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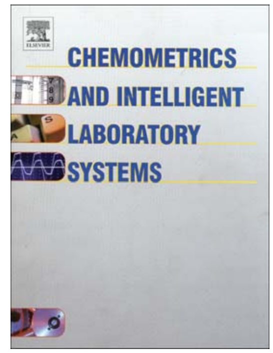

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State-Space Independent Component Analysis for Nonlinear Dynamic Process Monitoring

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Abstract

The cost effective benefits of process monitoring will never be over emphasised. Amongst monitoring techniques, the Independent Component Analysis (ICA) is an efficient tool to reveal hidden factors from process measurements, which follow non-Gaussian distributions. Conventionally, most ICA algorithms adopt the Principal Component Analysis (PCA) as a pre-processing tool for dimension reduction and de-correlation before extracting the independent components (ICs). However, due to the static nature of the PCA, such algorithms are not suitable for dynamic process monitoring. The dynamic extension of the ICA (DICA), similar to the dynamic PCA, is able to deal with dynamic processes, however unsatisfactorily. On the other hand, the Canonical Variate Analysis (CVA) is an ideal tool for dynamic process monitoring, however is not sufficient for nonlinear systems where most measurements follow non-Gaussian distributions. To improve the performance of nonlinear dynamic process monitoring, a state space based ICA (SSICA) approach is proposed in this work. Unlike the conventional ICA, the proposed algorithm employs the CVA as a dimension reduction tool to construct a state space, from where statistically inde-

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pendent components are extracted for process monitoring. The proposed SSICA is applied to the Tennessee Eastman Process Plant as a case study. It shows that the new SSICA provides better monitoring performance and detect some faults earlier than other approaches, such as the DICA and the CVA.

Keywords: Dynamic system, Nonlinearity, Principal component analysis, Canonical variate analysis, Independent component analysis, Probability density function, Kernel density estimation, Process monitoring.

1 Introduction

Process monitoring techniques are employed to detect abnormal deviations of process operation conditions and diagnose the causes for these deviations to maintain high quality products and process safety. The Principal Component Analysis (PCA) is a dimension reduction technique that summarises the variation in a set of correlated variables to a set of de-correlated principal components (PCs), each of which is a linear combination of the original variables. The PCA exploits the correlation amongst a large number of measured variables and is popular for its simplicity. The PCA by reducing the dimension of the process variables is able to eliminate noise and retain only important process information. MacGregor and Kourti [1] established a PCA model from the training data and judged the behaviour of online processes against the PCA model to detect deviations from the normal operating process. Wang et al. [2] also presented a PCA approach based on visualization using parallel co-ordinates with the Manresa Waste Water Treatment Plant as a case study.

The widely applied PCA is a static approach that assumes that the observations are in a steady-state, which is time independent. Furthermore, the PCA is normally associated with the Hotelling's T^2 statistic, which, in order to determine the upper control limit, assumes that the principal components derived by the PCA follow a Gaussian distribution. However, the assumption of time-independence may not be valid for processes subject to dynamic disturbances. The assumption of normality may also be invalid for most chemical processes where strong nonlinearity makes variables driven by noise and disturbances non-Gaussian. In these situations, the PCA is not an appropriate tool for process monitoring.

A solution to address the limitation of Gaussian assumption associated with the PCA is the Independent Component Analysis (ICA) [3–5]. The ICA technique recovers a few statistically independent source signals from collected process measurements by assuming that these independent signals are non-Gaussian. A set of variables are said to be statistically independent from each other when the value of one variable cannot be predicted by giving the value of another variable. Unfortunately in process systems, such independent sources are in general not directly measurable, but mixing each other in measurement variations. To identify the unmeasured ICs from measurements, the ICA algorithm involves a pre-processing stage known as the whitening stage to eliminate the cross correlation between the process variables before extracting the independent components [3–10]. Although the ICA is sometimes considered as an extension of the PCA [3], the objectives of the ICA are clearly different from those of the PCA. The ICA decomposes process measurements into statistically (high-order statistics) ICs of a lower dimension whereas the PCA decomposes the process measurements into a set of de-correlated (second order statistics) PCs of a lower dimension. Therefore, the ICA is able to extract more useful information than the PCA [4, 5] and as a result performs better than the PCA based monitoring techniques.

Process monitoring based on the ICA approach aims to extract the essential ICs, that drive a process, for detecting underlying faults. Lee *et al.* [4] in their ICA approach employed the Euclidean norm to determine the number of ICs to retain in the ICA model. The ICs in the model space were described as the dominant ICs while the ignored ICs were described as the excluded ICs. Three monitoring metrics; the I_d^2 for the dominant ICs, the I_e^2 for the excluded ICs and the Q-metric for the residual space were determined and then kernel density estimations (KDE) employed to derive the control limit for all three statistics.

Albazzaz and Wang [8] in another way, employed all the extracted ICs for process monitoring because it was argued that no single IC was more important than another. In addition, a box-cox transformation was applied to change the non-Gaussian coordinates of the ICs to a Gaussian distribution in order to justify the use of the control limits estimated based on the Gaussian assumption. Their technique was applied to the Manresa Waste Water treatment plant in Spain to demonstrate its efficiency.

Conventionally, most published ICA studies have utilised the PCA for whitening and dimension reduction in the pre-processing stage, allowing the ICs to be interpreted by the simple geometry of the PCA [7]. However, the connection of the ICA with PCA makes such ICA approaches not appropriate for dynamic process monitoring due to the static nature of the PCA. For most industrial processes, variables driven by noise and disturbances are strongly auto-correlated and time-varying making the PCA and the ICA inappropriate for monitoring of such dynamic processes. This means that a dynamic process would require a monitoring technique that will take the serial correlations of the process data into account in order to achieve efficient dynamic process monitoring. For this reason, Lee et al. [6] extended the ICA methods and proposed the dynamic ICA (DICA) approach to improve the monitoring performance. In the so called DICA approach, a dynamic extension of the PCA (DPCA) is applied to an augmented data set in the pre-processing stage, where each observation vector is augmented with the previous observations and stacked together to account for the auto-correlations, then the ICs are extracted from the decomposed principal components (PCs). However, the DICA, like the DPCA, is not the best approach to capture the dynamic behaviour from process measurements [11]. As a result, the statistical advantage of the ICA is not fully exploited by the DICA and the performance of the DICA in dynamic process monitoring is still not satisfactory.

