Improved PCA with Optimized Sensor Locations for Process Monitoring and Fault Diagnosis

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Abstract: Process monitoring and fault diagnosis using principal component analysis (PCA) were studied intensively and applied to industry processes. The emphasis of most PCA-based works has been mainly on procedures to perform monitoring and diagnosis given a set of sensors, and little attention is paid to the actual location of sensors for efficient detection and identification of process faults. In this paper, graph-based techniques are used to optimize sensor locations to ensure obtaining the maximum fault resolution. Based on the optimized sensor network, an improved PCA is proposed by introducing two new statistics of *PVR* and *CVR* to take place the *Q* statistic in the conventional PCA. The improved PCA can efficiently detect weak changes, and give an insight into the root cause of process fault. Simulation results of a CSTR process show that the improved PCA with optimized sensor locations is superior to the conventional methods.

Keywords: Principal component analysis, Sensor location, Fault diagnosis

1. Introduction

In chemical process operation and control, principal component analysis (PCA) is one of the most popular statistical methods for extracting information from measured data. Reports related to PCA show a wide application range including multivariate processes monitoring (Kresta et al, 1991), process understanding (Konsanovich et al, 1996), fault diagnosis (Dunia et al, 1998), data rectification (Tong and Crowe, 1995), and so on.

Although process performance monitoring can be performed efficiently using PCA, fault diagnosis is less well developed. Miller et al. (1994) proposed the use of residual and score contribution charts to identify variables indicative of non-conforming operation. But contribution chart is a qualitative technique in nature, and can not give an explicit presentation about process behavior. Gertler et al. (1999) proposed a structured residual method to find out the root cause for process deviation. Raich et al (1996) used different PCA models for each fault to detect and identify process faults. Both methods require empirical knowledge on all possible faults and are useful only for limited applications. There are many difficulties in applying PCA-based approach to fault diagnosis problem due to the implicit statistical assumption, which assumes the future “good” behavior should continue to resemble past “good” behavior and any statistically significant deviation from this hypothesis is simply classified as a special event or a fault. Therefore, the PCA based approach is “nondirectional” (MacGregor et al., 1994). That is, it would detect the abnormal behaviors of process, but can’t find out the root cause of a specific process malfunction. Some fundamental issues, such as the detectability and identifiability of process changes or failures have not been systematically considered and solved in the PCA frameworks.

Dunia and Qin (1998) proposed a subspace approach to realize fault detection, identification, isolation and diagnosis. Due to the difficult of isolating faults from normal process changes when only the T^2-test is violated, their method is based on the Q-statistic and the T^2 index is not utilized. However, any data-based empirical modeling methods, e.g. PCA and other multivariate statistical analysis methods, can not solve the process monitoring and fault diagnosis problem as a whole if no other information about process is efficiently utilize. Specifically, the emphasis of most PCA-based works has been more on procedures to perform monitoring and diagnosis given a set of sensors and less on the actual location of sensors for efficient detection and identification of process malfunctions (Raghuraj et al, 1999). Fortunately, many researches in other fields have been taken to design various sensor networks based on the graph theory (Iri et al, 1979; Ali and Narasimhan, 1993; Raghuraj et al, 1999). If sensors were suitably located based on the knowledge of fault propagation manner within the process, PCA with the optimized sensor locations would obtain a great improvement in detecting and identifying process faults.

Furthermore, information provided by the Q statistic in the conventional PCA does not well match with that of the T^2 statistic provided. The T^2 statistic mainly describes behavior of process variables which are

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significant correlated with the principal components (PCs), while the Q index is related with all monitored variables. Hence, This shortcoming may cause confusions in some situations and thus not favorable.

In this paper, the graph-based techniques are used to optimize sensor locations. Issues of the fault detectability and identifiability are explored to ensure the designed sensor network obtaining the maximum possible fault resolution. Then two new statistics of *PVR* and *CVR* are introduced to take place the Q statistic in the conventional PCA. The improved PCA can efficiently detect weak changes and give an insight into the root cause of process fault. A simulated CSTR process using the improved PCA with optimized sensor locations demonstrates superior performance with comparison to the conventional methods.

