Amalgamation of anomaly-detection indices for enhanced process monitoring

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Abstract
Accurate and effective anomaly detection and diagnosis of modern industrial systems are crucial for ensuring reliability and safety and for maintaining desired product quality. Anomaly detection based on principal component analysis (PCA) has been studied intensively and largely applied to multivariate processes with highly cross-correlated process variables; however conventional PCA-based methods often fail to detect small or moderate anomalies. In this paper, the proposed approach integrates two popular process-monitoring detection tools, the conventional PCA-based monitoring indices Hotelling’s $T^2$ and $Q$ and the exponentially weighted moving average (EWMA). We develop two EWMA tools based on the $Q$ and $T^2$ statistics, $T^2$-EWMA and $Q$-EWMA, to detect anomalies in the process mean. The performances of the proposed methods were compared with that of conventional PCA-based anomaly-detection methods by applying each method to two examples: a synthetic data set and experimental data collected from a flow heating system. The results clearly show the benefits and effectiveness of the proposed methods over conventional PCA-based methods.

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1. Introduction

1.1. The state of the art

Identifying anomalies in modern automate process is central to process safety and maintaining product quality. Because anomalies in complex processes are common and some can be the source of serious degradations, their early detection is desirable. Accurate and effective anomaly detection and diagnosis of modern engineering systems are crucial for ensuring reliability and safety and for maintaining desired product quality; most importantly detection may prevent disasters in the cases of equipment failure. Early anomaly detection is favorable for reducing operational and maintenance costs and system down-time, while increasing levels of safety. The purpose of anomaly detection is to identify any event in the process behavior that is deviation from its nominal behavior (Isermann, 2006).

Early and accurate anomaly detection is important for increasing process safety and for limiting losses caused by abnormal and faulty states. The operation of a plant or a process has motivated the various anomaly detection and diagnosis methodologies proposed in the literature (Serpas et al., 2013; Venkatasubramanian et al., 2003a, c; Qin, 2012). These techniques can be broadly classified into three main categories: (i) data-based or model-free techniques, (ii) model-based techniques and (iii) knowledge-based techniques. Knowledge-based anomaly detection is usually a heuristic process (Venkatasubramanian et al., 2003a). Techniques in this category are mostly based on causal analysis, expert systems (Kim et al., 2005), possible cause and effect graphs (Wilcox and Himmelblau, 1994), failure modes and effects analysis (Wirth et al., 1996), hazard and operability analysis (Venkatasubramanian et al., 2003b) or Bayesian networks (Verron et al., 2008). These methods are best suited to small-scale systems with a small number of variables, and thus may not be appropriate for monitoring complex processes. Model-based monitoring methods compare process-measured variables with information obtained from a mathematical model, which is usually developed based on some fundamental understanding of the process under fault-free conditions (Gertler, 1998; Staroswiecki, 2001). This approach relies on the concept of analytical redundancy (Kinjaert, 2003). More specifically, after a model is developed, it is
used to compute the process residuals, which are then evaluated to detect the presence of anomalies. The residuals, which are the difference between the measurements and the model prediction, can be used as an indicator of the presence or absence of anomalies in a monitored process (Kinnaert, 2003; Staroswiecki, 2001). When the monitored process is under normal operating conditions (no anomaly), the residual is zero or close to zero in cases of modeling uncertainties and measurement noise. When an anomaly occurs, the residuals deviate significantly from zero, indicating the presence of a new condition that is significantly distinguishable from the normal faultless working mode (Kinnaert, 2003; Harrou et al., 2014). The model-based anomaly-detection approaches include observer-based approaches (Kinnaert, 2003), parity-space approaches (Staroswiecki, 2001) and interval approaches (Benothman et al., 2007). Naturally, the effectiveness of these monitoring methods depends on the accuracy of the models used; however, deriving accurate models of monitored systems can be difficult, especially for complex processes. In addition, anomalies that have not been considered in the modeling stage may not be detected at all. Consequently, this problem, data-based anomaly-detection techniques are more commonly used.

Data-based monitoring methods, also known as process-history-based methods or black-box methods (Venkatasubramanian et al., 2003c), use the process data collected during normal operating conditions to build an empirical model that describes the nominal behavior of the process. This model is then used estimate true value of new measurements and evaluate the estimated residuals to detect and diagnose anomalies in future data (Venkatasubramanian et al., 2003c). Normally, the data-based anomaly-detection approach involves three steps: 1) model training, 2) residual generation and 3) residual evaluation. This approach uses information derived directly from input data and requires no explicit models for which development is usually costly or time consuming. Therefore, data-based methods are more attractive for practical applications to complex systems, although their performance mainly depends on the availability of an adequate amount of quality for different input data. Because each of these monitoring methods has advantages and disadvantages for different problems, the problem will determine which method is most suitable. This work focuses on the use of data-based methods for anomaly detection.