Nevertheless, the state-space models like the Canonical Variate Analysis (CVA) on the other hand are reported to be efficient tools for dynamic process monitoring [11–17]. The CVA is a dimension reduction technique that is based on state variables and is well suited for auto-correlated and cross-correlated process measurements. This makes the CVA based approaches a better choice than the PCA based approaches for dynamic process monitoring. However, on the other hand, the states obtained from the standard CVA, like the PCs are only de-correlated, but not statistically independent, hence are not efficient enough for nonlinear process monitoring.

To derive an efficient tool for nonlinear dynamic process monitoring, in this paper, the CVA, rather than the PCA, is proposed as the pre-processing tool to associate with the ICA resulting in a novel State Space ICA (SSICA) approach. In the approach, the CVA is adopted as a dimension reduction tool to construct a state space and perform the dynamic whitening in the pre-processing stage. Then, the ICA is applied to the constructed state space in order to identify the statistically independent components. The SSICA approach is developed for nonlinear dynamic process monitoring and applied to the Tennessee Eastman Process Plant as a case study. It demonstrates that generally, the proposed SSICA is able to improve the process monitoring performance over the existing DICA technique, which is reported to be an improvement of the traditional ICA [6]. Also, the overall performance of the SSICA is better than the CVA, which was reported to be an efficient dynamic monitoring tool [11–17]. The performance improvements of the SSICA over the DICA and the CVA include increases in detection reliability and decreases in both detection delay and false alarms.

This paper is organised as follows: Section 2 describes the SSICA technique in details, which include the CVA, SSICA and KDE algorithms. The SSICA is then applied to the Tennessee Eastman Process Plant in section 3. Finally, this work is concluded in section 4.

2 State Space Independent Component Analysis

The development of process monitoring techniques is geared towards applying these techniques to industrial processes in order to improve process performance monitoring. It is well known that most real time processes to which the monitoring techniques are applied are dynamic and nonlinear. The SSICA approach is developed to deal with such processes. Firstly, from a general nonlinear dynamic system, a linearized state space model can be constructed from normal operation data through the CVA. The non-Gaussian collective modelling errors are then extracted as statistically independent components through the SSICA. The obtained state space independent components together with the residuals are used for process monitoring by comparing the upper control limits estimated through the KDE approach. These algorithms are described in details as follows.

2.1 Canonical Variate Analysis

Consider a nonlinear dynamic plant represented as:

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{f}(\mathbf{x}_k) + \mathbf{w}_k \\ \mathbf{y}_k &= \mathbf{g}(\mathbf{x}_k) + \mathbf{v}_k \end{aligned} \tag{1}$$

where $\mathbf{x}_k \in \mathbb{R}^n$ and $\mathbf{y}_k \in \mathbb{R}^m$ are state and measurement vectors respectively, $\mathbf{f}(\cdot)$ and $\mathbf{g}(\cdot)$ are unknown nonlinear functions, whereas $\mathbf{w}_k$ and $\mathbf{v}_k$ are plant disturbances and measurement noise vectors respectively. Clearly, it is difficult to monitor such unknown nonlinear dynamic systems directly. Fortunately, under normal operation conditions, the plant in Equation (1) can be approximated by a linear stochastic state space model as:

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{A}\mathbf{x}_k + \boldsymbol{\varepsilon}_k \\ \mathbf{y}_k &= \mathbf{C}\mathbf{x}_k + \boldsymbol{\eta}_k \end{aligned} \tag{2}$$

where $\mathbf{A}$ and $\mathbf{C}$ are unknown state and output matrices respectively, whereas $\boldsymbol{\varepsilon}_k$ and $\boldsymbol{\eta}_k$ are collective modelling errors partially due to the underlying nonlinearity of the plant, which has not been included in the linear model, and partially associated with process disturbance and measurement noise, $\mathbf{w}_k$ and $\mathbf{v}_k$ respectively. Note, as a result of the nonlinearity of the physical plant represented in Equation (1), the collective modelling errors, $\boldsymbol{\varepsilon}_k$ and $\boldsymbol{\eta}_k$ in Equation (2) generally will be non-Gaussian although $\mathbf{w}_k$ and $\mathbf{v}_k$ might be normally distributed.

To monitor the linear dynamic process represented in (2) without knowing matrices $\mathbf{A}$ and $\mathbf{C}$, the CVA is employed to extract the state variables $\mathbf{x}_k$ from process measurements, $\mathbf{y}_k$. The CVA is based on the so called *subspace identification*, where the process measurements are stacked to form the past and future spaces through the past, $\mathbf{y}_{p,k}$ and future, $\mathbf{y}_{f,k}$ observations defined as follows.

$$\mathbf{y}_{p,k} = \begin{bmatrix} \mathbf{y}_{k-1} \\ \mathbf{y}_{k-2} \\ \vdots \\ \mathbf{y}_{k-q} \end{bmatrix} \in \mathbb{R}^{mq}, \quad \tilde{\mathbf{y}}_{p,k} = \mathbf{y}_{p,k} - \bar{\mathbf{y}}_{p,k} \tag{3}$$

$$\mathbf{y}_{f,k} = \begin{bmatrix} \mathbf{y}_{k} \\ \mathbf{y}_{k+1} \\ \vdots \\ \mathbf{y}_{k+q-1} \end{bmatrix} \in \mathbb{R}^{mq}, \quad \tilde{\mathbf{y}}_{f,k} = \mathbf{y}_{f,k} - \bar{\mathbf{y}}_{f,k} \tag{4}$$

where the first subscripts of $\mathbf{y}_{p,k}$ and $\mathbf{y}_{f,k}$ indicate the past (p) and the future (f) observations respectively, whilst the second subscripts stand for the reference sampling point, where the past and future observations are defined. The sample means of the past and future observations are represented as $\bar{\mathbf{y}}_{p,k}$ and $\bar{\mathbf{y}}_{f,k}$ respectively, whilst $\tilde{\mathbf{y}}_{p,k}$ and $\tilde{\mathbf{y}}_{f,k}$ are the pre-processed past and future observations with zero means.