2. Sensor Locations with Maximum Fault Resolution

The importance of the problem of sensor locations is evident, as most fault diagnosis techniques are based on a given set of sensors.

The criteria of locating sensors could be described as observing all variables (Vaclavek and Loucka, 1976; Ali and Narasimhan, 1993), formulating the fault propagation behavior (Iri et al, 1979) and obtaining maximum fault resolution (Ragharaj et al, 1999) etc. Basic concepts and terminology of the graph theory, as well as some sensor location algorithms, can be found in these documents. However, few researches tried to incorporate the sensor location problem with specific fault diagnosis approach, e.g. PCA. In fact, if some properties of PCA were considered, the task of locating sensors would be alleviated. Similarly, a properly designed sensor network may greatly improve the performance of PCA for fault detection and diagnosis. Here our aim is to bring them together and analyze the special advantages obtained from this combination.

To utilize the rich store of theoretical results available from the graph theory to locate sensors, a directed graph (DG) or digraph model should be built firstly to represent cause and effect relationships among process variables. DG model is particularly appealing because it provides a qualitative pictorial representation of the interactions among the important process variables and can be easily developed from empirical relationships or fundamental principles (Iri et al, 1979). As a illustrating example, consider a buffer tank system shown in Figure 1, where F_1, F_2 and F_3 denote flow rates, L denotes the level of the tank, and V_1, V_2, and V_3 the apertures of the valves.

The DG model shown in Figure 2 can qualitatively represent the topology structure of this process. Here, two new concepts of the *structure detectability* (SD) and *method detectability* (MD) will be introduced. SD refers to the condition that every defined fault of the process can be observed (or detected) by at least one sensor. SD condition is related with the "structure" or topology of the sensor network. However, SD condition alone can not ensure that each fault is detected in practice. That is, SD is only a necessary condition while not a sufficient one. The final detectability of a fault is also relevant to the performance of specific monitoring method, e.g., PCA. This method-dependent detectability is referred as MD condition and will be discussed at the next section. Only when both the SD and MD conditions are satisfied, faults could be ultimately detected. One of the SD conditions for buffer tank system, for example, is that a sensor placed at the node F_3. Also, sensors placed at node L or at each node of F_1, F_2, and F_3 simultaneously satisfy the MD condition. Hence, there is a minimum sensor set that meets the SD condition. However, the fault resolution of a minimum sensor set is very poor. For instance, a sensor at the node F_3 or L would be able to detect out changes caused by some fault or disturbance in the system, but can not tell whether the change is due to the failure of controller C_F, the leakage of the tank, or other system malfunctions. Therefore, more sensors should be located besides the minimum sensor set to obtain a satisfied fault resolution.