The data-based anomaly-detection techniques referenced in the bibliography can be broadly categorized into two main classes: univariate and multivariate techniques (Montgomery, 2005). Univariate statistical monitoring methods such as, the EWMA (exponentially weighted moving average) chart and CUSUM (cumulative sum) chart, are used to monitor essentially only one process variable (Harrou and Nounou, 2014). However, because modern industrial processes often present a large number of highly correlated process variables, univariate anomaly-detection methods are unable to explain different aspects of the process and, therefore, are not appropriate for modern day processes. Thus, multivariate statistical monitoring methods, which take into account correlation between process variables have developed to monitor several different process variables simultaneously. Multivariate data-based monitoring methods include latent variable methods, (e.g., partial least-squares regression (Harrou et al., 2015), principal component analysis (PCA) (Harrou et al., 2013), canonical variate analysis, independent component analysis (Chiang et al., 2001), neural networks (Neumann and Deerberg, 1999), and support vector machine based methods (Dehestani et al., 2011)). Data-based monitoring methods, especially those that utilize PCA or its extensions, have been applied across a wide range of industries, for example in the chemical industry (Singhal et al., 1997), for water treatment (George et al., 2009), and in ecological studies (Jankevics and Novák, 2012).

Data-based process monitoring using PCA, a well-known multivariate statistical method, has received considerable attention in the last few years (Qin, 2012; Harrou et al., 2013). PCA is a linear dimensionality reduction modeling technique that is very helpful when dealing with data sets that have a high degree of cross correlation among variables. The central idea of PCA is to reduce the dimensionality of highly correlated data, while retaining the maximum possible amount of variability present in the original data set (MacGregor and Kourti, 1995). This reduction is achieved by transforming correlated variables into a set of new uncorrelated variables, which are called principal components (PCs), each of which is a linear combination of the original variables. By reducing the dimension of the process variables, PCA is able to eliminate noise and retain only important process information; it can be employed to compress noisy and correlated measurements into a smaller informative subspace for measurement data sets. PCA-based anomaly detection is popular for use in practice because no prior knowledge about the process model is necessary and a good historical database describing the normal process operation is the only information needed.

1.2. Motivation and contribution

Detecting small or incipient anomalies in highly correlated input–output multivariate data is one of the most crucial and challenging tasks in the area of anomaly detection and diagnosis. Indeed, detection of small anomalies can provide an early warning and help to avoid catastrophic damage and subsequent financial loss. Unfortunately, conventional PCA-based monitoring indices, such as \( T^2 \) and \( Q \) statistics, often fail to detect small or moderate
changes. Although univariate, the EWMA chart has the capacity to
detected smaller faults in the mean process than conventional PCA-
based methods. We selected this combination of monitoring pro-
cesses to marry the multivariate PCA with the more sensitive fault
detection of EWMA to create the amalgamate $T^2$-EWMA and Q-
EWMA detectors. These new detectors are expected to provide
better anomaly detection in the process mean at multivariate data
sets by reducing the rate of missed detections and false alarms that
are associated with PCA monitoring methods.

The following section briefly reviews how PCA anomaly detec-
tion is performed, and Section 3 introduces the EWMA monitoring
chart and its use in anomaly detection. Next, the concept of
marring the two is presented in Section 4. In Section 5, the per-
fomances of the proposed methods are illustrated through two
simulated examples, one using synthetic data and the other using
flow heating system data. Finally, Section 6 concludes this study,
paving the way for future research.

2. PCA based statistical monitoring

PCA is a linear dimensionality reduction modeling method that
can be helpful when handling data with a high degree of cross
relation among variables. PCA is based on the eigenvalue anal-
ysis to orthogonalize the components of the input vector so that
they are uncorrelated with each other. The PCA method is
becoming increasingly popular in process industries due to its
ability to reduce dimensionality. The main idea behind PCA is
briefly introduced in this section and more details can be found in
(MacGregor and Kourti, 1995).

2.1. PCA modeling

Let us consider the following raw data matrix

$$
X = [x_1, \ldots, x_n]^T \in \mathbb{R}^{n \times m}
$$

consisting of $n$ observations and $m$ corre-
lated variables. Data are collected when the monitored process is
under normal operating conditions so that the PCA can build a
model that represents a reference of normal process behavior.
Before computing the PCA model, the raw data matrix $X$ is usually
pre-processed by scaling every variable to have zero mean and unit
variance. This is because variables are measured with various
means and standard deviations in different units. This
pre-processing step puts all variables on an equal basis for analysis
(Ralston et al., 2001). Let $X_s$ denote the autoscaled matrix of $X$.
Using singular value decomposition, PCA transforms the data ma-
trix $X_s$ into a new matrix $T = [t_1, t_2, \ldots, t_m] \in \mathbb{R}^{m \times m}$ of uncorrelated
variables called score or PCs. Each new variable is a linear combi-
nation of the original variables, such that $T$ is obtained from $X_s$ by
an orthogonal transformations (rotations) designed by

$$
P = [p_1, p_2, \ldots, p_m] \in \mathbb{R}^{m \times m}
$$

which is given as the following:

$$
T = X_s P
$$

where the column vectors $p_i \in \mathbb{R}^m$ of the matrix $P \in \mathbb{R}^{m \times m}$ (also
known as the loading vectors) are formed by the eigenvectors
associated with the covariance matrix of $X_s$, (i.e., $\Sigma$). The covariance
matrix, $\Sigma$, is defined as follows:

$$
\Sigma = \frac{1}{n-1}X_s^T X_s = P \Lambda P^T \text{ with } PP^T = P^T P = I_n,
$$

where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_m)$ is a diagonal matrix containing the ei-
genvalues in a decreasing order ($\lambda_1 > \lambda_2 > \cdots > \lambda_m$) and $I_n$ is the
identity matrix (Jackson and Mudholkar, 1979).