The past and future truncated Hankel matrices $\mathbf{Y}_p$ and $\mathbf{Y}_f$ are then defined in Equation (5) and Equation (6) respectively.

$$\mathbf{Y}_p = \begin{bmatrix} \tilde{\mathbf{y}}_{p,(q+1)} & \tilde{\mathbf{y}}_{p,(q+2)} & \cdots & \tilde{\mathbf{y}}_{p,(q+M)} \end{bmatrix} \in \mathbb{R}^{mq\times M} \tag{5}$$

$$\mathbf{Y}_f = \begin{bmatrix} \tilde{\mathbf{y}}_{f,(q+1)} & \tilde{\mathbf{y}}_{f,(q+2)} & \cdots & \tilde{\mathbf{y}}_{f,(q+M)} \end{bmatrix} \in \mathbb{R}^{mq\times M} \tag{6}$$

From the Hankel matrices defined above, the covariance of the past, future and cross-covariance matrices are estimated as follows:

$$\boldsymbol{\Sigma}_{pp} = E(\tilde{\mathbf{y}}_{pk}\tilde{\mathbf{y}}_{pk}^T) = \mathbf{Y}_p\mathbf{Y}_p^T(M-1)^{-1} \tag{7}$$

$$\boldsymbol{\Sigma}_{ff} = E(\tilde{\mathbf{y}}_{fk}\tilde{\mathbf{y}}_{fk}^T) = \mathbf{Y}_f\mathbf{Y}_f^T(M-1)^{-1} \tag{8}$$

$$\boldsymbol{\Sigma}_{fp} = E(\tilde{\mathbf{y}}_{fk}\tilde{\mathbf{y}}_{pk}^T) = \mathbf{Y}_f\mathbf{Y}_p^T(M-1)^{-1} \tag{9}$$

The goal of the CVA is to find the best linear combinations, $\mathbf{a}^T\tilde{\mathbf{y}}_{fk}$ and $\mathbf{b}^T\tilde{\mathbf{y}}_{pk}$ of the future and past observations so that the correlation between these combinations is maximised. The correlation can be represented as:

$$\rho_{fp}(\mathbf{a},\mathbf{b}) = \frac{\mathbf{a}^T\boldsymbol{\Sigma}_{fp}\mathbf{b}}{(\mathbf{a}^T\boldsymbol{\Sigma}_{ff}\mathbf{a})^{1/2}(\mathbf{b}^T\boldsymbol{\Sigma}_{pp}\mathbf{b})^{1/2}} \tag{10}$$

Let $\mathbf{u} = \mathbf{\Sigma}_{ff}^{1/2}\mathbf{a}$ and $\mathbf{v} = \mathbf{\Sigma}_{pp}^{1/2}\mathbf{b}$. The optimization problem can be casted as:

$$\begin{aligned} \max_{\mathbf{u},\mathbf{v}} \quad & \mathbf{u}^T(\mathbf{\Sigma}_{ff}^{-1/2}\mathbf{\Sigma}_{fp}\mathbf{\Sigma}_{pp}^{-1/2})\mathbf{v} \\ s.t. \quad & \mathbf{u}^T\mathbf{u} = 1 \\ & \mathbf{v}^T\mathbf{v} = 1 \end{aligned} \tag{11}$$

The solution of this problem can be obtained through the singular value decomposition (SVD) on the scaled Hankel matrix, $\mathbf{H}$ as indicated in Equation (12).

$$\mathbf{H} = \mathbf{\Sigma}_{ff}^{-1/2}\mathbf{\Sigma}_{fp}\mathbf{\Sigma}_{pp}^{-1/2} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \tag{12}$$

where $\mathbf{U} = \begin{bmatrix}\mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_{mq}\end{bmatrix} \in \mathbb{R}^{mq\times mq}$, $\mathbf{V} = \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_{mq}\end{bmatrix} \in \mathbb{R}^{mq\times mq}$
$\mathbf{\Sigma} = \begin{bmatrix}\sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \ddots & \vdots & \\ 0 & 0 & \cdots & \sigma_{mq}\end{bmatrix} \in \mathbb{R}^{mq\times mq}$

From Equation (12) above, the canonical variate, $\mathbf{z}_k \in \mathbb{R}^{mq}$ based on the past measurements can be derived as in Equation (13).

$$\mathbf{z}_k = \begin{bmatrix} {b_1}^T \\ {b_2}^T \\ \vdots \\ b_{mq}^T \end{bmatrix} \tilde{\mathbf{y}}_{p,k} = \begin{bmatrix} {v_1}^T \\ {v_2}^T \\ \vdots \\ v_{mq}^T \end{bmatrix} \mathbf{\Sigma}_{pp}^{-1/2}\tilde{\mathbf{y}}_{p,k} = \mathbf{V}^T\mathbf{\Sigma}_{pp}^{-1/2}\tilde{\mathbf{y}}_{p,k} = \mathbf{J}\tilde{\mathbf{y}}_{p,k} \tag{13}$$

where $\mathbf{J} = \mathbf{V}^T{\mathbf{\Sigma}_{pp}}^{-1/2} \in \mathbb{R}^{mq\times mq}$ is the transformation matrix, which transforms the mq-dimensional past measurements to the mq-dimensional canonical variate space. The canonical variate estimated in (13) can be separated into the state and residual spaces based on the order of the system, n. According to the magnitude of the singular values, the first n dominant singular values are determined and the corresponding n elements of the canonical variate retained as the state variables where $n < mq$. In addition, the remaining $(mq - n)$ elements of the canonical variate are said to be in the residual space. Equation (14) below shows the entire canonical variate space ($\mathbf{z}_k \in \mathbb{R}^{mq}$) is spanned by the state variables ($\mathbf{x}_k \in \mathbb{R}^n$) and the residuals ($\mathbf{d}_k \in \mathbb{R}^{mq-n}$), both of which are subsets of the canonical variate, $\mathbf{z}_k$.

$$\mathbf{z}_k = \begin{bmatrix} \mathbf{x}_k{}^T & \mathbf{d}_k{}^T \end{bmatrix}^T \tag{14}$$

The previous work [17] showed that the state variables, $\mathbf{x}_k$ obtained through CVA provides a tool better than directly using the past or future observations to monitor the dynamic systems in (1). However, as shown in (2), the states are combinations of statistically independent non-Gaussian sources. To make process monitoring more efficient, identifying these sources from the states is desired. The corresponding algorithm is to be developed in the next section.

