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Kernel Vertices PCA: A Novel Interval-Valued PCA Approach for Fault Detection in Nonlinear Complex Systems

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Abstract

Interval-valued data techniques are widely utilized in fault detection to enhance robustness against uncertainty. Among these, Vertices Principal Component Analysis (VPCA) is one of the most commonly applied methods. Constructing a VPCA model involves transforming the interval data matrix into a vertices matrix. This study introduces a novel data-driven approach for fault detection in uncertain nonlinear processes called Kernel VPCA (K-VPCA), which extends the VPCA method to handle nonlinear interval data. Specifically, the data are mapped into a high-dimensional kernel feature space before applying VPCA, allowing nonlinear relationships to be effectively modeled. The K-VPCA approach maintains robustness against false alarms without compromising fault detection performance. The proposed method is validated using data from a cement rotary kiln, confirming its effectiveness in fault detection.

Keywords: Fault Detection, Interval-Valued data, KPCA, Vertices Principal Component Analysis, Cement rotary kiln.

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1. Introduction

Principal Component Analysis (PCA) is a widely utilized data-driven method for monitoring and diagnosing complex systems [1]–[3]. Despite its success, PCA's performance in monitoring industrial systems with nonlinear dynamics is often limited due to its inherently linear nature, which prevents it from effectively modeling the nonlinear relationships present in such data [4], [5]. To overcome these limitations, various nonlinear extensions of PCA have been developed, with Kernel Principal Component Analysis (KPCA) being one of the most prominent approaches [6]. Originally introduced by Scholkopf ¨ [7], KPCA uses a nonlinear transformation to map the data into a higher-dimensional feature space, where linear PCA is then applied. This allows KPCA to capture the nonlinear characteristics of real-world processes, making it a robust tool for fault detection and diagnosis (FDD) [8]. As a result, KPCA has gained considerable attention for its ability to monitor and analyze nonlinear systems with higher precision [9]. However, a key limitation of KPCA lies in its assumption that sensor data is accurate and free from uncertainty, an assumption often violated in real-world applications where data is influenced by noise and approximations [10]. To overcome the challenges posed by uncertainty and nonlinearity in fault detection, researchers have developed algorithms tailored for interval-valued data [8], [11]. Examples of such methods include PCA vertices (VPCA), center PCA (CPCA), midpoint-radii PCA (MRPCA), and complete information PCA (CIPCA) [12]. Although these approaches show promise, their effectiveness is largely constrained to linear systems, limiting their applicability to nonlinear processes [13]. To address this limitation, recent research has focused on combining interval analysis with techniques capable of handling nonlinear systems [11]. This study introduces a new method, kernel vertices Principal Component Analysis (K-VPCA), which extends the VPCA framework by incorporating a nonlinear mapping that transforms the data into a higher-dimensional feature space. Within this space, interval-valued VPCA is applied, enabling K-VPCA to handle data uncertainties while effectively modeling nonlinear relationships. As a result, K-VPCA provides a robust and reliable solution for fault detection in complex, uncertain, and nonlinear processes. The effectiveness of the K-VPCA technique is validated using data from a rotary cement kiln, a complex industrial system characterized by significant non-linear behavior [14]. The results demonstrate that K-VPCA excels in minimizing false detections while maintaining high accuracy, without compromising detection speed or sensitivity to deviations. This establishes K-VPCA as a robust and dependable tool for fault detection in nonlinear systems, offering significant improvements over traditional PCA and other interval-based methods.

Additionally, the proposed method enhances fault detection reliability and provides a more comprehensive and precise diagnosis, contributing to improved process monitoring and control.

The structure of the paper is organized as follows: Section 2 outlines the theoretical foundations of the VPCA method as an interval-valued approach for process monitoring. Section 3 introduces the proposed K-VPCA method. In Section 4, the interval-based control chart for Hotelling's T^2, the squared predictive error Q, and the combined index Φ statistics is presented. Section 5 describes the cement plant setup, the application of the proposed method, and the resulting findings. Finally, Section 6 concludes with key remarks and future directions.

