can be obtained from the set of partial PCA models, the variables of which are differently selected according to the designed incidence matrix.

In an incidence matrix, the rows represent residuals while the columns represent corresponding faults. The number '1' in the matrix means the residual is sensitive to the corresponding fault, while the number '0' refers to the insensitivity of the residual to the fault [19]. In most cases, the incidence matrix is designed to be strongly isolating, which means that a misdetection of any residual does not result in a false isolation of the faults. Strong isolation ability can be guaranteed by the column canonical structure, which requires that each column has the same number of zeros and all the columns have a different pattern. An example of a strongly isolating incidence matrix is given in Table 1.

In addition to the constraints arising from the requirement of strong isolation, the design of the incidence matrices is also subjected to the constraints of the matrix $\mathbf{Q}'_R$. Firstly, for each row of the incidence matrix, the following condition

$$\text{Rank}(\mathbf{Q}'_R)^i \leq m-k-1 \quad (7)$$

should be satisfied [14], where $(\mathbf{Q}'_R)^i$ contains the columns of $\mathbf{Q}'_R$ that correspond to the incidence matrix columns that have the number '0'

Table 1
A strongly isolating incidence matrix

	f_{x1}	f_{x2}	f_{x3}	f_{x4}
r_1	1	1	1	0
r_2	1	1	0	1
r_3	1	0	1	1
r_4	0	1	1	1

in the i th row. This condition implies that the maximal number of zeros in each row of incidence matrix is $m-k-1$, due to the known fact that maximal $m-k-1$ variables can be eliminated out of $m-k$ linear relationship equations, that is $h \leq m-k-1$. Moreover, the condition also means that the primary residuals of each partial PCA model can only be decoupled from a maximal $m-k-1$ faults. Secondly, for each row of the incidence matrix, the following condition

$$\text{Rank} \left[\left(\mathbf{Q}'_R \right)^i, \mathbf{q}_j \right] = \text{Rank} \left[\left(\mathbf{Q}'_R \right)^i \right] + 1 \quad (8)$$

has to be satisfied [14], where $\mathbf{q}_j$ is any column of $(\mathbf{Q}'_R)_i$ and $(\mathbf{Q}'_R)_i$ contains the columns of $\mathbf{Q}'_R$ that correspond to the incidence matrix columns that have the number '1' in the i th row. This condition guarantees that the residuals of the partial PCA model, constructed according to the i th row of the incidence matrix, are sensitive to the faults as designed. Only if the above two conditions are satisfied is the designed incidence matrix considered as attainable. Finally, if any two columns of the matrix $\mathbf{Q}'_R$ are linearly dependent on each other, then no incidence matrix can isolate the faults corresponding to these two columns. In this case the incidence matrix is considered as non-isolatable.

According to the rows of the proper incidence matrix, subsets of variables can be selected and used to train a set of partial PCA models. The primary residuals for each partial PCA model, which are used as structured residuals, can be calculated according to Eq. (6). In the case $h < m-k-1$, i.e. the eliminated variables from the partial PCA model are less than $m-k-1$, more than one primary residual ($m-k-h$) are generated by Eq. (6), which respond to the same subset of faults as designed in the incidence matrix. Thus the final residuals from each partial PCA are generated by linearly combining the $m-k-h$ number of primary residuals in Section 2.4, in order to optimize the residuals' sensitivities to various faults.

2.3. Isolation-enhanced PCA

In isolation-enhanced PCA, the fault filter matrices are designed according to each row of the incidence matrix. The primary residuals of the full PCA model in Eq. (4) are filtered by the designed matrices to form the structured residuals.