2.2 State Space Independent Component Analysis

According to (2), $\mathbf{x}_k$ can be expressed as a linear combination of the initial state, $\mathbf{x}_0$ and the collective modelling errors, $\boldsymbol{\varepsilon}_j$, for $j = 0, 1, \ldots, k-1$.

$$\mathbf{x}_k = \mathbf{A}^k \mathbf{x}_0 + \sum_{j=0}^{k-1} \mathbf{A}^j \boldsymbol{\varepsilon}_{k-1-j} \tag{15}$$

Equation (15) indicates that if $\mathbf{x}_0$ and $\boldsymbol{\varepsilon}_j$, $j = 0, \ldots, k-1$ are mixtures of $m(\leq n)$ unknown independent components, $\mathbf{s}_j \in \mathbb{R}^m$, for $j = 0, \cdots, k-1$, then the states, $\mathbf{x}_k$, for $k = 1, \ldots M$ are also linear combinations of these unknown independent components. More specifically, the relationship can be expressed as follows.

$$\mathbf{X} = \mathbf{B}_x \mathbf{S}_x \tag{16}$$

where $\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_M \end{bmatrix} \in \mathbb{R}^{n \times M}$ is the state matrix, $\mathbf{B}_x = \begin{bmatrix} \mathbf{b}_1 & \cdots & \mathbf{b}_m \end{bmatrix} \in \mathbb{R}^{n \times m}$ is an unknown mixing matrix, and $\mathbf{S}_x = \begin{bmatrix} \mathbf{s}_{x,0} & \ldots & \mathbf{s}_{x,M-1} \end{bmatrix} \in \mathbb{R}^{m \times M}$ is unknown independent component matrix. The SSICA aims to estimate both mixing matrix, $\mathbf{B}_x$ and independent component matrix, $\mathbf{S}_x$, from the state matrix, $\mathbf{X}$ obtained through the CVA as described above.

The problem can be solved through an existing ICA algorithm, such as the FastICA [18] to find a de-mixing matrix, $\mathbf{W}$ such that the rows of the estimated independent component matrix,

$$\hat{\mathbf{S}}_x = \mathbf{W}_x \mathbf{X} \tag{17}$$

are as independent of each other as possible. Based on the "non-Gaussian represents independence" principle [18], the de-mixing matrix as well as the independent component matrix are obtained through iterative optimizations to maximize certain non-Gaussian criteria.

The ICA can be applied to the residual space spanned by $\mathbf{d}_k$. The independent component matrix in the residual space is obtained by applying the ICA algorithm to the residual matrix, $\mathbf{D}$ as follows.

$$\hat{\mathbf{S}}_d = \mathbf{W}_d\mathbf{D} \tag{18}$$

where $\mathbf{D} = \begin{bmatrix}\mathbf{d}_1 & \cdots & \mathbf{d}_M\end{bmatrix} \in \mathbb{R}^{(mq-n)\times M}$.

The ICA based process monitoring is frequently associated with the Mahalanobis distance I^2, also known as the D-statistic [4, 6, 10]. The I^2 metric is the sum of the squared independent components extracted from the ICA algorithm.

$$I^2_{x,k} = \hat{\mathbf{s}}^T_{x,k}\hat{\mathbf{s}}_{x,k} \tag{19}$$

$$I^2_{d,k} = \hat{\mathbf{s}}^T_{d,k}\hat{\mathbf{s}}_{d,k} \tag{20}$$

where $\hat{\mathbf{s}}_{x,k}$ and $\hat{\mathbf{s}}_{d,k}$ are the k-th columns of $\hat{\mathbf{S}}$ and $\hat{\mathbf{S}}_d$, respectively. The M $I^2_{x,k}$ and $I^2_{d,k}$ values for $k = 1, \ldots, M$ are then used to derived the upper control limits, $I^2_{x,\mathrm{UCL}}(\alpha)$ and $I^2_{d,\mathrm{UCL}}(\alpha)$ using the KDE algorithm described in the next section.

For online monitoring, the ICs of the state and residual spaces is calculated from the new measurements, $\tilde{y}^{\mathrm{new}}_{p,k}$ using the transformation matrix, $\mathbf{J} = \begin{bmatrix}\mathbf{J}_x^T & \mathbf{J}_d^T\end{bmatrix}^T$ and the de-mixing matrices, $\mathbf{W}_x$ and $\mathbf{W}_d$ respectively.

$$\hat{\mathbf{s}}^{\mathrm{new}}_{x,k} = \mathbf{W}_x\mathbf{J}_x\tilde{\mathbf{y}}^{\mathrm{new}}_{p,k} \tag{21}$$

$$\hat{\mathbf{s}}^{\mathrm{new}}_{d,k} = \mathbf{W}_d\mathbf{J}_d\tilde{\mathbf{y}}^{\mathrm{new}}_{p,k} \tag{22}$$

The corresponding I^2 metrics for the new measurements are then obtained as follows.

$$I^{2,\mathrm{new}}_{x,k} = (\hat{\mathbf{s}}^{\mathrm{new}}_{x,k})^T\hat{\mathbf{s}}^{\mathrm{new}}_{x,k} \tag{23}$$

$$I^{2,\mathrm{new}}_{d,k} = (\hat{\mathbf{s}}^{\mathrm{new}}_{d,k})^T\hat{\mathbf{s}}^{\mathrm{new}}_{d,k} \tag{24}$$

A fault condition is then detected if either I^2 metric is larger than the corresponding UCL.