2. VERTICES PRINCIPAL COMPONENT ANALYSIS (VPCA)

VPCA is a two-step analysis that begins with numerical coding of a box's vertices and ends with a standard PCA on the coded data [13], [15]. Each observation in *Rm* can be represented as a hyperrectangle with $2m$ vertices and the total number of vertices is $n \times 2m$. Therefore, from the interval data:

$$[X] = \begin{pmatrix} \begin{bmatrix} \underline{x_1}(1) & \cdots & \underline{x_m}(1) \\ \vdots & \ddots & \vdots \\ \overline{x_1}(1) & \cdots & \overline{x_m}(1) \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \underline{x_1}(n) & \cdots & \underline{x_m}(n) \\ \vdots & \ddots & \vdots \\ \overline{x_1}(n) & \cdots & \overline{x_m}(n) \end{bmatrix} \end{pmatrix} \tag{1}$$

VPCA does not directly summarize the interval-valued data matrix *X*, it is replaced by a single-valued data matrix obtained as follows. Each interval-valued row is transformed into the numerical matrix X_i as follows:

$$[X] = \begin{pmatrix} \begin{bmatrix} \underline{x_1}(k) & \underline{x_2}(k) & \underline{x_3}(k) & \cdots & \underline{x_{m-1}}(k) & \underline{x_m}(k) \\ \overline{x_1}(k) & \underline{x_2}(k) & \underline{x_3}(k) & \cdots & \underline{x_{m-1}}(k) & \underline{x_m}(k) \\ \underline{x_1}(k) & \overline{x_2}(k) & \underline{x_3}(k) & \cdots & \underline{x_{m-1}}(k) & \underline{x_m}(k) \\ \overline{x_1}(k) & \overline{x_2}(k) & \underline{x_3}(k) & \cdots & \underline{x_{m-1}}(k) & \underline{x_m}(k) \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ \overline{x_1}(k) & \overline{x_2}(k) & \overline{x_3}(k) & \cdots & \overline{x_{m-1}}(k) & \overline{x_m}(k) \end{bmatrix} \end{pmatrix} \tag{2}$$

By stacking below, each other all the matrices *Xi's*, $i = 1, \ldots, n$, we get the new data matrix X_{VPCA} with $nx2^m$ rows and m columns:

$$X_{VPCA} = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_m \end{pmatrix} \tag{3}$$

VPCA entails performing PCA on 3. As with standard PCA, it is best to pre-process the data to avoid unwanted differences between variables. The matrix in 3 can be pre-processed in the same way that the standard single-valued case is. The application of PCA to the matrix X_{VPCA} will give $\hat{X}_{VPCA} = T_{VPCA}\, P^T$, and if B is chosen to be column-wise orthonormal, we have $X_{VPCA} = T_{VPCA}\, P^T$. To facilitate the interpretation of the solution, for each observation unit, for each component, the segment containing all component scores for vertices associated with this observation unit. Specifically, with respect to the k^{th} component, $k = 1, \ldots, p$, if n_i denotes the set of all the vertices for the i^{th} observation unit, $i = 1, \ldots, n$. The dimension of matrix X_{VPCA} is huge which will make the PCA of a such matrix practically impossible. This computational problem can be overcome by considering a special property of PCA. Specifically, it is well known that the columns of the component loadings matrix are the eigenvectors obtained from the eigen-decomposition of the cross-products matrix. Note that the eigenvectors are arranged in such a way that the first ones are associated with the highest eigenvalues [16]. Dealing with the cross products matrix $\Sigma_V = X_{VPCA}^T X_{VPCA}$, after simplification the covariance matrix Σ_V can be written as in equ. 4.