In the case of collinear processes, the dimensionality reduc-
tion of the $m$-dimensional space is obtained by retaining only the first ($l$)
largest principal components which are corresponding to the
largest eigenvalues of the covariance matrix. The first ($l$) largest
principal components normally describe the most of the variance of the
data (Fig. 1). On the other hand, the smallest principal com-
ponents are considered as a noise contributor. An important step
in the building of a PCA model is to determine the number of PCs, $l$,
that are required to adequately capture the major variability in the
data sets. Various techniques have been proposed to select the
number of PCs including a Scree plot (Zhu and Ghodsi, 2006), cu-
nulative percent variance (CPV), parallel analysis, sequential tests,
resampling, profile likelihood (Zhu and Ghodsi, 2006; Jolliffe, 2002)
and cross validation (Li et al., 2002). In this study, the CPV technique
will be used to determine the number of PCs in the PCA model. The
CPV is defined as,

$$
CPV(l) = \frac{\sum_{i=1}^{l} \lambda_i}{\sum_{i=1}^{m} \lambda_i} \times 100.
$$

Once the number of PCs, $l$, is determined, the data matrix $X_s$ can
be represented using the PCA as the sum of two orthogonal parts:
an approximated data matrix $\hat{X}$ and a residual data matrix $E$; that is

$$
X_s = \hat{X} + E,
$$

where $T \in \mathbb{R}^{n \times l}$ and $E \in \mathbb{R}^{n \times (m-l)}$ are matrices containing the $l$
retained and the $(m-l)$ ignored PCs, respectively, and $\hat{X} \in \mathbb{R}^{l \times l}$ and
$E \in \mathbb{R}^{m \times (m-l)}$ are matrices containing the $l$ retained eigenvectors and
the $(m-l)$ ignored eigenvectors, respectively (Jackson and
Mudholkar, 1979).

2.2. Anomaly detection with PCA

In PCA-based process monitoring, first the PCA creates a refer-
ence model using the fault-free data collected from the normal
process. Any new process behavior can now be compared with the
predefined one by the monitoring system to that any changes to
normal operating conditions are noted. When an anomaly occurs,
the process moves out of the normal operation regions indicating
that a change in the process behaviors has occurred. Typically, the
Hotelling $T^2$ statistic (Hotelling, 1933) and the sum of squared

Fig. 1. Principle of PCA.
prediction error (Box, 1954), which is also known as the Q statistic (Romagnoli and Palazoglu, 2006), are used in PCA-based monitoring to elucidate the pattern variations in the model and residual subspaces, respectively. The $T^2$ statistic is defined by the Mahalanobis distance, whereas the Q statistic is defined by the Euclidean distance to avoid ill-conditioning due to small eigenvalues (Qin, 2003) (see Fig. 2). The $T^2$ statistic is used to detect anomalies associated with abnormal variations within a PC’s subspace. The PCA-based $T^2$ chart based on the first I PCs is defined as (Hotelling, 1933):

$$T^2 = \sum_{i=1}^{I} \frac{t_i^2}{\lambda_i}$$

(5)

where $\lambda_i$ is the $i$th eigenvalue of the covariance matrix $\Sigma$. For new testing data, when the value of $T^2$ exceeds the value of the threshold, $T_{null}^2$, given in (Hotelling, 1933), an anomaly is declared.

Meanwhile, the Q statistic indicates how well each sample conforms to the model, measured by the projection of a data sample on the residual subspace (see Fig. 2), which is defined as (Qin, 2003):

$$Q = \left\| (P^T) x_i \right\|^2$$

(6)

Accordingly, the Q statistic indicates whether the current model is valid or not. When a vector of new data is available, the Q statistic is calculated and compared with the threshold value $Q_e$, given in (Jackson and Mudholkar, 1979). A fault is detected if the Q statistic exceeds $Q_e$. These confidence limits are calculated based on the assumptions that measurements are time independent, multivariate and normally distributed.