If the additive faults $\Delta \mathbf{x}(t)$ are considered for the n variables as:

$$\mathbf{x}(t) = \mathbf{x}^0(t) + \Delta \mathbf{x}(t) \quad (9)$$

then the primary residuals of the full PCA model in Eq. (4) are modified to

$$\mathbf{e}(t) = \mathbf{Q}'_R \mathbf{x}(t) = \mathbf{e}^0(t) + \mathbf{Q}'_R \Delta \mathbf{x}(t) = \mathbf{Q}'_R \Delta \mathbf{x}(t). \quad (10)$$

It can be seen from the above equation that the primary residuals $\mathbf{e}(t)$ are sensitive to all the possible faults related to the n variables. In order to form the structured residuals, the fault filter matrix $\mathbf{V}_i$ is designed according to the i th row of the incidence matrix such that the i th filtered residuals

$$\varepsilon_i(t) = \mathbf{V}_i \mathbf{e}(t) = \mathbf{V}_i \mathbf{Q}'_R \Delta \mathbf{x}(t) \quad (11)$$

only respond to a subset of faults. In order to decouple the residuals $\varepsilon_i(t)$ from corresponding faults, the matrix $\mathbf{V}_i$ needs to be

$$\mathbf{V}_i \left(\mathbf{Q}'_R \right)^i = 0 \quad (12)$$

Eq. (7) should be satisfied in order to guarantee the existence of the solution of Eq. (12) for matrix $\mathbf{V}_i$ [14]. In addition, for the faults which are sensitive to the residuals $\varepsilon_i(t)$,

$$\mathbf{V}_i \left(\mathbf{Q}'_R \right)_i \neq 0 \quad (13)$$

is required. To guarantee the above equation, Eq. (8) should be satisfied [14]. Moreover, in order to isolate all the designed faults, no two columns of $\mathbf{Q}'_R$ should be linearly dependent. Thus it can be stated that the design of the incidence matrix in isolation-enhanced PCA is the same as that of the partial PCA method.

Note that Eq. (12) can be solved for $\mathbf{V}_i$ by finding an orthonormal basis for the null space of $(\mathbf{Q}'_R)^i$. In the Matlab environment, this can be performed with the null command. The dimension of the matrix $\mathbf{V}_i$ is then $(m-k-h) \times (n-m-k)$, where $h = \text{Rank}(\mathbf{Q}'_R)^i$ is the number of zeros in the i th row of the incidence matrix. As with the partial PCA method, in the case of $h < m-k-1$ more than one structured residuals $\varepsilon_i(t)$ ($m-k-h$) are generated by Eq. (11), which respond to the same subset of faults as in the design. The final residuals are optimized in Section 2.4 with respect to the residuals' sensitivities to various faults.

2.4. Fault sensitivity optimization

Apart from the fact that the sensitivity of the structured residuals generated both in the partial PCA method and the isolation-enhanced PCA method might be too small compared with the noise to be detected, there is a possibility to increase the fault sensitivity of the structured residuals. The improvement is offered by the linear combination of the multiple structured residuals, which respond to the same subset of faults in the case $h < m-k-1$.

Gertler and Cao [19] proposed the ratio of the fault-gain to noise standard deviation as the measure of the fault sensitivity of the structured residuals. Furthermore, the worst fault sensitivity for a specific structured residual was maximized in their work only for the partial PCA method.

However, the maximization of the worst sensitivity of a structured residual will lead to compromising its sensitivities to various faults. Thus its sensitivity to each fault cannot reach the maximal. In order to avoid this problem, the sensitivity of the structured residual for each fault is maximized individually.

In the partial PCA method, the optimal residual of the i th partial PCA model with respect to the j th fault $\Delta x_j(t)$ among all the considered faults $\Delta \mathbf{x}_{n-h}(t)$, is calculated by linearly combining the $m-k-h$ structured (primary) residuals from that partial PCA model as

$$r_i^j(t) = \mathbf{s}_i^j \cdot \mathbf{e}_i(t) \quad (14)$$

where $\mathbf{s}_i^j$ is a unitary row vector that needs to be designed, and $\mathbf{e}_i(t)$ are the primary residuals of the i th partial PCA model calculated by Eq. (6).