$$\Sigma_V = 2^{m-2} \begin{pmatrix} 2\sum_{k=1}^{n}\left(\overline{x}_1^2(k) + \underline{x}_1^2(k)\right) & \sum_{k=1}^{n}((\overline{x}_1(k) + \underline{x}_1(k))(\overline{x}_2(k) + \underline{x}_2(k))) & \cdots & \sum_{k=1}^{n}((\overline{x}_1(k) + \underline{x}_1(k))(\overline{x}_m(k) + \underline{x}_m(k))) \\ \sum_{k=1}^{n}((\overline{x}_2(k) + \underline{x}_2(k))(\overline{x}_1(k) + \underline{x}_1(k))) & 2\sum_{k=1}^{n}\left(\overline{x}_2^2(k) + \underline{x}_2^2(k)\right) & \cdots & \sum_{k=1}^{n}((\overline{x}_2(k) + \underline{x}_2(k))(\overline{x}_m(k) + \underline{x}_m(k))) \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{k=1}^{n}((\overline{x}_m(k) + \underline{x}_m(k))(\overline{x}_1(k) + \underline{x}_1(k))) & \sum_{k=1}^{n}((\overline{x}_m(k) + \underline{x}_m(k))(\overline{x}_2(k) + \underline{x}_2(k))) & \cdots & 2\sum_{k=1}^{n}\left(\overline{x}_m^2(k) + \underline{x}_m^2(k)\right) \end{pmatrix} \tag{4}$$

Then, the components can be extracted by performing the eigen-decomposition on Σ_V , indeed the obtained loading matrix P is column-wise orthonormal. However, this would require that we nevertheless use the huge matrix X_{VPCA}, we use a shortcut to define what we may call the positive and negative component loadings matrices, respectively, $P^+$and P^- with generic elements

$$p_{jk}^{+} = \begin{cases} p_{jk}, & if \;\; p_{jk} \geq 0 \\ 0, & otherwise \end{cases} \tag{5}$$

$$p_{jk}^{-} = \begin{cases} p_{jk}, & if \ p_{jk} \leq 0 \\ 0, & otherwise \end{cases} \qquad (6).$$

Where p_{jk} gives the loading of variable j on component k. In matrix notation, the bounds of the component scores matrix are given by:

$$\begin{cases} \underline{t}(k) = \overline{X}(k)P^{-} + \underline{X}(k)P^{+} \\ \overline{t}(k) = \overline{X}(k)P^{+} + \underline{X}(k)P^{-} \end{cases} \qquad (7)$$

Thus, it can be seen that score matrices were computed without explicitly having to compute all the component scores for all the vertices. It follows that this computational approach to VPCA finds the same component loadings and the same segments for the observation units, as the original computational approach to VPCA. We only lose the component scores of all individual vertices, but not of the segments that enclose them. Estimates of interval measurements are also computed as mentioned before

$$\hat{X}_{VPCA} = T_{VPCA}\, P^{T} \qquad (8)$$

The estimated interval-valued measurements for the principal components are then computed as:

$$\begin{cases} \underline{\hat{x}}_j(k) = \underline{t}(k)P^{-} \\ \overline{\hat{x}}_j(k) = \overline{t}(k)P^{+} \end{cases} \qquad (9)$$

3. THE PROPOSED METHOD KERNEL VERTICES PCA (K-VPCA)

Let X *be* a training data matrix of n samples (or observations) and m variables (or features). That is $X \in R^{nxm}$, where

$$X = [X_1, X_2, \ldots, X_n]^T \qquad (10).$$

These data points are mapped to a higher-dimensional feature space

$$\Phi : \ X_i \in \mathcal{R}^m \rightarrow \Phi\,(X_i) = \ \Phi_i \in \mathcal{F} \qquad (11)$$

Note that the feature space F has an arbitrarily large, possibly infinite, dimensionality equal to $\mathcal{H}$ [7]. An essential property of the feature space is the dot product of two vectors, $\Phi\ (x_i)$ and $\Phi\ (x_i)$, i, j = 1, . . . n. It is calculated as follows:

$$\phi(x_i)^T.\phi(x_j) = \mathbf{k}(x_i,\ x_J) \qquad (12)$$

where **k** is the kernel function. In the literature, several core functions have been presented, the most common of which is the radial basis function (RBF), which is provided by the following:

$$k(x_i,\ x_J) = exp[\frac{-|x_i - x_J|}{2\sigma^2}] \qquad (13)$$

where σ is the width of a Gaussian function that controls the flexibility of the kernel. A common choice for σ is the average minimum distance (d) between two points in the training data set.

