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Recursive Diagonal Contributions Method for Time Varying Chemical Processes Monitoring

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Abstract. This paper proposes a Recursive Diagonal Contributions (RDC) method for fault isolation of time-varying chemical processes. The proposed fault isolation method depends on recursive calculating of the contribution of each process variable in the fault detection indices of the principal component analysis (PCA) model. The overall performance of the proposed scheme is validated by using a non-isothermal continuous stirred tank reactor (CSTR) chemical process. The isolation results of the proposed RDC method are superior to traditional methods in the sense of isolating the correct faulty variable and of decreasing the false alarm rates

Keywords: Principal Component Analysis (PCA), Recursive PCA, Process monitoring

1. Introduction

The classical PCA is a time invariant process monitoring model, whereas, most chemical processes are time varying. Accordingly, this may lead to inefficient and unreliable process monitoring [1]. To deal with this problem, extention of PCA to time varying processes monitoring have been developed. Several recursive approaches for adaptive process monitoring have been reported in the literature [2-5]. The most important challenge faced by the recursive adaptation of PCA model is the high computation costs, due to repeated eigenvalue decomposition (EVD) or singular value decomposition (SVD). Recently, Elshenawy et al. introduced two recursive principal component analysis (RPCA) methods for fault detection in time varying processes [6].

After detecting a fault, it is important to identify the root cause of the fault. While much work has been reported in fault detection using data-correlation based models, only a few methods are available for fault isolation [7]. A good overview of different methods for fault isolation can be found in [8].

The objective of this study is to present a fault isolation method for time varying chemical processes. The proposed RDC method depends on recursive calculating of the process variables contributions in the fault detection indices, the Hotelling's T^2 and *SPE*. The adaptive scheme depends on a low computation cost adaptation method, first-order perturbation (FOP) analysis that is proposed in [6]. This adaptive isolation method is used to identify the faults that may occur in the sensors. These faults include bias, drift, precision degradation, and complete failure.

This paper is organized as follows: Section (2) gives a brief review of recursive PCA model based on FOP analysis. Section (3) defines the proposed RDC method for the T^2 and *SPE* fault detection indices; this is followed by a complete scheme for the proposed adaptive fault detection and isolation approach. A simulated chemical process is used in section (4) to demonstrate the effectiveness of the proposed RDC method. Section (5) concludes the paper.

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2. Recursive PCA based on FOP Analysis

According to the first-order perturbation theory, the eigen-structure of the correlation matrix is updated as a whole, instead of the correlation matrix itself as follows:

$$R_k = R_{k-1} + \varepsilon\left[x_k x^T{}_k - R_{k-1}\right] \tag{1}$$

where $R_k \in \Re^{m\times m}, \varepsilon$ is a small positive number ($\varepsilon \to 0$), $x_k \in \Re^m$ is the sample data vector at the k^{th} time instant. The final relations of the updated eigenvalues and eigenvectors are:

$$\lambda_{k,i} = (1-\varepsilon)\lambda_{k-1,i} + f_i^2 \tag{2}$$

$$v_{k,i} = v_{k-1,i} + \sum_{j=1}^{m} b_{ji} v_{k-1,j} \tag{3}$$

With

$$f_i = v_{k-1}^T x_k \tag{4}$$

$$b_{ji} = \begin{cases} 0 & j = i, \\ -b_{ji} = \dfrac{f_j f_i}{(\lambda_{k-1,i} - \lambda_{k-1,j} -}) & j \neq i \end{cases} \tag{5}$$

where $i, j = 1, \ldots, m$.

The complete FOP analysis-based recursive PCA is given in [6].

3. The proposed Recursive Diagonal Contributions Method

The proposed Recursive Diagonal Contributions (RDC) method can be described as in the following. We will begin with the recursive contribution of T^2 index. Equation (6) presents the recursive calculation of the T^2 statistic based on the diagonal contribution formula.

$$T_k^2 = x_k^T A_k x_k = x_k^T I A_k I x_k = x_k^T (\sum_{i=1}^{m} \zeta_i \zeta_i) A_k (\sum_{i=1}^{m} \zeta_i \zeta_i) x_k = \sum_{i=1}^{m} x_k^T \zeta_i \zeta_i^T A_k \zeta_i \zeta_i^T x_k \tag{6}$$

The contribution of each variable i in the T^2 index is then:

$$C_{D_{k,i}}^{T^2} = x_k^T \zeta_i \zeta_i^T A_k \zeta_i \zeta_i^T x_k \tag{7}$$

The definition of the contribution for the SPE index is calculated according to the following relation:

$$SPE_k = x_k^T B_k x_k = x_k^T I B_k I x_k = x_k^T (\sum_{i=1}^{m} \zeta_i \zeta_i) B_k (\sum_{i=1}^{m} \zeta_i \zeta_i) x_k = \sum_{i=1}^{m} x_k^T \zeta_i \zeta_i^T B_k \zeta_i \zeta_i^T x_k \tag{8}$$