The main disadvantage of using PCs in process monitoring is the lack of physical interpretation (Kourti and MacGregor, 1996). In addition, in a previous study (Romagnoli and Palazoglu, 2006), showed that the $T^2$ statistic can result in false negatives (missed detection) due to the latent space sometimes being insensitive to small process upsets, which is because each latent variable is a combination of all process variables. A specific disadvantage of the $T^2$ statistic is that anomalies in the process mean that are orthogonal to the first PCs are not detected (Mastrandrello et al., 1996). The Q statistic, however, is more sensitive to additive anomalies than the $T^2$ statistic because additive anomalies propagate to the model error. The Q statistic is more sensitive to modeling errors and its performance largely depends on the choice of the number of retained PCs (Mastrangelo et al., 1996). If an incorrect number of PCs is chosen to be used in the model, may residuals be autocorrelated, which will affect the confidence limits for the Q test. In the illustrative examples presented later in Section (5), $T^2$ and Q statistics are used as benchmark for anomaly detection using PCA. To improve the performance of these conventional PCA-based detection methods, we develop an alternative anomaly-detection approach with PCA as the modeling framework for anomaly detection using an EWMA based on the conventional PCA metric, $T^2$-EWMA or Q-EWMA. More details about the EWMA and how it can be used in anomaly detection are presented next.

3. EWMA statistical control scheme

The aim of statistical process control is to monitor a process to detect abnormal behavior. Statistical control charts (also referred to as monitoring charts) are one of the most commonly used tools in SPC and have been extensively used in quality engineering as a monitoring tool to detect the presence of possible anomalies in the mean or variance of process measurements (Montgomery, 2005). Control charts play a crucial role in detecting whether a process is still working under normal operating conditions (usually termed in-control) or not (out-of-control) (Montgomery, 2005). Numerous control charts have been developed to monitor the mean of a process variable over time, including the Shewhart chart, the CUSUM chart (Page, 1954) and the EWMA chart (Hunter, 1986; Kadi et al., 2016). Shewhart control charts, the first method proposed to test the hypothesis, are very popular in statistical process control and can be effectively used to detect large shifts in the process mean (Human et al., 2010). A key disadvantage of Shewhart charts, however, is that they only use the last data sample of an inspected process and do not carry a memory of the previous data (i.e., ignore any potential information contained in past samples) (Montgomery, 2005). These shortcomings motivate the use of other alternatives, such as EWMA and CUSUM charts, which are better suited to detecting smaller shifts in the process mean (Montgomery, 2005). This is because CUSUM and EWMA charts take into account the information contained in the entire process history. The CUSUM chart gives equal weights to the entire process history of the observations when it accumulates all useful information as historical data (Hawkins and Olwell, 1998). However, since EWMA uses a weighted average of all past and current observations, it is a lot less sensitive to violating the normality assumption than are CUSUM charts (Lucas and Saccucci, 1990). Also, CUSUM is relatively slow to respond to large shifts. Therefore, EWMA-based charts are an appropriate monitoring scheme to be adopted when dealing with individual observations (Hunter, 1986; Montgomery, 2005). According to the literature, EWMA is one of the most frequently used control charts for process monitoring because of its flexibility and sensitivity to small shifts (Montgomery, 2005).

The EWMA control scheme was first introduced by Roberts (Roberts, 1959) and has since been used extensively in time series analysis. In the EWMA control scheme, the moving average is calculated by multiplying the historical observations by a weight that decays exponentially with time (Montgomery, 2005). The EWMA decision statistic is described by the following recursive formula:

$$z_t = \gamma x_t + (1 - \gamma) z_{t-1}$$

(7)

where $\gamma$ is a weighted parameter, with $0 < \gamma \leq 1$, and $x_t$ is the value of the supervised variable at time $t$. The starting value $x_0$ is set equal to the process in-control mean, $\mu_0$. Generally, smaller values of $\gamma$ increase the chart’s sensitivity to smaller shifts in the process mean, while larger values of $\gamma$ increase its sensitivity to larger shifts (Lucas and Saccucci, 1990). The standard deviation of $z_t$ is defined as $\sigma_{z} = \sigma_0 \sqrt{\frac{\gamma (2 - \gamma) [1 - (1 - \gamma)^{2t}]}{\gamma - 1}}$, where $\sigma_0$ is the standard deviation of the fault-free or preliminary data set. The EWMA control scheme declares an anomaly when the value of $z_t$ falls outside of the interval between the control limits. The upper and lower control limits, UCL and LCL, are set as (Montgomery, 2005):
In this section, three statistics are combined for anomaly detection: \( T^2 \), \( Q \), and EWMA charts. \( T^2 \) and \( Q \) are multivariate statistics, while EWMA is univariate statistic. Although all have been widely used historically in process monitoring of industrial quality control applications (Montgomery, 2005). Unlike all the snapshot Shewhart-type monitoring charts, such as the \( T^2 \) or \( Q \) statistics, the EWMA control chart has the advantage of considering the information contained in the entire process history and has shown a greater sensitivity for detecting small changes. However, it can only be used to monitor single variables. Thus, the main goal of this paper is to merge the advantages of conventional PCA-based monitoring statistics and EWMA charts to enhance their performances and widen their practical applicability. The current study proposes the use of a version that comprises these three statistics. More specifically, in this work, EWMA is used to enhance process monitoring through its integration with conventional PCA-based monitoring statistics. PCA is used to represent a matrix of the system measurements as the sum of two orthogonal parts (an approximated data matrix and a residual data matrix), as shown in Equation (4). Detection of possibility of an anomaly occurring in the monitored process is further achieved through the amalgamated EWMA monitoring charts, \( T^2 \)-EWMA and \( Q \)-EWMA, by applying them to the PCs and residuals, respectively, as a basis for multivariate statistic. The \( T^2 \)-based EWMA statistic is used to monitor the space spanned by the retained components, while the \( Q \)-based EWMA statistic is used to monitor the space spanned by those components not included in the established model. This work proposes an amalgamation of the conventional \( T^2 \), \( Q \) and EWMA schemes by exploiting the advantages, the features of their design of each, as described in the following section.