The suggested method's fundamental idea is to map data into a feature space via a nonlinear mapping, and then execute a linear interval-valued VPCA in feature space. The flow chart of Fig. 1 explains the procedure of the work.

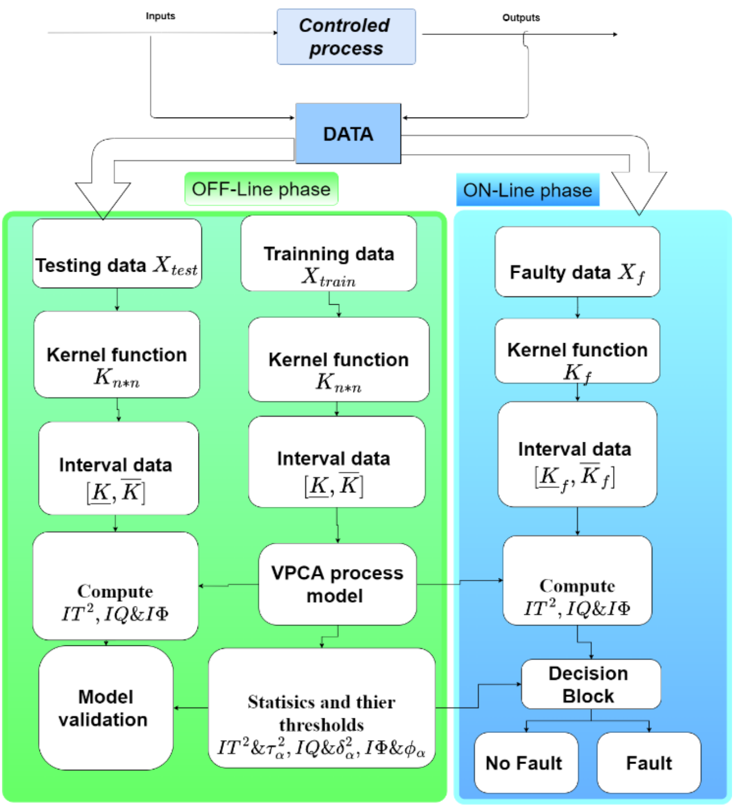

Figure 1. K-VPCA flowchart.

4. FAULT DETECTION USING K-VPCA METHOD

In this part, we present numerous fault detection indices based on K-VPCA for interval-valued data approaches to obtain the highest degree of robustness against uncertainty. In multivariate fault detection using a KPCA model, many statistics that quantify variances in distinct projection subspaces are utilized. The most often used fault indicators are T^2 and SPE (Q-statistic).

4.1. Interval-valued indices

The interval $[T^2]$ statistic is computed for the first interval principal components using a combination of interval eigenvalues and interval principal components as follows:

$$\begin{cases} \underline{T}^2(k) = \underline{\hat{t}}^T(k)\Delta_l^{-1}\underline{\hat{t}}(k) \\ \overline{T}^2(k) = \overline{\hat{t}}^T(k)\Delta_l^{-1}\overline{\hat{t}}(k) \end{cases} \tag{14}$$

For the interval-valued case, the Q statistic is computed as in the classical case, providing an interval [SPE] ([Q]) with upper and lower limits that correspond to the upper and lower bounds of the estimated residuals, as follows:

$$\begin{cases} \underline{Q} = \|\underline{e}(k)\|^2 = \underline{e}^T(k)\underline{e}(k) \\ \overline{Q} = \|\overline{e}(k)\|^2 = \overline{e}^T(k)\overline{e}(k) \end{cases} \tag{15}$$

Given that $\underline{e}(k) = [\underline{e}_1(k), \ldots, \underline{e}_m(k)]$, $\overline{e}(k) = [\overline{e}_1(k), \ldots, \overline{e}_m(k)]$.