The ratio of the fault-gain to noise standard deviation is used as the measure of the sensitivity of the residual to faults. Firstly, the gain of the residual r_i^j to the j th fault is given as

$$g_i^j = |\mathbf{s}_i^j \cdot \mathbf{q}_{n-h,j}| \quad (15)$$

where $\mathbf{q}_{n-h,j}$ is the corresponding column of $\mathbf{Q}'_{R,n-h}$ of the i th partial PCA model. Secondly, the standard deviation of the noisy residual r_i^j is calculated by

$$\sigma_i^j = \sqrt{\frac{(\mathbf{s}_i^j)^2 \cdot [\lambda_{n-m+k+1} \cdots \lambda_{n-h}]}{N}} \quad (16)$$

where λ_i are the last $m-k-h$ eigenvalues of the i th partial PCA model, and N is the number of observations in the training data [19]. Finally, the sensitivity measurement of the residual r_i^j to the j th fault is given as

$$k_i^j = g_i^j / \sigma_i^j. \quad (17)$$

The row vector $\mathbf{s}_i^j$ is designed by solving the following optimization problem

$$\mathbf{s}_i^j = \arg \max_{\mathbf{s}_i^j} (k_i^j) \text{ Subject to } \|\mathbf{s}_i^j\| = 1. \quad (18)$$

Thus $n-h$ optimal structured residuals r_i^j (define r_i as the set of all r_i^j) are generated for the i th partial PCA model. As a result, the incidence matrix needs to be modified accordingly due to the fact that each row in the original incidence matrix expands to $n-h$ rows. The modification of the incidence matrix in Table 2 is given below as an example.

From the above modified incidence matrix, it can be seen that the fault signature of each fault is constructed from different residuals. For example, the fault signature of f_{x1} is formed from the residuals $r_1^1, r_2^1, r_3^1, r_4^1, r_5^1$ and r_6^1 . The first three residuals are optimized for the fault f_{x1} , and the last three are decoupled from this fault.

A similar optimization procedure can be applied to the isolation-enhanced PCA method with minor modifications.

In the isolation-enhanced PCA method, the optimal residual r_i^j with respect to the j th fault $\Delta x_j(t)$ among all the considered faults $\Delta \mathbf{x}(t)$ is calculated by

$$r_i^j(t) = \mathbf{s}_i^j \mathbf{e}_i(t) = \mathbf{s}_i^j \mathbf{V}_i \mathbf{e}(t). \quad (19)$$

In order to design the unitary row vector $\mathbf{s}_i^j$, the fault gain of the residual r_i^j to the j th fault is calculated as

$$g_i^j = |\mathbf{s}_i^j \mathbf{V}_i \mathbf{q}_j| \quad (20)$$

where $\mathbf{q}_j$ is the corresponding column of $\mathbf{Q}_k$. The standard deviation of the residual r_i^j is given as:

$$\sigma_i^j = \sqrt{\frac{(\mathbf{s}_i^j \mathbf{V}_i)^2 \cdot [\lambda_{n-m+k+1} \cdots \lambda_n]}{N}} \quad (21)$$

where λ_i are the last $m-k$ eigenvalues of the full PCA model. Thus the row vector $\mathbf{s}_i^j$ is designed by solving the optimization problem

$$\mathbf{s}_i^j = \arg \max_{\mathbf{s}_i^j} (k_i^j) \text{ Subject to } \|\mathbf{s}_i^j\| = 1 \quad (22)$$

where $k_i^j = g_i^j / \sigma_i^j$. Similarly, the incidence matrix is modified as shown in Table 2.

2.5. Residual evaluation

In order to form the fault signature, the optimal residuals need to be evaluated by a fault detection algorithm. The bootstrap technique

and the double sided CUSUM method of Hinckley [15], which can detect both positive and negative jumps in the mean of a noisy residual, are combined to fulfil this task.

The basic concept of the bootstrap technique is to sample the available data with replacement, and then estimate the interesting statistics. In this paper, the statistic 99th percentile of each fault-free residual is estimated off-line by the bootstrap technique. The estimated values are used as the parameter of minimal detectable change for the CUSUM method.