### 4.1. The amalgamated \( T^2 \)-EWMA monitoring scheme

In this approach, the EWMA control scheme is applied on the computed PCA-based \( T^2 \) statistic. The \( T^2 \) statistic measures the variations in the PCs at different time samples. \( T^2 \) is defined in Equation (5). If the vector of \( T^2 \) measurements is defined as \( T^2 = [t^2_1, \ldots, t^2_2, \ldots, t^2_n] \), then the EWMA decision function can be computed using the \( T^2 \) measurements as follows:

\[
 z_{t, j}^{T^2} = \gamma t_{j}^{T^2} + (1 - \gamma)z_{t-1, j}, \quad j \in [1, n].
\]

This approach can only detect the presence of faults not their locations.

### 4.2. The amalgamated \( Q \)-EWMA monitoring scheme

In this subsection, a brief description of the \( Q \)-EWMA monitoring chart is introduced. The EWMA scheme is applied using \( Q = [q_1, \ldots, q_{[0, \ldots, q_n]} \) measurements, which is defined in Equation (6). Then, the \( Q \)-EWMA decision function can be computed as follows:

\[
 z_{t, j}^{Q} = \gamma q_t + (1 - \gamma)z_{t-1, j}, \quad t \in [1, n].
\]
where, $\varepsilon_i$ represents measurement errors, that follow a zero-mean Gaussian distribution with a standard deviation of 0.095. The variables $u_1$ and $u_2$ represent a pseudo-random binary sequence and a quad-chirp signal (sinusoidal waveform with quadratically increasing frequency), respectively. The above model is used to simulate 500 fault-free training data samples. These data, which are shown in Fig. 4, are scaled (for zero mean and unit variance) and then used to develop a PCA model.

\begin{align}
    x_1 &= u_1 + \varepsilon_1, \\
    x_2 &= u_1 + \varepsilon_2, \\
    x_3 &= u_2 + \varepsilon_3, \\
    x_4 &= 2x_1 + 2x_2 + \varepsilon_4, \\
\end{align}

(10)

5.1.2. Training the PCA model

The scaled fault-free training data matrix is used to construct a PCA model. In PCA, most of the important variations in the data are usually captured by the few PCs that correspond to the largest eigenvalues. An important issue in PCA model building is the selection of the number of retained PCs. Using a CPV threshold value of 90%, only the first two PCs were retained, capturing 72% and 27% of the total variations in the data as shown in Fig. 5.

After building of PCA model, two case studies were performed to evaluate the performance of the anomaly-detection charts: one with a single additive anomaly and the other with multiple additive anomalies. We also conducted the same tests for the conventional PCA method and compared the results. These simulated case studies with known anomalies are helpful because they allow theoretical comparisons between the various techniques. Rates of false alarm and missed detection were used to evaluate the performance of the monitoring charts; from a practical point of view these are important detection performance criteria. A false alarm is an indication of an anomaly when no anomaly has occurred, while missed detection denotes that faulty data were misclassified as faultless data. Missed detection rate (MDR) is the number of faulty data points that do not exceed the control limits (missed detection) over the total number of faulty data points.

\begin{align}
    \text{MDR} &= \frac{\text{missed detection}}{\text{faulty data}} \times 100 \%. \\
    \text{FAR} &= \frac{\text{false alarms}}{\text{faultless data}} \times 100 %. \\
\end{align}

(11) (12)

The smaller values of the miss detection and false alarm rates show the better performance of the corresponding monitoring chart.

Fig. 3. A schematic diagram of the proposed anomaly-detection algorithms.

Fig. 4. A sample training fault-free data set used in the synthetic example.