4.2 The interval fault detection index

The interval fault detection index was developed owing to the ambiguity in fault detection decisions due to the interval structure of statistics presented above. When each bound draws a different conclusion about the appearance of faults [13]. The interval fault detection index presented here is denoted by the interval square prediction error (IQ), which is defined as:

$$IQ(k) = ||[e(k)]||^2 = \sum_{j=1}^{m}\|[e_j(k)]\|^2 \tag{16}$$

Where

$$||[e(k)]||^2 = \underline{e}_j^2(k) + \underline{e}_j(k)\overline{e}_j\ (k) + \overline{e}_j^2(k)) \quad (17).$$

Similarly, the interval Hotelling T^2 statistic (IT^2) is computed as follows:

$$IT^2\ (k) = \left\| \frac{[\hat{t}(k)]}{[\Delta_l]^{\frac{1}{2}}} \right\| \quad (18)$$

The combined index, Φ, is evaluated as a combination of the principal subspace indicator, T^2, and the residual subspace indicator, SPE (Q). For interval data, the interval Φ depends on both T^2 and $[Q]$ as described by the following equation:

$$\begin{cases} \underline{\phi} = \frac{\underline{T}^2}{\overline{\tau}_\alpha^2} + \frac{\underline{Q}}{\overline{\delta}_\alpha^2} \\ \overline{\phi} = \frac{\overline{T}^2}{\underline{\tau}_\alpha^2} + \frac{\overline{Q}}{\underline{\delta}_\alpha^2} \end{cases} \quad (19)$$

The new interval statistic $I\Phi$ also based on the combined interval fault detection indices IT^2 & IQ could be calculated as follows:

$$I\Phi = \frac{IT^2(k)}{\tau_\alpha^2} + \frac{IQ(k)}{\delta_\alpha^2} \quad (20)$$

where τ_α^2 and δ_α^2 are the threshold of $IT^2\ (k)$ and $IQ\ (k)$ respectively.

5. APPLICATION ON CEMENT ROTARY KILN

This section provides an overview of the cement plant process and describes the signals employed for fault detection. Additionally, it details the fault detection methodology by specifying the types and sizes of datasets collected for the development and evaluation of the monitoring methods' performance

5.1 *Process description*

The rotary kiln plays a pivotal role in cement production and comprises several key components, including the head-sealing device, tail-sealing device, and hood. During normal operation, the kiln is driven by a primary motor through a reducer, which powers a large gear ring attached to the cylinder near the kiln tail via a spring plate. Raw materials are fed into the kiln from the top and transported through the rotating chamber to the opposite end, where they undergo high-temperature decomposition. In indirect-fired rotary kilns, heat is supplied by an external burner, whereas in indirect-fired kilns, the heat source is located within the chamber, maintaining the integrity of the raw materials. The rotation speed and temperature of the cylinder are adjusted to accommodate different materials and operational requirements. After calcination, the clinker undergoes initial cooling within the chamber before being transferred to the cooler for further cooling. Detailed descriptions of the various process variables can be found in [4].

5.2 Application of the Proposed Monitoring Scheme

The proposed K-VPCA technique is applied to monitor industrial cement production in this part. 44 sensors are used to monitor the process. These variables were picked from a pool of 55 to build a strong monitoring strategy and evaluate its detection capacity based on data from process computers in real time. Because standard PCA and its interval variants are already noise separation techniques, preprocessing or filtering the data is unnecessary.

The software used in the simulation was MATLAB. The data utilized in this article are of two types:

1) A healthy dataset which are divided into training (11000 samples), and testing (768 samples) data.
2) A faulty dataset that contains an actual involuntary process fault. It consists of 2084 samples.

The flowchart in fig 1 explains the steps that have been done.