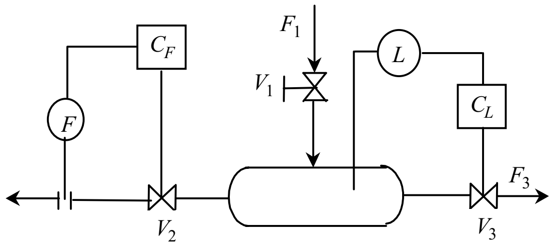

Fig. 1 Buffer tank

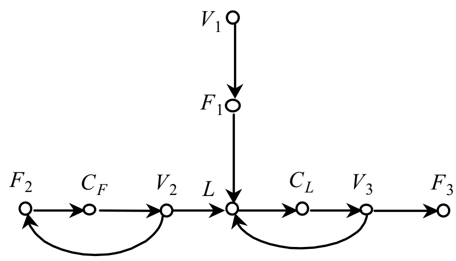

Fig.2 Directed graph of buffer tank

A sensor set with maximum fault resolution means that it not only satisfies SD condition but also resolve faults to the maximum possible extent. Raghuraj et al. (1999) presented a searching algorithm for sensor location with maximum fault resolution. Their method was based on DG instead of signed graph (SDG) which is more prevalent in sensor network design literature (Kramer and Palowitch, 1987; Iri et al., 1979). DG is adopted (also in our example of buffer tank) for its easy access and no plant-specific information is required for the signs as in SDG. Since Raghuraj et al. actually solved the maximum fault resolution problem based on the SD condition (although the concept of SD condition was not introduced and used in their paper), their obtained sensor set does not guarantee faults could be ultimately detected. Furthermore, some faults would still not be able to isolated and identified by their sensor location scheme whereas the fault resolution is maximized in some sense. However, if MD condition and other properties of PCA were considered, it would be find the searching algorithm of Raghuraj et al. suffices the sensor location problem. Integration of the improved PCA with the algorithm of Raghuraj et al. will be illustrated in next sections.

Here the steps of sensor location with maximum fault resolution can be formulated as follows

1) Build DG model for the monitored process. It can be implemented by using empirical relationships or fundamental mathematical model of the process.
2) Use searching algorithm proposed by Raghuraj et al (1999) to decide the location of sensors. The obtained sensor network satisfies SD condition and thus the fault detectability issues could be solved if MD condition is also satisfied.

Based on this optimized sensor location, the improved PCA is then used to guarantee the MD condition and enhanced fault resolution is obtained.

3. Improved PCA and Associated Statistics

Mathematically, PCA can be generally considered as a subspace decomposition technique where the process measurement space is divided into two orthogonal subspaces, that is, the principal component (PC) subspace and residual subspace.

3.1 PCA Principles Consider a normalized data matrix $\boldsymbol{X}(m\times n)$ composed of m sample vectors and n process variables collected under normal operation conditions. PCA transforms the matrix $\boldsymbol{X}$ to a linear combination of variables as follows

$$\boldsymbol{X} = \boldsymbol{T}\boldsymbol{P}^T + \hat{\boldsymbol{T}}\hat{\boldsymbol{P}}^T = \boldsymbol{T}\boldsymbol{P}^T + \boldsymbol{E} \tag{1}$$

where $\boldsymbol{P}(n\times k)$ are the first $k(<n)$ principal component loadings, $\boldsymbol{T}(m\times k)$ are corresponding scores. Matrices $\hat{\boldsymbol{P}}$ and $\hat{\boldsymbol{T}}$ consist of the last n-k column vectors of loadings and row vectors of scores, respectively. Matrix $\boldsymbol{E}(m \times n)$ is correspond to the residual subspace consisted by the abandoned information in PC subspace. Obviously, the principal component subspace $\boldsymbol{T}\boldsymbol{P}^T$ is orthogonal to the residual subspace $\boldsymbol{E} = \hat{\boldsymbol{T}}\hat{\boldsymbol{P}}^T$. The decomposition of data matrix $\boldsymbol{X}$ in Eq.1 can be implemented by singular value decomposition of correlation matrix $\boldsymbol{R}$ as

$$\boldsymbol{R} = \boldsymbol{U}\boldsymbol{\Lambda}^{1/2}\boldsymbol{U}^T \tag{2}$$

where $\boldsymbol{R}=(\boldsymbol{X}^T\boldsymbol{X})/(n\text{-}1)$, $[\boldsymbol{P}^T \quad \hat{\boldsymbol{P}}^T] = \boldsymbol{U}$ and $[\boldsymbol{T} \quad \hat{\boldsymbol{T}}] = \boldsymbol{U}\boldsymbol{\Lambda}^{1/2}$, and matrix $\boldsymbol{\Lambda}$ is a diagonal one composed of the eigenvalues of the matrix $\boldsymbol{R}$.