The CUSUM method is able to provide more robust detection in a noisy environment in comparison to the simple threshold method, even though there is some degree of detection lag. For a positive mean jump of the residual r , the following applies.

$$\begin{aligned} \sum(t) &= \sum(t-1) + r(t) - \mu_0 - \beta/2 \\ \sum_{\min}(t) &= \min(\sum_{\min}(t-1), \sum(t)) \end{aligned} \quad (23)$$

where β is the minimum detectable change obtained from the bootstrap technique, and μ_0 is the expected mean of the fault-free residual, which is usually considered to be zero. Whenever $\sum(t) - \sum_{\min}(t) > \lambda$, the residual is declared as faulty. The parameter λ is tuned such that the satisfactory false alarm rate and miss alarm rate are achieved. A more general procedure can be developed on the basis of the simple positive jump case for detecting two-directional changes and the residual recovery back to the normal situation.

2.6. General design procedure

The general design procedure for both the partial PCA method and the isolation-enhanced PCA method is presented in the following:

1. Preprocess the training data (mean centred and scaled by standard deviation) and perform the full PCA. Determine the number $m-k$ and matrix $\mathbf{Q}_k$
2. Design a proper incidence matrix on the basis of the number $m-k$ and the matrix $\mathbf{Q}_k$
- 3(a). For the partial PCA method, construct a set of partial PCA models on the basis of the incidence matrix. Design the row vector $\mathbf{s}_i^j$ optimizing the fault sensitivity of the residuals r_i from the set of partial PCA models. Modify the incidence matrix on the basis of the optimal residuals.
- 3(b). For the isolation-enhanced PCA method, design the fault filter matrix $\mathbf{V}_i$ on the basis of the incidence matrix. Design the row vector $\mathbf{s}_i^j$ optimizing the fault sensitivity of the residuals r_i and modify the incidence matrix accordingly.
4. Generate the fault-free residuals with the training data set for both the partial PCA method and the isolation-enhanced PCA method; apply the bootstrap technique to the fault-free residuals in order to obtain the parameter of the minimal detectable change for the CUSUM method.

In this work, both partial PCA and isolation-enhanced PCA are applied and evaluated on a dynamic, first principles paper machine simulator.

3. Case study

This paper describes a case study on fault detection and isolation carried out on a paper machine simulator. In the remainder of this section, the paper machine process and the simulation environment used are described together with an explanation of the experiment.

3.1. Process description

The paper machine can be divided into 3 main parts: the wire section, the press section and the dryer section. Diluted stock with a consistency of approximately 1% is sprayed from the hydraulic head-box onto the wire at a constant speed. The stock is dehydrated on the wire to form a wet web. About 98% of the water and 54% of the filler

Table 2

A modified incidence matrix from Table 1

	f_{x1}	f_{x2}	f_{x3}	f_{x4}
r_1^1	1	–	–	0
r_2^1	–	1	–	0
r_3^1	–	–	1	0
r_1^2	1	–	0	–
r_2^2	–	1	0	–
r_3^2	–	–	0	1
r_1^3	1	0	–	–
r_2^3	–	0	1	–
r_3^3	–	0	–	1
r_1^4	0	1	–	–
r_2^4	0	–	1	–
r_3^4	0	–	–	1

‘–’ denotes the residual is not considered for this fault.

and fibre pass through the wire and flow into the wire pit as white water.

In the press section, additional water is removed by mechanically pressing the paper between the press cylinders, leaving the exiting paper with a dry content of approximately 50%. In the dryer section, steam heated cylinders evaporate off most of the water remaining in the paper after the press section. The dryer section is divided into several dryer groups, each comprising several drying cylinders. Fresh, high-pressure steam is first fed to the last drying group, after which it is reused in the preceding groups at lower pressures.

The paper on the reel typically has a moisture content of approximately 8%. In the approach system before the paper machine, mechanical pulp, chemical pulp and broke are pumped into a blending chest and mixed according to a given recipe. The stock is then pumped from the blending chest to the machine chest. The consistency of the stock between the blending chest and the machine chest is controlled to a setpoint of approximately 3%.