Finally, the i^{th} variable contribution based on the diagonal approach is:

$$C_{D_{k,i}}^{SPE} = x_k^T \zeta_i \zeta_i^T B_k \zeta_i \zeta_i^T x_k \tag{9}$$

Where $A_k = \hat{P}_k \Lambda_k^{-1} \hat{P}_k^T$ and $B_k = \tilde{P}_k \tilde{P}^T$. $\hat{P}_k$ and $\tilde{P}_k$ are the principal components and residual loading matrices, respectively. Let $\zeta_i = \begin{bmatrix} 0 & 0 & \cdots & 1 & 0 \end{bmatrix}^T$ is the i^{th} column of the identity matrix and represents the direction of x_i.

Therefore, the proposed adaptive fault detection and isolation (FDI) scheme can be divided into two stages, building the monitoring model off-line and updating the monitoring model indices after collecting new process measurements on-line. The complete strategy of the proposed adaptive FDI scheme is depicted in Fig. (1). Here $\Lambda_k \in \Re^{m\times m}$ is a diagonal matrix whose diagonal elements are the eigenvalues of the correlation matrix R. The number of the principal components (PCs) can be determined by using different techniques [9].

4. Simulation Results

This section shows the utility of the proposed adaptive FDI scheme using a simulated chemical process. This process is a non-isothermal Continuous Stirred Tank Reactor (CSTR). The schematic diagram and the variables of this process are shown in Fig. 2. The reaction is of the first order (A → B), where reactant A premixed with a solvent, converts into product B with a rate:

$$r = \beta_r k_o e^{-E/(RT)} C \tag{10}$$

The dynamic behavior of this system is described as follows:

$$V\frac{dC}{dt} = F(C - C_i) - V_r \tag{11}$$

$$V\rho C_P \frac{dT}{dt} = \rho C_P F(T_i - T) - \frac{UA}{1 + UA/2F_c\rho_c C_{\rho c}}(T - T_c) + (-\Delta H_r)Vr \tag{12}$$

where UA is the heat transfer coefficient which is related to the coolant flow by the empirical relation $UA = \beta_{UA} a F_c^b$. The inlet reactant concentration C_i obtained from the two feed streams, the reactant and the solvent, is calculated as

$$C_i = \frac{(F_a C_a + F_s C_s)}{(F_a + F_s)} \tag{13}$$

The outlet temperature (T) and concentration (C) are regulated with a proportional-integral (PI) controller by manipulating both the inlet coolant flow rate (F_c) and the inlet reactant flow rate (F_a), respectively. The details of the controller and model parameters are given in [6].

200 samples were generated to build the normal PCA model. Another 800 samples were generated to update the adaptive FDI scheme on-line. The performance of the proposed FDI scheme is tested through (i) slow parameter variation, i.e., a slow drift in process parameter βr; (ii) an abrupt change in one of the process set-points, i.e., the outlet concentration C that changes from 0.8 to 0.85 $Kmole/m^3$ at sample time 300. Faulty sensors are simulated as shown in table 1. In this study, the number of significant principal components l_k is calculated by using Cumulative Percent Variance (CPV) [6], such that the variance explained is approximately 99% of the total variance.