Process monitoring and fault diagnosis can then be carried out based upon statistical hypothesis tests in these two subspaces. Two indices, the *Hotelling*-T^2 and the Q statistics are used to describe process behavior, and subsequently detect process change and faults. In PC subspace, the hypothesis tests is done by using T^2 statistic, which is defined as

$$T^2 = \boldsymbol{t}\,\boldsymbol{\Lambda}_k^{-1}\boldsymbol{t}^T \tag{3}$$

where $\boldsymbol{\Lambda}_k^{-1}$ is a diagonal matrix consisted by reciprocals of the k largest eigenvalues of matrix $\boldsymbol{R}$. In residual subspace, the Q statistic is used for statistical test, it is defined as follows

$$Q = \boldsymbol{e}\boldsymbol{e}^T = \boldsymbol{x}(\mathbf{I} - \hat{\boldsymbol{P}}\hat{\boldsymbol{P}}^T)\boldsymbol{x}^T \tag{4}$$

The confidence restriction for T^2 and Q-statistics can be found in Jackson (1991).

3.2 *PVR* and *CVR* Statistics The definition of T^2 index in Eq.3 indicates the value of T^2 is related with the score vector t. Note the score vector t is the linear combination of process variables and combination weights are exactly the correlation coefficients of corresponding variables to the load vectors. If a variable is greatly correlated with the loads, then this variable will be well explained by the resulting score vectors. In other words, the T^2 statistic in conventional PCA (corresponding to the PC subspace) mainly describes behavior of process variables that have significant correlation with PCs. While the Q statistic (corresponding to the residual subspace) is related with all monitored variables. Hence, the information provided by the Q statistic does not well accord with that of the T^2 statistic provided. For example, the violation of Q statistic would mean the advent of a fault that violates the PCA model. While a significant increase in T^2 but not in Q statistic could be due to a fault (include process fault and sensor fault) or a normal process change (or disturbance) in the process that conserves the PCA model. This drawback may cause confusions in some situation and is the reason of T^2 index was not utilized in the paper of Dunia and Qin (1998). Therefor, if the process information contained in the residual subspace could be divided into more details to match with information in the PC subspace, the performance of PCA would be improved.

***Definition* 1.** Suppose there are s variables in the variable set $\{x_i\}_{i=1}^n$ that are significant correlated with PCs, refer these variables as principal-component-related variable (PV) and other (n-s) variables are common variable (CV). The project of PV in the residual subspace comprises a new statistic of *PVR* (PV Residuals) and corresponding statistic of the CV is *CVR* (CV Residuals). Here *PVR* and *CVR* statistics are defined as

$$PVR = \boldsymbol{x}_s \cdot (\mathbf{I} - \boldsymbol{P}_s \boldsymbol{P}_s^T) \cdot \boldsymbol{x}_s^T$$
$$CVR = \boldsymbol{x}_{n-s} \cdot (\mathbf{I} - \boldsymbol{P}_{n-s} \boldsymbol{P}_{n-s}^T) \cdot \boldsymbol{x}_{n-s}^T \tag{5}$$

where the subscript s and n-s denote PV and CV elements in the corresponding matrixes, respectively.

Comparing Eq.5 with Eq.4, one can see the residual subspace is divided into two parts. One is represented by *PV* (and *PVR* statistic), and the other is by *CV* and the *CVR* statistic. The advantage of partition of the residual subspace is that the information represented by *PVR* statistic now is mainly related with PCs, and thus consists with T^2 statistic in the PC subspace.

Before calculating the confidence limits of *PVR* and *CVR* statistics, PV needs to be selected out from process variables. By calculating the *multiple correlation* (MC) coefficients between each process variable and PCs, PV could be determined as variables whose MC coefficients are larger than a predefined threshold. The MC coefficient between the i-th variable $x_i^{(m\times1)}\in\boldsymbol{X}^{(m\times n)}$ and PCs is defined as

$$\rho\left(x_i, \boldsymbol{T}\right) = \arg\max_{\beta} \left\{ \operatorname{cov}\left(x_i, T\beta\right) / \left[\operatorname{Var}\left(x_i\right) \times \operatorname{Var}\left(T\beta\right)\right]^{1/2} \right\} \tag{6}$$

where $\boldsymbol{T}^{(m\times k)}=\{t_1, \ldots, t_k\}$ is the score matrix, and $\beta^{(k\times1)}$ is a parameter vector.