Closely interconnected to the paper machine is the short circulation, which starts after the machine chest. The thick stock is pumped to the wire pit and mixed with white water and filler. The diluted stock is pumped by a fan pump via the hydro-cyclones to the deculator, where impurities and air are removed. After that the fibre suspension of correct consistency is pumped into the headbox and sprayed onto the wire, from where most of the water drains off. The collected white water is used for the later thick stock dilution, which forms the material circulation called the short circulation. By acting as the intermediate process between stock preparation and the former, the short circulation process is very important for paper quality control. Firstly, control of the basis weight and filler rate of the final paper is implemented here. Secondly, control of the formation and fibre orientation of the paper is

also located in the short circulation. Finally, the material circulation in the short circulation improves the total retention of the fibres and fillers, i.e. the transportability of the raw material to the final product.

3.2. Simulation environment

For the case study in this paper, the Advanced Process Simulator (APROS) was used to construct the paper machine model. A general description of the APROS simulator is given on the APROS website [17]. The APROS simulator provides first principle models for the necessary components used in constructing and parameterizing the model for the paper machine. An automation system with 12 control loops was also constructed. The quality variables, basis weight, ash rate and moisture of the paper are controlled in cascade control loops. In the headbox, the stock jet ratio is controlled in the cascade loop by manipulating the setpoint of the inner pressure control loop. In the stock preparation section, the stock consistency in the machine chest is controlled by manipulating the dilution water valve. In the dryer section, the setpoints of the pressures in the steam system are obtained from the moisture control loop. Fig. 1 shows the model used for this case study.

A static test for linearity has earlier been performed on the process simulator in order to motivate the use of linear methods [18]. The test showed that the process behaves almost linearly over the studied range.

3.3. Experiment description

The experiment has two steps: the design phase and the monitoring phase. In the design phase, the training data set containing 9781 observations (sampling time 10 s) and the 18 variables listed in

Fig. 1. Part of the APROS model of the paper machine [17].

Table 3

The variables observed in the case study

Variable no.	Description
1	Machine chest consistency (M: measurement)
2	Basis weight valve control signal (A: actuator)
3	Filler valve control signal (A)
4	Headbox pump control signal (A)
5	4th dryer upper valve control signal (A)
6	4th dryer lower valve control signal (A)
7	5th dryer upper valve control signal (A)
8	5th dryer lower valve control signal (A)
9	4th dryer input pressure (M)
10	4th dryer output pressure (M)
11	5th dryer input pressure (M)
12	5th dryer output pressure (M)
13	Paper moisture (M)
14	Paper basis weight (M)
15	Paper filler rate (M)
16	Headbox pressure (M)
17	Headbox jet ratio (M)
18	Mass flow out of machine chest (M)

Table 3 was first collected from the APROS simulator with all the control loops closed. In addition, the process was perturbed during data generation by changing the basis weight, filler rate, moisture, headbox jet ratio and the machine chest stock consistency; setpoints in the ranges 50 to 55 g/m², 18 to 22% filler, 7 to 10 wt.% H₂O, 1.00 to 1.03 and 3.43 to 3.7%, respectively. The reason for using the close loop data for training is that the control constraints can be removed from the generation of the structured residuals by operating the feedback loops at different setpoints (at least two) [14] [20]. Six variables (the 2nd, 3rd, 7th, 13th, 14th and 16th variables in Table 3) outside the training data set are illustrated in Fig. 2.

Fig. 2. PCA training data.**Table 4**

The studied faults

Fault no.	Fault	Type	Size/slope
1	Basis weight actuator fault	Abrupt	Size: 0.03
2	Filler actuator fault	Abrupt	Size: 0.05
3	5th dryer upper valve actuator fault	Incipient	Size: 0.05 Slope: 0.00125/min
4	Moisture sensor fault	Abrupt	Size: 0.35%
5	Basis weight sensor fault	Incipient	Size: 2.5 g/m ² Slope: 0.06 g/m ² /min
6	Headbox pressure sensor fault	Abrupt	Size: 10 kPa

For the sake of simplicity, the case study was limited to the six possible additive sensor or actuator faults in the variables shown in Fig. 2. With the training data set, both the partial PCA method and the isolation-enhanced PCA method were designed for these six possible faults according to the procedures presented in Section 2.6. The studied faults are summarized in Table 4.