After transforming the interval data into single-valued data, the PCA model is constructed based on the Cumulative Percentage of Variance (CPV) rule. The performance of the proposed technique is evaluated using several metrics:

- False Alarm Rate (FAR): This metric is calculated as:

$$FAR = 100 \times \frac{N_{h,f}}{N_h}\%.$$

where $N_{h,f}$ represents the number of samples exceeding the threshold while the system is healthy, and N_h is the total number of healthy samples.

- Missed Detection Rate (MDR): This metric is calculated as:

$$MDR = 100 \times \frac{N_{f,f}}{N_f}\%.$$

where $N_{f,f}$ is the number of samples below the threshold while the system is faulty, and N_f is the total number of faulty samples.

- Fault Detection Time Delay (DTD):

$$\text{DTD} = t_d - t_o.$$

DTD is the number of samples while the system is faulty before it exceeds its threshold, t_d and t_o are the detection time and occurrence time of a fault, respectively.

Table 1 compares the False Alarm Rate (FAR) for T^2, Q and Φ statistics across PCA, VPCA, and K-VPCA methods for training and testing datasets. In the training set, PCA exhibits a FAR of 10% for all metrics, whereas VPCA and K-VPCA consistently achieve a lower FAR of 5%, indicating greater reliability in handling training data. For the testing set, PCA shows significant variability, with a low FAR for T^2, (5.07%) but much higher values for Q (18.7%) and Φ (12.5%), highlighting its sensitivity to uncertainty. In contrast, VPCA demonstrates consistent and reduced FAR values (T^2 = 6.07%, Q = 6.00%, Φ = 6.04%), showcasing improved robustness. K-VPCA further enhances performance, achieving the lowest FAR across all metrics (T^2= 5.55%, Q = 6.00%, Φ = 5.33%), particularly reducing false alarms in Φ. Overall, the results establish K-VPCA as the most robust and reliable method for fault detection in uncertain nonlinear systems.

Table 1. FAR % contributed by T 2, Q and Φ statistics, for the training and testing sets.

Data Set	Training Set			Testing Set		
Statistics	T^2	Q	Φ	T^2	Q	Φ
PCA [12]	10.0	10.0	10.0	5.07	18.7	12.5
VPCA [12]	5.00	5.00	5.00	6.07	6.00	6.04
K-VPCA	5.00	5.00	5.00	5.55	6.00	5.33

5.2 Real process fault detection

Table II presents the False Alarm Rate (FAR), Missed Detection Rate (MDR), and Detection Time Delay (DTD) for the faulty dataset based on three statistical indices (T 2, Q, and Φ) across PCA, VPCA, and K-VPCA methods. PCA shows a high FAR, particularly for Q (94.8%) and Φ (98.4%), with T^2 also contributing significantly (30%), indicating frequent false alarms. Additionally, PCA has an MDR and DTD of zero across all indices, suggesting it fails to detect faults effectively. VPCA reduces FAR substantially, with T^2 and Φ achieving zero, but exhibits an MDR of 61.2% for Q and a high DTD for Q (115) and T^2 (15), indicating delayed and missed fault detections in some cases.

Table 2. FAR, MDR & DTD of the faulty dataset contributed by the three statistic indices.

Data Set	FAR			MDR			DTD		
Statistics	T^2	Q	Φ	T^2	Q	Φ	T^2	Q	Φ
PCA [12]	30.0	94.8	98.4	0.00	0.00	0.00	0.00	**0.00**	**0.00**
VPCA [12]	0.00	6.22	0.00	1.40	61.2	0.00	15.0	**115**	20.0
K-VPCA	5.00	5.00	5.00	5.55	6.00	5.33	0.00	**26.0**	**0.00**

K-VPCA achieves the best balance, with minimal FAR (Q = 0.00%), reduced MDR (Q = 2.14%), and significantly lower DTD compared to VPCA, particularly for Q (26). Overall, K-VPCA demonstrates superior fault detection performance with fewer false alarms, improved detection accuracy, and faster response times, making it the most robust method among the three. Concerning the data of the real fault, Fig. 2, shows the result of the proposed interval approach K-VPCA method where the first 450 samples are healthy; the remaining ones are related to the real fault.