2.3 Control Limit Through Kernel Density Estimations

The ICs are not Gaussian. Therefore, the UCL for the I^2 metric cannot be derived analytically. The kernel density estimation (KDE) is a well established approach to estimate the PDF of random processes [19–21]. Hence, it is a natural selection using the KDE to determine the UCL [17]. Considering both I^2 metrics are positive, a KDE algorithm with lower bound support is adopted in this work to estimate the UCL.

Let $y > 0$ be the random variable under consideration. Firstly, the bounded y is converted into unbounded x by defining $x = \ln(y)$. Then, the density function $p(x)$ can be estimated by the normal KDE algorithm. Finally, the density function of y is $p(\ln(y))/y$ as derived in (25).

$$P(y < b) = P(x < \ln(b)) = \int_{-\infty}^{\ln(b)} p(x)dx = \int_{0}^{b} p(\ln(y))\frac{1}{y}dy \tag{25}$$

Therefore, by knowing $p(x)$, an appropriate control limit can be determined for a specific confidence bound, α using Equation (25). The estimation of the probability density function $\hat{p}(x)$ at point x through the kernel function, $K(\cdot)$ is defined as follows

$$\hat{p}(x) = \frac{1}{Mh}\sum_{k=1}^{M} K\left(\frac{x - x_k}{h}\right). \tag{26}$$

where x_k, $k = 1, 2, \cdots, M$ are samples of x and h is the bandwidth. The bandwidth selection in KDE is an important issue because selecting a bandwidth too small will result in the density estimator being too rough, a phenomenon known as under-smoothed while selecting a bandwidth too big will result in the density estimator being too flat. There is no single perfect way to determine the bandwidth. However, a rough estimation of the optimal bandwidth h_{opt} subject to minimising the approximation of the mean integrated square error can be derived in Equation (27), where σ is the standard deviation [22].

$$h_{opt} = 1.06\sigma N^{-1/5} \tag{27}$$

To use both I_x^2 and I_d^2 metrics together, the joint distribution of these two metrics has to be considered. In general, the joint probability of two random variables, x and y is defined as follows.

$$P(x < a, y < b) = \int_{-\infty}^{a} \int_{-\infty}^{b} p(x, y) dx dy \tag{28}$$

However, for the SSICA and the DICA, I_x^2 and I_y^2 are independent. Hence,

$$P(x < a, y < b) = P(x < a)P(y < b) \tag{29}$$

Equation (29) can also be approximately applied to T^2 and Q metrics for the CVA because $\mathbf{x}$ and $\mathbf{d}$ in (14) are uncorrelated [23]. This means the joint PDF estimation can be simplified by two univariate PDF estimations.

By replacing x_k in Equation (26) with $I_{x,k}^2$ and $I_{d,k}^2$ obtained in (19) and (20) respectively, the above KDE approach is able to estimate the underlying PDFs of the I_x^2 and I_d^2 metrics. The corresponding control limits, $I_{x,\mathrm{UCL}}^2(\alpha)$ and $I_{d,\mathrm{UCL}}^2(\alpha)$ can then be obtained from the PDFs of the I_x^2 and I_d^2 metrics for a given confidence level, α by solving the following equations respectively.

$$\int_0^{I_{x,\mathrm{UCL}}^2(\alpha)} \frac{p(\ln(I_x^2))}{I_x^2} dI_x^2 \int_0^{I_{d,\mathrm{UCL}}^2(\alpha)} \frac{p(\ln(I_d^2))}{I_d^2} dI_d^2 = \alpha \tag{30}$$

$$\int_0^{I_{x,\mathrm{UCL}}^2(\alpha)} \frac{p(\ln(I_x^2))}{I_x^2} dI_x^2 = \sqrt{\alpha} \tag{31}$$

$$\int_0^{I_{d,\mathrm{UCL}}^2(\alpha)} \frac{p(\ln(I_d^2))}{I_d^2} dI_d^2 = \sqrt{\alpha} \tag{32}$$

In this work, a fault is then identified ($F_k = 1$) if either $I_{x,k}^{2,\mathrm{new}} > I_{x\mathrm{UCL}}^2(\alpha)$ or $I_{x,d}^{2,\mathrm{new}} > I_{d\mathrm{UCL}}^2(\alpha)$ conditions are satisfied, i.e.

$$F_k = (I_{x,k}^{2,\mathrm{new}} > I_{x,\mathrm{UCL}}^2(\alpha)) \oplus (I_{d,k}^{2,\mathrm{new}} > I_{d,\mathrm{UCL}}^2(\alpha)) \tag{33}$$

where $\oplus$ represents a logical "OR" operation.

3 APPLICATION - Tennessee Eastman Process Plant

The Tennessee Eastman Process (TEP) plant has 5 main units which are the reactor, condenser, separator, stripper and compressor [13, 24, 25]. A graphical description of the TEP plant is presented in Figure 1.