Fig. 5. Fraction of variance captured by each principal component of the synthetic data.
5.1.3. Simulation results

5.1.3.1. Case A: single-bias anomaly. In this case study, we investigated the problem of detecting single-bias anomalies, by building a PCA model with historical normal data is used for anomaly detection. The testing data, comprising 150 samples were separate from the fault-free training data, were simulated using Equations in (10). This data set was first scaled with the mean and standard deviation of the training data. After deciding on the number of PCs, \( T_a^2 \) and \( Q_a \) with a 95% confidence limit were calculated at \( T_a^2 = 6.05 \) and \( Q_a = 0.01 \). Two examples are presented here to assess the ability of \( T^2 \)-EWMA and Q-EWMA to detect bias anomaly. In the first example, we added the anomaly to the variable \( x_3 \) between samples 50 and 70. This anomaly is a constant bias of amplitude equal to 50% of the total variation in \( x_3 \). The results of \( T^2 \) and Q monitoring indices based on the testing data are shown in Fig. 6a and b, respectively. The red dashed lines represent the 95% confidence limit used to identify possible anomalies, and the green-shaded area represents the zone where the anomaly is introduced to the testing data. The red crosses in each plot denote the presence of false alarms. For this anomaly. This result may be explained by the fact that the \( Q \) statistic fails to detect a few faults. Thus, the Q statistic is a better detector for this anomaly. This result may be explained by the fact that the \( T^2 \) statistic provides a measure of the deviation in the PCs that are of greatest importance to the operation of normal processes. The normal operating region defined by the \( T^2 \) confidence limits is thus usually larger than that defined by the Q control limits. Therefore, anomalies with moderate amplitudes can easily exceed the Q threshold but not the \( T^2 \) threshold, which means that typically the Q statistic will be more sensitive for this type of anomaly. Fig. 6c and d depict the \( T^2 \)-EWMA and Q-EWMA plots of the testing data, respectively. The parameters of the EWMA are the same: the smoothing parameter, \( \gamma = 0.25 \), and the control limit width, \( L = 3 \). Fig. 6c shows that the confidence limits of \( T^2 \)-EWMA have been exceeded, which means that the anomaly has been detected, although a few faults were not detected. Fig. 6d demonstrates that the Q-EWMA violates the confidence limits, evidencing the ability of this method to correctly detect anomalies of this type without any false alarms. Note that enhanced anomaly detection can be achieved by \( T^2 \)-EWMA and Q-EWMA.

In the second example, a lower bias level of 30% of the total variation in \( x_3 \) is injected into the input variable \( x_3 \) between samples 50 and 70. Results of the \( T^2 \) statistic indicate that no anomaly was detected (Fig. 7a). Thus, the \( T^2 \) chart is completely unable to detect this simulated anomaly. Result of the Q statistic reveals that when an anomaly occurs the Q falls slightly below the control limit, resulting in a missed detection rate of 60% (Fig. 7a). Fig. 7c reveals that when an anomaly occurs, the \( T^2 \)-EWMA threshold is too high to detect the majority of anomaly resulting in several missed detections (Fig. 7c). The Q-EWMA chart in Fig. 7d detects the majority of this anomaly. The superiority of the Q-EWMA anomaly detection chart over the conventional PCA approaches is evident by comparing Fig. 7a and d. This result explains the general tendency in the literature to use the residual subspace rather than the PC’s subspace in anomaly detection. Potentially this chart gains its advantage from the memory effect of the EWMA scheme.

5.1.3.2. Case B: multiple-bias anomalies. To illustrate the performance of the developed anomaly-detection algorithms in the case of multiple anomalies, additive-bias anomalies were simultaneously introduced into variables \( x_3 \) and \( x_4 \) (each of which is represented by a bias of a magnitude equal to 10% of the variation in its corresponding variable) between samples 50 and 70. The time evolution of \( T^2 \) and Q statistics for this testing data are shown in Fig. 8a and b, respectively. Results show that neither the conventional PCA-based \( T^2 \) (Fig. 8a) or Q (Fig. 8b) were able to detect this additive anomaly; the Q index has a missed detection rate of 55%. \( T^2 \)-EWMA index was also unable to detect this anomaly (Fig. 8c), but Q-EWMA algorithm missed only a few detection (Fig. 8d) for both single and multiple-bias anomalies. These results testify to the superior performance of Q-EWMA over all other indices.

Results of the monitoring charts were evaluated by calculating the percentage of false alarms and missed detections; performances are summarized in Table 1. A reduction in missed detection confirms the efficiency advantages of Q-EWMA over the other indices, particularly in the case of multiple anomalies.

5.2. Monitoring of an air flow heating system

5.2.1. Data sources

In this section, the performance of the developed anomaly-detection methods are illustrated through their application to monitor a flow heating system, as shown in Fig. 9. Such a system comprises a duct equipped with a heating resistor and a fan. When an electrical voltage, \( U_2 \), is applied to the heating resistor, a quantity...
of heat proportional to the power supply voltage is produced. Air flow is generated by controlling the fan speed using the input voltage, \( U_f \). Three temperature sensors (platinum temperature transducers), \( s_1 \), \( s_2 \) and \( s_3 \), located at three different points are used to measure the temperature inside the duct. Fan speed is measured using a tachometer, and the measurement signals are automatically recorded by the digital logger. Over a 5.35 s, 3210 measurements of fault-free data (measurements temperature and fan speed) were collected and used to develop the reference models shown in Fig. 10a, b and d.