Directly calculating MC coefficients by the definition equation of Eq.6 is difficulty. Fortunately, there is a straightforward approach in the PCA framework to solve this problem, as indicated by the following equation (Johnson and Wichern, 1988)

$$\rho\left(x_i, \boldsymbol{T}\right) = \left(\sum_{j=1}^{k} \lambda_j p_{i,j}^2 \right)^{1/2} \tag{7}$$

where $\lambda_j \in \boldsymbol{\Lambda}$ is the eigenvalue of matrix $\boldsymbol{R}$, and $p_{i,j}$ is the corresponding element of loading matrix $\boldsymbol{P}$.

After PV is determined, CV comprises the other left variables. Obviously the confidence limits of *PVR* and *CVR* statistics could be calculated independently as *Q* statistics using methods provided by Jackson (1991). However it is worth noting the following linear relationship between the *Q* statistic and *PVR* and *CVR* statistics

$$Q_i = \sum_{j=1}^{n} (x_{i,j} - \hat{x}_{i,j})^2 = \sum_{j\in PV} (x_{i,j} - \hat{x}_{i,j})^2 + \sum_{j\in CV} (x_{i,j} - \hat{x}_{i,j})^2 = PRV^{(i)} + CVR^{(i)} \tag{8}$$

where subscript i denotes the i th measurement vector. It shows confidence limits of *PVR* and *CVR* statistics (denoted as λ_{PVR} and λ_{CVR}) are relevant to that of the *Q* statistic (denoted as λ_Q). The control limits λ_{PVR} and λ_{CVR} could be derived directly by given different weight to λ_Q, respectively.

$$\lambda_Q^{(\alpha)} = \lambda_{PVR}^{(\alpha)} + \lambda_{CVR}^{(\alpha)} = w_{PVR}\lambda_Q^{(\alpha)} + w_{CVR}\lambda_Q^{(\alpha)}$$
$$\text{with } w_{PVR} + w_{CVR} = 1 \tag{9}$$

where the superscript α is a predefined significant level, w_{PVR} and w_{CVR} are weighting coefficients. Due to the linear relationship in Eq.8, the weight would be taken as the percentage of information of variables described by PCs. Because the square of the MC coefficient approximately reflects the percentage of a variable represented by PCs, the weights are taken as follow

$$w_{PVR} = 1 - \sum_{i\in PV} \rho_i^2 \Big/ \sum_{i=1}^{n} \rho_i^2$$
$$w_{CVR} = 1 - \sum_{i\in CV} \rho_i^2 \Big/ \sum_{i=1}^{n} \rho_i^2 = 1 - w_{PVR} \tag{10}$$

Thus, the framework of the improved PCA is established. The *PVR* and *CVR* statistics, together with the T^2 statistic constitute a new process monitoring and fault diagnosis strategy for multivariate processes.

4. Simulation Examples

The improved PCA based on the optimized sensor locations is used to monitor and diagnose a simulated CSTR system as shown in Figure 3. In this example, an exothermic reaction of *A* to *B* takes place in a stirred-tank reactor. Temperature control is implemented by recycling part of the reactor outlet stream to the reactor through a heat exchanger. The recycle flow rate is controlled, and the reactor residence time is controlled by maintaining the level of the reactor. Some ideal properties about this reaction procedure are assumed, and controller parameters are determined to guarantee a satisfied performance by means of simulation. This CSTR system was used by many authors to solve the sensor network design problem (Kramer and Palowitch, 1987; Raghuraj et al, 1999).

The DG model of this CSTR system is shown in Figure 4 (Raghuraj et al., 1999). Nodes 1~13 are defined as the root nodes (corresponding to faults). Nodes 14~23 are those where sensors can be placed. Raghuraj et al. studied the design problem of sensor network with maximum fault resolution, and their searching algorithms gave out nodes [15, 17, 18, 19, 20, 21, 23] as the optimized sensor set. Based on this sensor set, all faults (F1~F13) are structurally detectable, that is, SD conditions of all these faults are satisfied. But some faults still can not be isolated from others due to the non-redundant requirement of Raghuraj et al.'s algorithms.