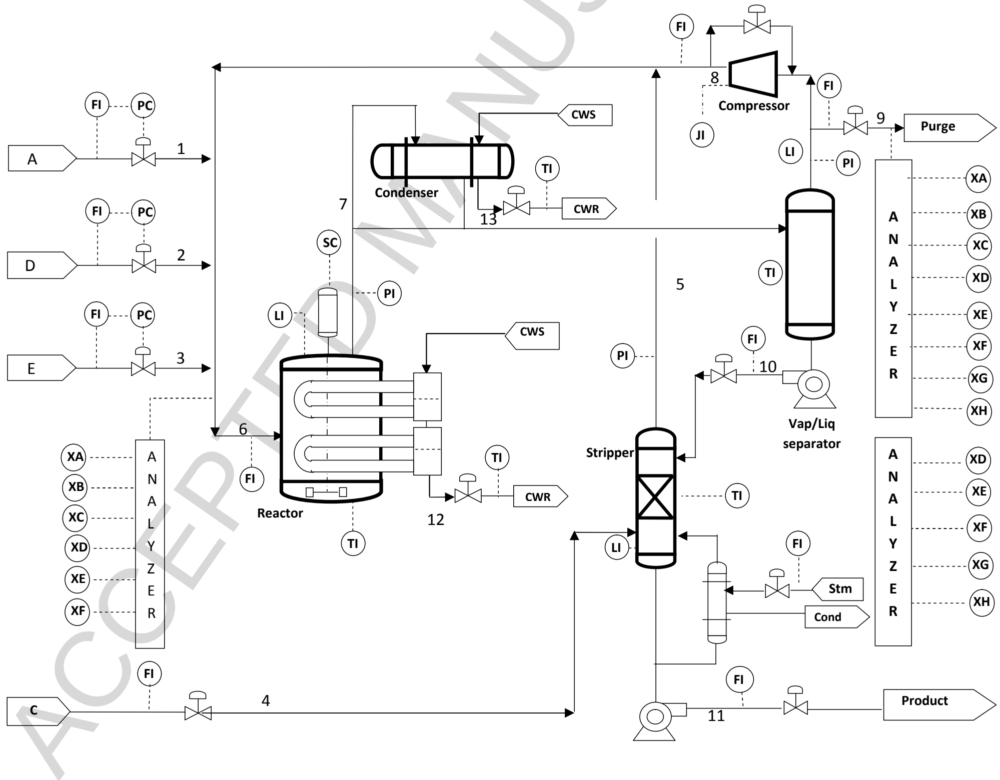

Figure 1 Graphical Description of the TEP Plant

The TEP process is a large dimensional, nonlinear process with unknown mathematical representation as the simulation is intentionally distributed as an undocumented FORTRAN program [24, 25]. The TEP data consists of two blocks; the training and test data sets each of which has 22 continuous process measurements, 12 manipulated variables and 19 composition measurements sampled with time delays. There are also 21 scenarios corresponding to Faults $0 - 20$, with Fault 0 being the data simulated at normal operating condition (no fault) and Faults 1 - 20 corresponding to data sets from the simulated fault processes, each with a specified fault as listed in Table 1.

Table 1 Brief Description of TEP Plant Faults

Fault	Description	Type
1	A/C Feed Ratio, B Composition Constant (Stream 4)	Step
2	An increase in B while A/C Feed ratio is constant (stream 4)	Step
3	D Feed Temperature (Stream 2)	Step
4	Reactor Cooling Water Inlet Temperature	Step
5	Condenser Cooling Water Inlet Temperature	Step
6	A loss in Feed A (stream 1)	Step
7	C Header Pressure Loss - Reader Availability (Stream 4)	Step
8	A,B,C Feed Composition (Stream 4)	Random variation
9	D Feed Temperature (Stream 2)	Random variation
10	C Feed Temperature (Stream 4)	Random variation
11	Reactor Cooling Water Inlet Temperature	Random variation
12	Condenser Cooling Water Inlet Temperature	Random variation
13	Reaction Kinetics	Slow drift
14	Reaction Cooling Water Valve	Sticking
15	Condenser Cooling Water Valve	Sticking
16	Unknown	Unknown
17	Unknown	Unknown
18	Unknown	Unknown
19	Unknown	Unknown
20	Unknown	Unknown

A total of 52 measurements are collected for each data set of length, $N = 960$ representing 48-hour operation with a sampling rate of 3 minutes. Among these measurements, 19 analyzer measurements, 14 of which are sampled at 6 minute interval whilst other 5 are sampled in every 15 minutes, have not been included in this study due to the measurement time delay, while 11 manipulated variables are treated the same as other measured variables because under feedback control, these variables are not independent any more. The simulation time of each operation run in the test data block is 48 hours and the various faults are introduced only after 8 hours. This means that for each of the faults, the process is in normal operation condition for the first 8 simulation hours before the process becomes abnormal after the introduction of the fault. Furthermore, all twenty TEP faults have also been studied to investigate the effectiveness of the proposed SSICA technique. The results are based on a $\alpha = 99\%$ confidence level ($\sqrt{\alpha} = 0.995$ for individual metrics).

The TEP plant is under closed-loop control, which by its nature, tries to overcome the abnormal deviations that occur as a result of the introduction of the various faults to the simulated TEP process. Due to the closed loop nature of the plant, deviations caused by some faults are relatively small such that these faults are difficult to be detected by most monitoring approaches, such as principal component analysis and partial least squares [17]. Different from these conventional methods, the SSICA proposed in this work aims to address both dynamic and nonlinear issues effectively.

The monitoring performance in this study is assessed by the percentage reliability, which is defined as the percentage of the samples outside the control limits [26]. Hence, a monitoring technique is said to have a better performance over another if the percentage reliability of this technique is numerically higher than the percentage reliability of another technique. Another criterion employed in this study to judge the performance of the monitoring techniques is the detection delay, which is how long it takes for a technique to identify a fault after the introduction of the fault. A monitoring technique is said to be better than another if it is able to detect a fault earlier than another technique. The false alarm rate, which is the percentage of samplings classified as abnormal during the 8 hour normal operation period before introducing a fault, is also considered for performance comparison.

To demonstrate the efficiency of the proposed SSICA, the monitoring performance of the proposed SSICA is compared with the monitoring performance of the DICA technique, an existing dynamic extension of the ICA. The SSICA is also compared with the CVA to demonstrate the improvement by performing ICA on the state space obtained by the CVA. For the pre-processing CVA described above, the number of state variables to retain in the dominant space is normally determined by the dominant singular values from the scaled Hankel matrix $\mathbf{H}$ in Equation (32). However, applying the CVA to the TEP case study showed that using the dominant singular values left an unrealistically large number of state variables in the dominant space.