In the monitoring phase of the experiment, the above faults were simulated in the APROS simulator with the control loop closed by adding an extra fault signal to the corresponding control or sensor signal. If any of these faults were to occur in a real paper machine, they would seriously jeopardize the operation of the process and lead to an inferior end product quality.

The six fault scenarios were simulated individually for 9000 s, the corresponding faults being introduced after 3000 s. The faults lasted for 3000 s before they disappeared. All the data were scaled according to the training data before the methods were applied. The produced residuals from both methods were evaluated by the CUSUM method to form the fault signatures. A comparison was made between the two enhanced PCA-based methods and between these methods and the classical T^2 , SPE contribution plot methods in order to evaluate their performance.

In order to test the ability of the partial PCA and isolation-enhanced PCA methods to diagnose previously unknown faults, an abrupt additive fault (size: 5%) in the control signal of the headbox feedpump was simulated in APROS and tested with the two methods.

4. Results

4.1. Results of partial PCA

In the design phase, the full PCA is first applied to the training data set. The eigenvalues of the covariance matrix are listed in Table 5.

Table 5

Eigenvalues of the full PCA

PC no.	Eigenvalues	Variance captured (%)
1	8.40	46.7
2	2.95	63.1
3	2.66	77.8
4	1.84	88.0
5	1.03	93.8
6	0.65	97.4
7	0.13	98.1
8	8.05e-2	98.6
9	6.85e-2	99.0
10	6.52e-2	99.3
11	4.95e-2	99.6
12	3.45e-2	99.8
13	1.68e-2	99.9
14	1.04e-2	99.9
15	2.12e-3	99.9
16	7.74e-4	100
17	2.79e-4	100
18	1.8e-16	100

Nine principal components were selected according to the above table, because the rest of the eigenvalues were relatively smaller than the ones selected. The number $m-k$ is thus determined as 9. Therefore, in the design of the incidence matrix, the maximal zeros we can put in each row is $h=m-k-1=8$. Considering the degree of freedom that we can exploit for the fault sensitivity optimization of the residuals, we try to put as few zeros in each row as possible. One possible incidence matrix is given in Table 6, and proved to be according to the obtained matrix $\mathbf{Q}_R'$. Six partial PCA models with nine principal components were constructed on the basis of the incidence matrix.

The corresponding vectors $\mathbf{s}_i^j$ were designed for each partial PCA models according to Eqs. (14)–(18). In addition, the incidence matrix was modified accordingly as shown below.

In the last step of the design phase, the bootstrap technique was applied to estimate the 99 percentile of the fault-free residuals generated by Eq. (14), which was used as the parameter of the minimal detectable change of the CUSUM method. As an example, the results of the residual r_1^3 are shown in Fig. 3 in the case where 10,000 repetitions were carried out with each sample size as 4000. The first plot shows the noisy residual and its estimated 99 percentile for both positive values and negative values. The histograms of these two statistics show their statistical distribution, as given in the lower two plots.

In the monitoring phase, the collected data set for each fault scenario were evaluated by the set of partial PCA models. The residuals were generated according to Eq. (14) and evaluated by the CUSUM method. The fault signatures were formed with the corresponding detection results, and compared with the incidence matrix in Table 7.

For the sake of brevity, only the results for the third fault (incipient actuator fault) and sixth fault (abrupt sensor fault) are shown in Figs. 4 and 5, respectively. The results for all six scenarios are shown in Table 8.

It can be seen from Fig. 4 that, during the faulty period, the residuals r_1^3 , r_2^3 , r_3^3 , r_4^3 and r_5^3 were detected as faulty, while the residuals r_6^3 , r_7^3 , r_8^3 , r_9^3 were fault free. The corresponding detection results determined by the CUSUM method are shown as dashed lines in the figures. Thus the fault signature for fault 3 was formed as

$$[r_1^3 \ r_2^3 \ r_3^3 \ r_4^3 \ r_5^3 \ r_6^3 \ r_7^3 \ r_8^3 \ r_9^3] = [1100000111]. \quad (24)$$

According to the incidence matrix in Table 7, the obtained fault signature is the same as that of fault 3, and therefore the detected fault was identified as the third fault.