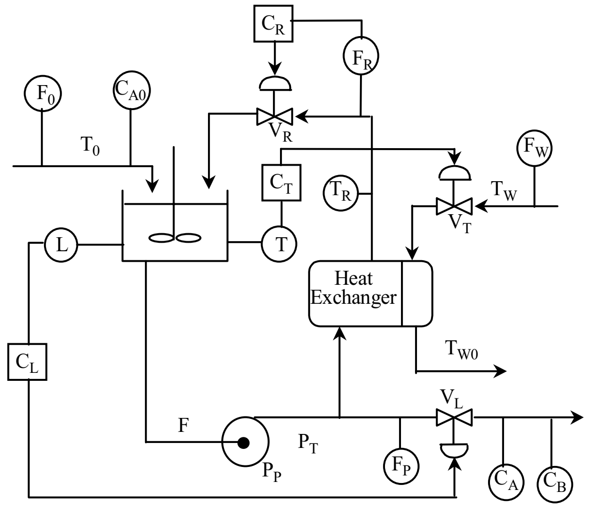

Fig.3 Process diagram of a CSTR System

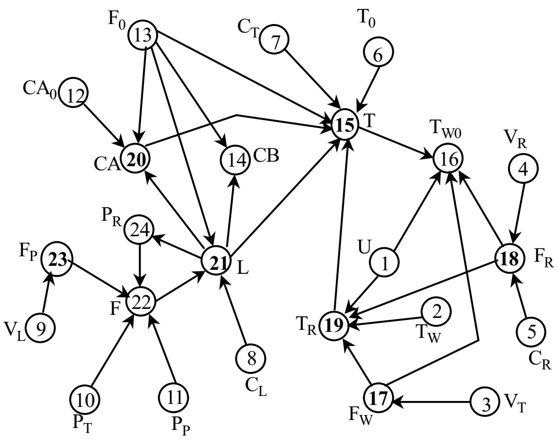

Fig.4 DG model of a CSTR System

These 7 sensor variables S15, S17, S18, S19, S20, S21, and S23 are then used as measured variables to provide process information of the CSTR system. The advantage of using this optimized sensor set is that more information about the system is utilized, and some basic properties as detectability and identifiability are already partially guaranteed before PCA has been used to monitor the system behavior.

As mentioned above, the performance of PCA determines whether a fault can be ultimately detected. Only both the SD and MD conditions of a fault were satisfied, this fault could be detected in practice. As an illustration example, a process change of 5 percent concentration increase of inlet stream *A* is studied. Before this change occurs, a conventional PCA model is built using 720 samples of the 7 selected variables under nominal process conditions. The singular value decomposition of the correlation matrix as Eq. 2 shows the cumulated variance ratio of first 2 PCs is 80.571%. Thus the retained number of PCs is taken as 2, and corresponding confidence limits of T^2 and Q indices are 10.733 and 9.058 (99%), respectively. The monitoring result of the change of CA_0 (F12 node) by conventional PCA is shown as figure 5, altogether 60 samples.

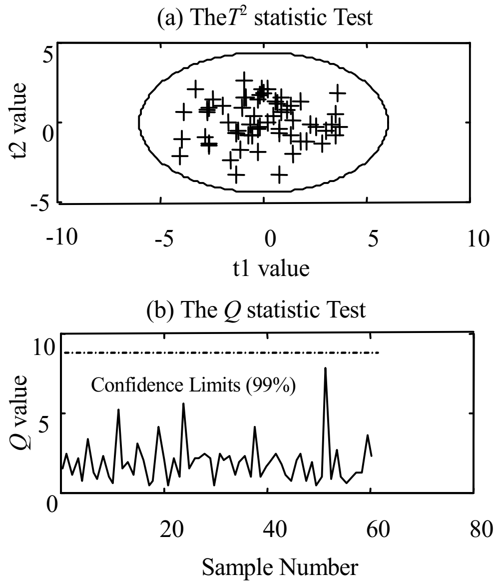

Fig. 5 Results of fault detection of F12 node (Conventional PCA)

Because the change of CA_0 is small, both T^2 and Q indices do not be significant changed. In fact, as the DG model shows in figure 4, the change of CA_0 only influences two sensors in the selected sensor set, i.e., sensors S15 and S20. Intuitively, due to other 5 variables are not greatly changed, the weak change of CA_0 would be disguised by the relatively large control limit of Q statistic. Nevertheless the more profound reason is due to the intrinsic conservation of PCA in the detection of weak process disturbance or faults.