Hence a more realistic number of state variables 28 were retained in the dominant space so that 28 state variables were retained from the pre-processing stage of CVA. To make a fair comparison with the proposed SSICA, in the DICA, equal number of latent variables were retained in the dominant spaces while the rest of the latent variables spanned the excluded spaces. The percentage reliability and the detection delay of all twenty TEP faults for the proposed SSICA technique is compared with that of the CVA and DICA techniques and presented in Table 2. The corresponding false alarm rate of all faults is 0.6849% for the DICA and 0% for both the CVA and the SSICA.

Table 2 Performance Comparison

Fault	**Reliability (%)**			**Detection Delay (minute)**		
	SSICA	**CVA**	**DICA**	**SSICA**	**CVA**	**DICA**
1	99.75	99.75	99.75	9	9	9
2	99.63	99.63	99.50	12	12	15
3	73.03	70.04	19.48	15	21	21
4	99.88	99.88	99.88	6	6	6
5	99.88	99.88	99.88	6	6	6
6	99.88	99.88	99.88	6	6	6
7	99.88	99.88	99.88	6	6	6
8	99.00	98.88	98.75	18	30	33
9	91.64	90.01	46.82	18	39	48
10	96.75	96.38	96.13	18	90	96
11	99.38	99.38	99.38	18	18	18
12	99.50	99.50	99.50	15	15	15
13	96.25	96.13	96.13	18	96	96
14	99.88	99.88	99.88	6	6	6
15	99.63	99.63	99.50	12	12	15
16	99.38	99.38	99.25	18	18	21
17	98.38	98.25	98.13	18	45	48
18	99.25	99.25	99.25	21	21	21
19	99.88	99.88	99.88	6	6	6
20	97.63	97.50	97.13	18	63	72

The superiority of the SSICA over the CVA and DICA techniques is demonstrated in Table 2. For 10 of the 20 faults (2,3,8,9,10,13,15,16,17 and 20), the SSICA is able to improve the monitoring performance over the existing DICA technique in both reliability and detection delay, while for the rest 10 faults, the SSICA maintains the same performance as the DICA does. This is achieved by the SSICA with a reduced false alarm rate for all faults. In the reliability, the improvement of the SSICA over the DICA is significant ($> 0.5\%$) for 4 of the faults (3,9,10 and 20). Particularly, for faults 3 and 9, the improvement is extremely significant, over 40%. Meanwhile, the SSICA is able to reduce the detection delay significantly (> 10 minutes) for 6 faults (8, 9, 10, 13, 17 and 20). The over one hour reduction in detection delay is achieved by using the SSICA on faults 10 and 13. In comparison between the SSICA and CVA, the performance of the SSICA is better than that of the CVA for 7 faults (3, 8, 9 10, 13, 17 and 20) in both the reliability and the detection delay, whilst these performance criteria of the remaining 13 faults are the same for both methods. In the reliability, the improvement on 2 faults (3 and 9) are significant (over 1%). Meanwhile, significant improvements in the detection delay (> 10 minutes) are observed for 6 faults (8, 9, 10, 13, 17 and 20), for two of which (10 and 13), the improvements are over one hour.

To appreciate the capability of the SSICA, fault detection by these three methods along with fault propagation is further analysed for Faults 3 and 9. As shown in Table 1, both Faults 3 and 9 relate to the temperature of D feed (stream 2), one for step change (Fault 3) and another for random variations (Fault 9). These faults directly result in small deviations in the reactor cooling water outlet temperature, which can be easily corrected by the closed-loop control system by manipulating the cooling water flow. Therefore, both faults are generally difficult to be detected by most monitoring approaches.

Figure 2 shows a comparison of the fault detection along with the propagation of Fault 3 for the SSICA (a), CVA (b) and DICA (c) techniques, using F_k derived from Equation (33), whilst Figure 3 shows the fault detection along with the propagated Fault 9 process for these three techniques.