Similarly for the sixth fault scenario, Fig. 5 shows that the residuals r_1^6 , r_2^6 , r_3^6 , r_4^6 and r_5^6 were detected as faulty, while the residuals r_6^6 , r_7^6 , r_8^6 , and r_9^6 were fault free. The fault signature formed for fault 6 was

$$[r_1^6 \ r_2^6 \ r_3^6 \ r_4^6 \ r_5^6 \ r_6^6 \ r_7^6 \ r_8^6 \ r_9^6] = [1111100000] \quad (25)$$

which matches that of fault 6 in the incidence matrix in Table 7.

Table 6
The incidence matrix with six faults and six residuals

	f_1	f_2	f_3	f_4	f_5	f_6
r_1	0	1	1	1	1	1
r_2	1	0	1	1	1	1
r_3	1	1	0	1	1	1
r_4	1	1	1	0	1	1
r_5	1	1	1	1	0	1
r_6	1	1	1	1	1	0

Fig. 3. The 99 percentiles for residual r_1^3 .

For comparison purposes, the results of the classical T^2 and SPE contribution plot methods are shown in Figs. 6 and 7 for fault scenarios 3 and 6, respectively. It can be clearly seen in Fig. 6 that the index SPE is able to detect and isolate the 3rd fault (in the 7th variable), while the index T^2 fails to perform either the fault detection or the fault isolation. In Fig. 7, both SPE and T^2 were able to detect the 6th fault (in the 16th variable); however, neither of them successfully isolated the fault.

Table 7
Modified incidence matrix from Table 6

	f_1	f_2	f_3	f_4	f_5	f_6
r_1^2	0	1	–	–	–	–
r_1^3	0	–	1	–	–	–
r_1^4	0	–	–	1	–	–
r_1^5	0	–	–	–	1	–
r_1^6	0	–	–	–	–	1
r_2^1	1	0	–	–	–	–
r_2^2	–	0	1	–	–	–
r_2^3	–	0	–	1	–	–
r_2^4	–	0	–	–	1	–
r_2^5	–	0	–	–	–	1
r_2^6	–	0	–	–	–	–
r_3^1	1	–	0	–	–	–
r_3^2	–	1	0	–	–	–
r_3^3	–	–	0	1	–	–
r_3^4	–	–	0	–	1	–
r_3^5	–	–	0	–	–	1
r_3^6	–	–	0	–	–	–
r_4^1	1	–	–	0	–	–
r_4^2	–	1	–	0	–	–
r_4^3	–	–	1	0	–	–
r_4^4	–	–	–	0	1	–
r_4^5	–	–	–	0	–	1
r_4^6	1	–	–	–	0	–
r_5^1	–	1	–	–	0	–
r_5^2	–	–	1	–	0	–
r_5^3	–	–	–	1	0	–
r_5^4	–	–	–	–	0	1
r_5^5	–	–	–	–	–	0
r_5^6	1	–	–	–	–	0
r_6^1	–	–	–	1	–	0
r_6^2	–	–	–	–	1	0

Fig. 4. Results for fault scenario 3 with partial PCA.

Note that both the partial PCA method and the isolation-enhanced PCA method are designed for a limited number of faults, and the capacity of these two methods to diagnose previously unknown faults in the monitoring phase is therefore poor. This is illustrated in Fig. 8 by evaluating the additive fault of the 4th variable (headbox pump control signal) with the designed partial PCA models. This fault was not designed for the partial PCA in this case study. The results in Fig. 8 show that the fault cannot be decoupled from any of the residuals r_i implying that, in general, previously unknown faults can be detected, but not explained or isolated.