Although the optimized sensor location ensures the change of CA_0 is structurally detectable (or observable), the conventional PCA fails to detect this change. That is, SD condition for the change of CA_0 is satisfied while the MD condition is not. For comparison, detection result of this weak change of CA_0 using the improved PCA is shown in figure 6. The T^2 plot is the same as that of the conventional PCA in figure 5 and not shown here again. A threshold of 0.78 is used to determine whether a variable is significantly correlated with PCs (MC coefficients of each process variable to the 2 PCs is not shown for space limitation). Hence, variables S15, S18, S19, S21 and S23 are PV, and variables S17 and S20 are CV. Control limits of *PVR* and *CVR* statistics calculated by Eqs. 9 and 10 are 1.595 and 7.463, respectively.

Figure 6 shows that *PVR* test is not violated but *CVR* test does. The change of CA_0 influences variables S15 and S20. Variable S15 is a PV that means the variation of this variable is well described by PCs and thus the projection of the CA_0 change to the *PV* space (contained in the residual subspace) will be small. In fact, even the CA_0 changed greatly, the contribution of S15 to the *PVR* index is relatively limited. Contrarily, information contained in a CV is poorly described by PCs and thus a small change of CV (here is the variable S20) would be instantly detected by *CVR* statistic. Since all variables are treated together by *Q* statistic in the conventional PCA, the weak variation in the CV would be disguised due to the relatively large control limit of the *Q* statistic. This is the reason why conventional PCA fails to detect the small change of CA_0 in the figure 5. This case indicates the improved PCA is more sensitive to small process changes than the conventional one, and MD condition is easier to be satisfied in this new method.

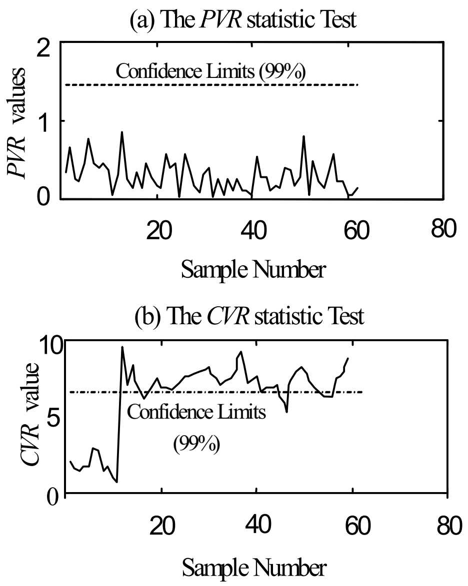

Fig. 6 Results of fault detection of F12 node (Improved PCA)

Another advantage of separating *Q* statistic into two parts is that an enhanced fault resolution can be obtained. Because the *PVR* index is direct related with PCs, the combination of T^2 plot and *PVR* plot will be helpful to identify a fault from a normal process change (disturbance), which is impossible in the conventional PCA or only based on DG model shown in figure 4. More details about this point refer to Wang et al. (2000). It is the combination of the optimized sensor locations and the improved PCA that gives an efficient solution.

5. Conclusions

The sensor location issue has not been paid enough attention in most PCA-based process monitoring and fault diagnosis approaches until now. In fact, as shown in this paper, the qualitative information contained in the graphic model (DG or SDG) is very important and useful to guarantee a satisfied fault detection and diagnosis result. The improved PCA using two new introduced statistics of *PVR* and *CVR* is also presented in this paper to overcome some drawbacks of the conventional PCA. The digraph model and optimized sensor networks ensure the SD conditions are satisfied for all defined faults and meanwhile provide maximum fault resolution. As a result, the improved PCA based on the optimized sensor locations meets the MD conditions and makes faults ultimately detectable.

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