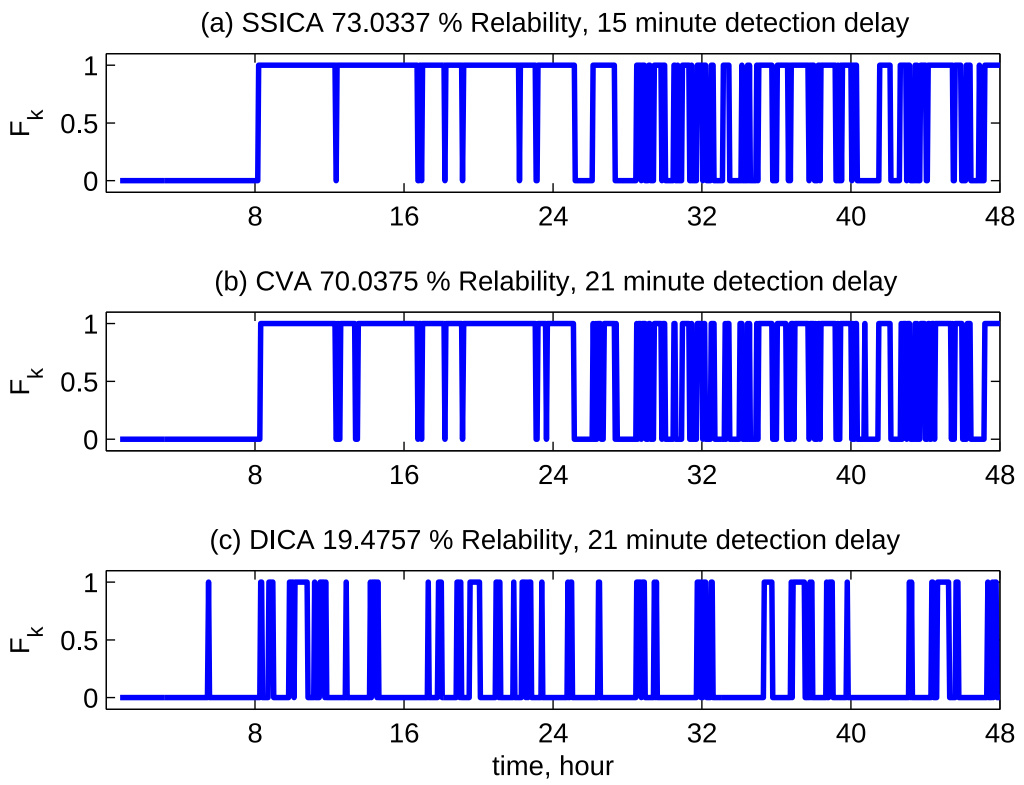

Figure 2 Comparison of fault detection along with the propagation of Fault 3

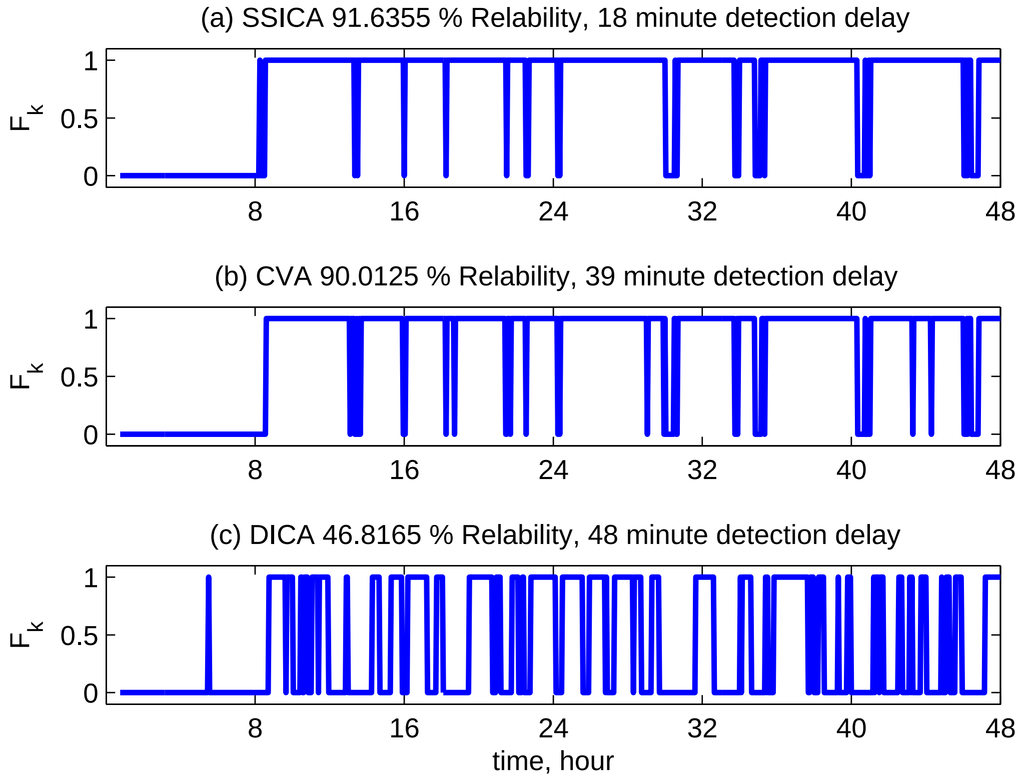

Figure 3 Comparison of fault detection along with the propagation of Fault 9

It is for such faults as Faults 3 and 9 that the superiority of the proposed SSICA technique over the CVA and particularly the DICA techniques is most outstanding as illustrated in Figure 2 and Figure 3. The performance of the SSICA is better than that of the CVA and DICA techniques for both Faults 3 and 9. Particularly, it is clear that for both faults the SSICA is able to show a significant improvement of fault detection over the DICA technique within a few hours of the early stage of fault propagation. The improvement in the early fault propagation stage is important since it will give more time for operators to deal with the detected fault.

Although the DICA, also referred to as the ICA with delays is reported to be a more efficient dynamic monitoring tool than the traditional ICA [6], the proposed SSICA technique is able to significantly improve the monitoring performance over the DICA technique for most of the faults considered in this work. This is because the pre-processing stage of the SSICA is based on the CVA, which is a more appropriate dynamic monitoring tool than the DPCA on which the DICA technique is firstly based on. Furthermore, the efficiency of the SSICA over the CVA is owed to the fact that the SSICA is more suited than the CVA to deal with non-Gaussian process measurement, separating the original sources to a greater degree than the CVA technique. The results illustrated above demonstrate that there were no faults for which either the CVA or DICA techniques outperformed the proposed SSICA technique.

It is worth to note that the CVA approach adopted in this work is able to cope with certain level of nonlinearities due to the use of the KDE to determine the UCL [17]. Moreover, the superiority of the CVA over the DICA indicates that the dynamic issue has more impact on the fault detection performance than the nonlinearity for the TE process. This might be due to the feedback control, which widely propagates the transient response caused by a fault, as well as restricts the variations caused by a fault to relatively small level. This restriction on variation causes some faults to be difficult to detect without taking into account the correlations in time. Meanwhile, the effect of nonlinearity on fault responses is also restricted so that the CVA with KDE approach is able to detect most faults adequately. This may also be the reason for most faults the performance of the SSICA and the CVA is very close.

4 Conclusion

In this study, an ICA model was developed based first on CVA in the pre-processing stage before applying the ICA algorithm and then control limits derived based on kernel density estimations with 99% joint confidence intervals. The proposed approach is applied to the Tennessee Eastman Process. The monitoring performance of the proposed SSICA is assessed and compared with those of the CVA and DICA techniques also considered in this study. The percentage reliability, detection delays as well as the false alarm rates were adopted to assess and compare the monitoring performance of the proposed approach with those of the CVA and DICA techniques. The percentage reliability of the SSICA was significantly higher than both of the DICA and the CVA for some of the faults although the significance of improvement over the CVA was not as high as that over the DICA. Moreover, the SSICA is also able to dramatically reduce the detection delay over both the CVA and the DICA for certain faults. In particular, the remarkable superiority of the SSICA is demonstrated in the faults that are more difficult to detect, emphasizing the efficiency of the proposed SSICA over the existing CVA and DICA techniques.

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