The results of the classical T^2 and SPE contribution plot methods for the fault on the 4th variable are compared in Fig. 9. It can be seen that both T^2 and SPE were able to detect the fault. However, only T^2 gave the correct fault isolation result.

To sum up, the partial PCA method is better than the classical T^2 and SPE contribution plot method in terms of fault isolation for the designed faults. However, the partial PCA method is not able to explain and isolate a previously unknown fault, even though the fault is detected.

4.2. Results with isolation-enhanced PCA

In the design phase of the isolation-enhanced PCA, the procedures presented in Section 2.6 were performed. The same incidence matrix in Tables 6 and 7 were used for the isolation-enhanced PCA.

In the monitoring phase, the faulty data sets were evaluated by the full PCA model. The residuals were produced according to Eq. (19), and evaluated by the CUSUM method to form fault signatures for the fault isolation. For the sake of brevity, only the results for the third and sixth fault scenarios are shown in Figs. 10 and 11, respectively, and compared with the results obtained using the partial PCA method. The results for all six scenarios are summarized in Table 8.

Fig. 10 shows the results for the third fault scenario with the isolation-enhanced PCA. The result is similar to that obtained with the partial PCA method. Fig. 11 also shows similar results to those in Fig. 5. Thus, in both fault scenarios, isolation-enhanced PCA was able to detect and isolate the fault as desired.

Fig. 5. Results for fault scenario 6 with partial PCA.

In the case of a previously unknown fault, i.e. the fault in the 4th variable, the isolation-enhanced PCA generated similar results as the partial PCA method. This implies that the ability of the isolation-enhanced PCA to diagnose or explain detected new faults is relatively poor.

5. Conclusions

In this paper two variations of the PCA approach for improved fault isolation have been evaluated on a realistic paper machine simulator. A residual optimization method was used for improving the detection ability of both methods. The bootstrap technique was applied to the fault-free residuals in order to obtain the parameter of the minimal detectable change for the residual evaluation method CUSUM.

Comparisons were made between the partial PCA, isolation-enhanced PCA, classical T^2 and SPE contribution plot methods. The results revealed similarity between the partial PCA method and the isolation-enhanced PCA method. In the tests, both methods were able to detect and isolate the faults as designed. Moreover, both of the PCA-based methods provided better fault isolation results than the classical T^2 and SPE contribution plot methods.

The ability of both of the PCA-based methods to diagnose a previously unknown fault was also evaluated. A new fault, which was not designed in either the partial PCA method or the isolation-

Table 8

Comparison of the results obtained with different methods for different fault scenarios

		Partial PCA	Isolation-enhanced PCA	T^2 and contribution plot	SPE and contribution plot
f_1	Detection	Yes	Yes	No	Yes
	Isolation	Yes	Yes	No	Yes
f_2	Detection	Yes	Yes	No	No
	Isolation	Yes	Yes	No	No
f_3	Detection	Yes	Yes	No	Yes
	Isolation	Yes	Yes	No	Yes
f_4	Detection	Yes	Yes	No	No
	Isolation	Yes	Yes	No	No
f_5	Detection	Yes	Yes	No	Yes
	Isolation	Yes	Yes	No	Yes
f_6	Detection	Yes	Yes	Yes	Yes
	Isolation	Yes	Yes	No	No
f_{new}^*	Detection	Yes	Yes	Yes	No
	Isolation	No	No	Yes	No

f_{new}^* denotes the fault in the 4th variable (headbox pump control signal).

Fig. 6. Results of the T^2 and SPE contribution plot for fault scenario 3.

Fig. 7. Results of the T^2 and SPE contribution plots for fault scenario 6.

enhanced PCA method, was analysed. The results showed that neither of these two methods was able to explain the detected fault.

For easy access, the results of the different methods are summarized in Table 8.

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Fig. 8. Results for the fault in the 4th variable with partial PCA.

Fig. 9. Results of the T^2 and SPE contribution plots for the fault in the 4th variable.

Fig. 10. Result obtained for fault scenario 3 with isolation-enhanced PCA.

Fig. 11. Result obtained for fault scenario 6 with isolation-enhanced PCA.