### 5.2.2. Development of the PCA model

In this section, the \( T^2 \)-EWMA and \( Q \)-EWMA algorithms are applied to detect single and multiple-bias sensor anomalies in the heating system described above. The performance of the developed methods is compared to that of the conventional PCA methods. As a kind of data-driven method, the empirical PCA model is determined entirely by the data collected from the system or process. The quality of the data samples directly determines the sensitivity and accuracy of the PCA model used for anomaly detection. Because it is necessary to have enough training data to capture the correlations among variables, the training data must be chosen carefully to improve the quality of the data and the sensitivity of the model. The measured data used in the training includes four variables: temperatures \( x_3 \) and \( x_4 \) between samples 50 and 70 (Case B). The horizontal dashed line denotes the control limit and the green shaded region represents the zone where the anomaly is introduced to the testing data. The red crosses in each plot denote the presence of false alarms. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

<table>
<thead>
<tr>
<th>Statistical chart</th>
<th>Case A – Example 1</th>
<th>Case A – Example 2</th>
<th>Case B</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T^2 )</td>
<td>0 100</td>
<td>0 100</td>
<td>0 100</td>
</tr>
<tr>
<td>( Q )</td>
<td>0 25</td>
<td>0 60</td>
<td>0 55</td>
</tr>
<tr>
<td>( T^2 )-EWMA</td>
<td>1.54 45</td>
<td>0 95</td>
<td>0 100</td>
</tr>
<tr>
<td>( Q )-EWMA</td>
<td>\textbf{3.85} 2.3</td>
<td>\textbf{4.65} 5</td>
<td></td>
</tr>
</tbody>
</table>

In bold: Fewer missed detection confirms the efficiency of the \( Q \)-EWMA chart over other charts.
then the eigenvalue decomposition of $\Sigma$ is performed to obtain the eigenvector matrix, $P$. In PCA models, most variations in the data are captured by a few PCs (those associated with large eigenvalues), while the remaining PCs represent mainly noise. To determine the optimal number of PCs, the CPV method, which is typically used in the literature for determining the number of PCs, is used in this work. In this study, the threshold of cumulative variance value is chosen to be 90%. In our PCA model, the first two PCs (which capture 72.44% and 25% of the total variations) are retained as shown in Fig. 11. Once the optimal number of PCs is determined, $P$ can be calculated and then the approximated data matrix, $X'$, and a residual data matrix, $E$, can be obtained. In this way, the PCA model of the researched system is built.

The control limits of PCA-based charts, such as $T^2$ and $Q$, are based on the assumption that data are normally distributed. Therefore, it is necessary to check whether the residual distribution follows a Gaussian distribution. The residuals here are columns of the error matrix, $E$, which were not captured by the PCA model. The residual normality hypothesis was verified in this study by examining the histogram. This simple graphical tool allows us to check the normality of the residual by visually checking the histograms of these four residual vectors, which are shown in Fig. 12. In each plot of Fig. 12, the solid curve overlay on the histogram is the normal distribution. It shows that the normality assumption appears to be a reasonable one.

Now, the performances of the different anomaly-detection techniques will be assessed. Two different cases of anomalies will be considered. In the first case study, it is assumed that the testing data sets contain only a single-additive-bias anomaly (case A). In the second case study, multiple-additive-bias anomalies were considered by contamination of the temperature measurement of sensors $S_2$ and $S_3$ (case B).

5.2.3. Simulation results

5.2.3.1. Case study 1: anomaly in one temperature sensor — single-bias anomaly. In this first case study, we investigated the problem of detecting sensor bias anomalies in a flow heating system. The testing data used to compare the four anomaly-detection methods, which consist of 1000 samples, are collected from the flow heating system described earlier. Two examples are presented here to illustrate the ability of the anomaly-detection methods to detect a single-additive anomaly.

To simulate a single anomaly in the temperature measurement $S_2$, an additive anomaly with a magnitude of 3% of the total variation in the temperature measurement, is introduced between samples 400 and 500. Fig. 13a shows that the $T^2$ values for the testing data are a little larger in the region of the bias anomaly but do not violate the confidence limits. Thus, this additive anomaly is undetectable by $T^2$ anomaly-detection methods. Fig. 13b illustrates that the $Q$ statistic successfully detected this single anomaly in the temperature measurement $S_2$ but with several false alarms, which are indicated by the red circles. The $T^2$-EWMA statistic detected this additive fault but with some false alarms, while the $Q$-EWMA control scheme effectively detected this fault without false alarms. The alarm condition is triggered between the samples where the anomaly was introduced when the $Q$-EWMA statistic surpasses the control limit. It is apparent that an anomaly occurred in the monitored system or that the system was under faulty operating conditions. Therefore, the advantage of the proposed control schemes is highlighted by these results. Results also validate that the anomaly-detection methods are capable of detecting single-bias anomalies in measurement sensors and that the PCA model is able to capture the major correlation and variance among the system variables.