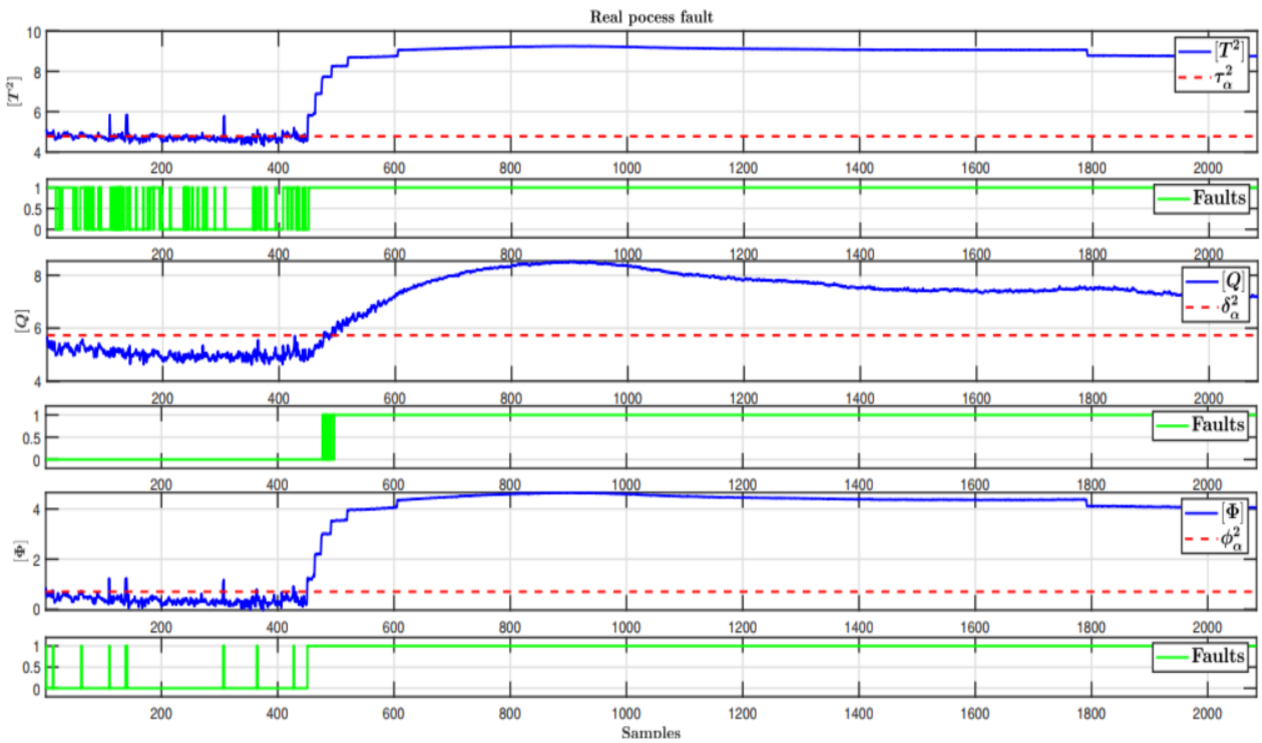

Figure 2. $\boldsymbol{T}^{2}$, Q, and Φ monitoring results of the faulty process operation, using the proposed K-VPCA method.

4. Conclusion

The interval nature of the projections ensures that approximation errors are eliminated during the fault identification and isolation process. This study introduces a novel data-driven approach for detecting faults in uncertain nonlinear processes. By incorporating sensor data and uncertainties through interval representation, interval-valued methods provide a robust strategy for fault detection and isolation (FDI). The objective was to evaluate the applicability and reliability of VPCA for

fault identification in nonlinear systems, utilizing data from a cement rotary kiln. The results demonstrated the effectiveness of the proposed K-VPCA technique compared to interval VPCA and traditional PCA approaches. This research aims to establish an efficient interval diagnosis methodology that addresses the limitations of existing interval-based methods.

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