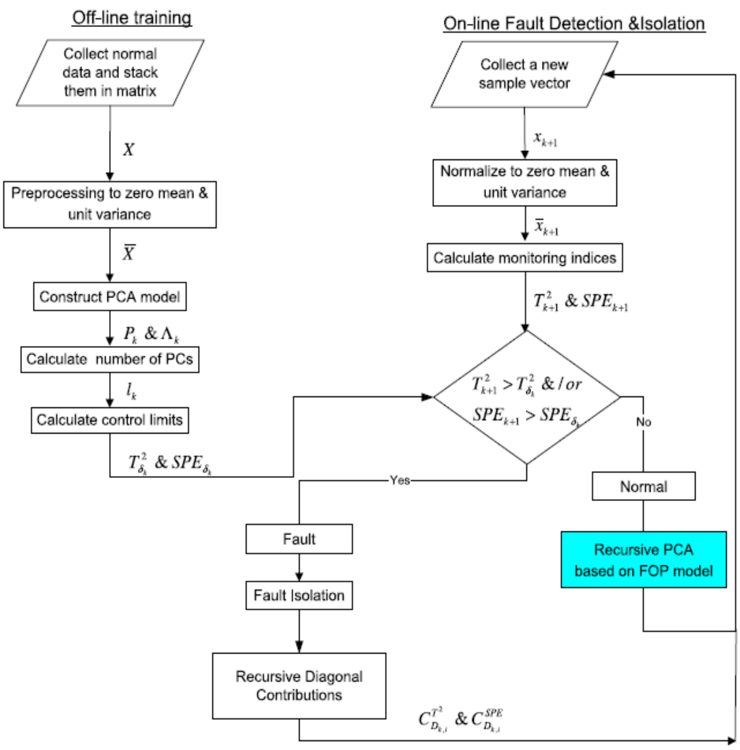

Fig. 1: Strategy of the proposed adaptive FDI scheme

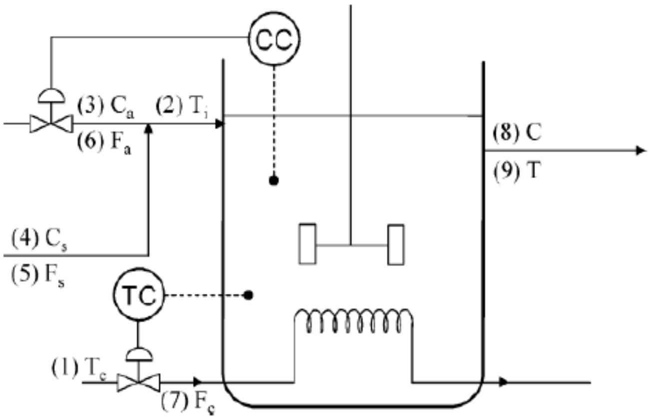

Fig. 2. Non-isothermal CSTR process and nine measured variables: (1) coolant temperature, (2) reactant mixture temperature, (3) reactant A concentration, (4) solvent concentration, (5) solvent flow rate, (6) solute flow rate, (7) coolant flow rate, (8) outlet concentration, and (9) outlet temperature.

Table 1: Sensor fault simulation

Cases	Faulty sensor	Fault Description	Fault time
1. Bias	T_i	$f_1(t) \approx U(2, 3)$	700
2. Drift	F_s	$f_2(t) = 0.05(t - t_f)$	701
3. Precision degradation	T_i	$f_3(t) = N(0, 5)$	698
4. Complete failure	T	$T(t) = 366$	701

To measure the capability of the adaptive FDI scheme, two indices are used. The first one is the rate of false alarms (FAR). The second one is the rate of correct fault isolation rate (IR). The false alarm rate is measured by calculating the number of violated samples to the number of normal data as:

$$FAR = \frac{Violated\ Samples}{Normal\ Data}\% \tag{14}$$

The isolation rate is determined by calculating the number of data of the faulty variable contribution (FVC) that can exceed the monitoring control limits according to the following relation:

$$IR = \frac{FVC}{Faulty\ Data}\% \tag{15}$$

Table 2 summarizes the false alarm rate of the conventional PCA and the recursive PCA model based on FOP analysis in the first part, and the fault isolation rate of the traditional Diagonal Contributions (DC) method and the proposed fault isolation (RDC) method in the second part. The table depicts the reliability of the proposed adaptive fault detection and isolation approach. Also, the largest rates are given when the contribution approaches that involve the combined *SPE* are used. That is not surprising because the T^2 index detects only a small group of large faults. It can be clearly seen that the isolation rates of the proposed recursive fault isolation method (RDC) increases significantly for different sensor faults. Although, the isolation results of the DC and RDC methods when the faults are detected with the *SPE* index are similar in some simulation cases, the simulation results of the traditional fault isolation DC method cannot give a totally unambiguous isolation. That means, the traditional contributions method could not isolate the main cause of the faults, but showed obvious contributions of many variables in the process. These results may cause some confusion to the operator. In contrast, the proposed recursive isolation method can clearly isolate most sensor faults.

Table 2: False alarm rate of the (conventional PCA and recursive PCA) models and fault isolation rate of the (traditional DC and proposed RDC) methods in simulated CSTR process

Cases	Conventional PCA		Recursive PCA		DC		RDC	
	T^2	*SPE*	T^2	*SPE*	T^2	*SPE*	T^2	*SPE*
1	40.5714	34.7143	1.7143	1.4286	0	100	99	100
2	33	30.2857	2.4286	4.4286	0	82	41	88
3	40.5714	34.7143	1.7143	1.4286	0	73	48	76
4	10.7143	4.4286	0.4286	0.8571	0	100	0	100

5. Conclusion

This paper presents the proposed Recursive Diagonal Contributions (RDC) method for fault isolation of time varying chemical processes. The proposed method performs the fault isolation after the detection of the fault by using the two PCA monitoring indices (T^2 and *SPE*). Two adaptive contribution indices for the Hotelling's T^2 and *SPE* are introduced, that are, $C_{D_{k,i}}^{T^2}$ and $C_{D_{k,i}}^{SPE}$, respectively. Four types of sensor faults: bias, drift, precision degradation, and complete failure are considered. The overall performance of the proposed scheme was validated by using CSTR system. The simulation results prove the adaptability, credibility and isolability of the proposed approach with compared to the traditional method.

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