In the second example, a small bias level, which is 3% of the total variation in the temperature measurement $S_2$, is injected into $S_2$ between samples 400 and 500. The time evolution of $T^2$ and $Q$ monitoring indices based on the testing data are shown in Fig. 14a and b, respectively. The dashed lines represent the 95% confidence limits used to identify the possible anomalies. As can be seen from Fig. 14a the conventional PCA-based $T^2$ monitoring index was unable to detect this small bias anomaly. Fig. 14b shows that the $Q$ index however is capable of detecting this anomaly but with multiple false alarms. The $T^2$-EWMA statistic shown in Fig. 14c shows that this extension of the $T^2$ statistic can detect this simulated anomaly but with a lot of missing detections, leading to a lot of false alarms even in the normal operating state. Meanwhile, Fig. 14d clearly indicates that the $Q$-EWMA anomaly-detection algorithm detects the introduced anomaly. Recall that the EWMA control schemes are set at $\gamma = 0.3$, and $L = 3$. Therefore, this index is effective for detecting this simulated anomaly, verifying that the Q-EWMA monitoring scheme can detect small or moderate anomalies that are difficult to detect by conventional PCA. Note that statistics quantifying variations in the residual space were usually more sensitive. Our own experience with the actual data confirms that the $Q$-EWMA test is more sensitive than the $T^2$-EWMA test.

5.2.3.2. Case study 2: anomaly in temperature sensors — multiple anomalies. In this case study, simultaneous additive anomalies in the temperature sensors $S_2$ (consisting of a bias of magnitude equal to 2% of the variation in its corresponding variable) and $S_3$ (an amplitude equal to 2% of its variation domain) are introduced between samples 400 and 500. In Fig. 15b, $Q$ moves above the red dashed line (threshold for $Q$), which indicates that the flow heating system has abnormal behavior. This anomaly is not observed in $T^2$. 

![Diagram of the experimental setup.](image-url)
chart in Fig. 15a, which reveals the possibility that an anomaly occurred in the residual subspace rather than in the PC’s subspace. It is clear from Fig. 15a and b that the anomaly is better detected by the Q statistic than by $T^2$; however, not from Fig. 15b that the Q statistic results in several false alarms. The false alarm rate and missed detection rate of the Q index are 47.39 and 1%, respectively.

Indeed, the presence of measurement noise and modeling errors increases the rate of false alarms, especially in the Q-based monitoring chart. Often, to improve the quality of detection by reducing the rate of false alarms (due to noise), the EWMA filter can be applied to the residuals obtained from the PCA model. As shown in Equation (4), the data matrix $X$ can be written as the sum of an approximated matrix $X^\hat{}$ and a residual matrix $E$. Defining $E = [e_1, \ldots, e_j, \ldots, e_m]$, where $e_j \in \mathbb{R}^n$, i.e., $e_j = [e_{j1}, \ldots, e_{jn}]$, and then the residuals filtered via EWMA filter can be computed using the residuals of the $j$th vector as follows:

$$z_j^t = \gamma e_j^t + (1 - \gamma)z_j^{t-1}, \quad j \in [1, m].$$  \hspace{1cm} (13)  

where $\gamma$ is a smoothing parameter that ranges between zero and one. A value of zero eliminates all features while a value of one returns the original data unchanged. The evolution of the Q statistic based on the filtered residuals for a weighting parameter $\gamma = 0.25$ are shown in Fig. 16a. These results show a slight improvement of the Q chart applied to the filtered data over unfiltered data, where the number of false alarms is minimally reduced from 47.39% to 45.5%. Fig. 16b shows that although the $T^2$-EWMA index, detected these multiple anomalies, it resulted in some false alarms (3%) and missed detections (16%). The Q-EWMA index, however, was capable of detecting these anomalies with lower false alarm rate (of 0.88%) than other methods. The superiority of the Q-EWMA over the conventional PCA-based charts and $T^2$-EWMA is confirmed.

In summary, the results of this example show that the Q-EWMA method outperforms the conventional PCA approach by detecting all anomalies with a smaller number of false alarms, especially for the case of multiple-bias anomalies. In addition the residual subspace gives a much clearer indication of the faulty samples compared to the PC’s subspace. These results also show that
applying the $Q$-based chart on pre-filtered residuals slightly enhanced its detection ability with a smaller number of false alarms. The proposed methods were successful in detecting both single and multiple-bias anomalies.

6. Conclusion

Anomaly-detection is a central problem with important impacts on safety, availability and reliability of the operation of complex industrial processes. By amalgamation the EWMA procedure with the conventional PCA-based monitoring statistics, $T^2$ and $Q$, novel anomaly-detection methods were proposed in this study. The effectiveness of $T^2$-EWMA and $Q$-EWMA demonstrated with synthetic data and data from a flow heater system. Results show that $Q$-EWMA effectively detected both single-bias and multiple-bias additive anomalies.
The anomaly-detection methods developed here rely on linear PCA (which is an input-space modeling technique) as a modeling framework. However, most environmental and chemical processes are nonlinear and may exhibit some dynamic characteristics. Therefore, in future work, we plan to extend the advantages of the Q-EWMA and $T^2$-EWMA anomaly-detection method to handle nonlinearities and input–output models.

References


