

# A New Fault Isolation Method Based on Unified Contribution Plots

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**Abstract:** Contribution plots are important to identify the unusual process variables for fault isolation. In this paper a new fault isolation method based on unified contribution plots was presented for linear and nonlinear principal component analysis. Principal component analysis based process monitoring was first analyzed and variable contributions to monitoring statistic were modified to bring a new unified framework for contribution calculation. Then this method was generalized to nonlinear kernel principal component analysis. Some issues were further discussed including negative contribution and confidence limit, and then relative contribution was introduced to give a more reasonable explanation on variable contribution. Simulations on a continuous stirred tank reactor system were performed to show the proposed method is effective to isolate fault variables.

**Key Words:** Contribution Plots, Fault Isolation, Kernel Principal Component Analysis

## 1 Introduction

Computer control systems of modern industrial processes allow large amounts of plant data to be collected and stored. This motivates the development of the data-driven fault diagnosis method, which is also referred to as the Multivariate Statistical Process Monitoring (MSPM) technique. One of well-known MSPM methods is principal component analysis (PCA) and recently some nonlinear principal component analysis methods have emerged in this field such as kernel principal component analysis (KPCA) and neural PCA. Both linear and nonlinear methods are effective in fault detection but have great difficulty in diagnosing the potential root causes. The main reason for this is that the monitoring charts based on detection statistics indicate the deviation from normal operating conditions but do not give information on what is wrong with the process, or which process variable causes the process out of control.

As a challenging research topic, the task of fault variable isolation has attracted much attention from researchers. This was firstly studied by Miller et al.[1] and MacGregor et al.[2] which proposed the contribution plots to isolate fault variables by comparing the contribution of each process variable to the monitoring statistic. In the contribution plots, the variable with the greatest contribution value usually indicates fault sources. Based on Miller's study, Westerhuis et al.[3], Alcalá et al.[4], Alawi et al.[5], Alvarez et al.[6] and Li et al.[7] made further discussion on the application and development of contribution plots. However most of studies on contribution plots were focused on calculating variable contribution to fault in a constructive way in linear PCA and these methods can not be generalized to nonlinear PCA. Cho et al.[8] indicates the contribution plot for PCA cannot be directly applied to the case of nonlinear kernel PCA. For the purpose of building a general contribution plots theory for linear and nonlinear PCA, this paper will analyze the contribution plots in PCA-based methods and present a new

contribution calculating framework for linear and nonlinear methods.

The rest of this paper is organized as follows. In Section 2, a brief review of contribution plots in PCA-based process monitoring is described and then new contribution plots are proposed to modify the traditional contribution plots. Section 3 will generalize the modified contribution plots to nonlinear PCA as KPCA. In Section 4 a new unified contribution calculating framework is summarized and some issues are further discussed. Case studies on a continuous stirred tank reactor (CSTR) system are given in Section 5. Finally we present our conclusions in Section 6.

## 2 Contribution Plots for PCA

### 2.1 Traditional contribution plots

In PCA, the data matrix  $\mathbf{X}$  is decomposed into principal component (PC) subspace and residual subspace.

$$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E} \quad (1)$$

where  $\mathbf{X} \in R^{n \times m}$  represents  $m$  variables with  $n$  samples,  $\mathbf{T}$  is score matrix in which each row is score vector  $\mathbf{t} = [t_1, t_2, \dots, t_k]$ ,  $\mathbf{P}$  is loading matrix,  $\mathbf{E}$  is residual matrix.

When PCA is used in fault detection, two monitoring statistics are constructed for monitoring.

$$T^2 = \mathbf{t}\mathbf{\Lambda}^{-1}\mathbf{t}^T = \mathbf{x}\mathbf{P}\mathbf{\Lambda}^{-1}\mathbf{P}^T\mathbf{x}^T \quad (2)$$

$$Q = \|\mathbf{e}\|^2 = (\mathbf{x} - \hat{\mathbf{x}})(\mathbf{x} - \hat{\mathbf{x}})^T = \mathbf{x}(\mathbf{I} - \mathbf{P}\mathbf{P}^T)\mathbf{x}^T = \mathbf{x}\mathbf{P}_r\mathbf{P}_r^T\mathbf{x}^T \quad (3)$$

where  $\mathbf{x}$  is a measurement vector with  $m$  variables and  $\hat{\mathbf{x}}$  is a reconstructed vector,  $\mathbf{\Lambda}$  is the diagonal matrix of the eigenvalues associated with score vectors,  $\mathbf{P}_r$  is an orthonormal matrix which meets  $\mathbf{P}_r\mathbf{P}_r^T + \mathbf{P}\mathbf{P}^T = \mathbf{I}$ .

Westerhuis et al.[3] discussed contribution plots theory in batch process and continuous process and extended it from PCA models to latent variable models with correlated scores. In their work, the contribution to the  $Q$ -statistic for process variable  $j$  is calculated as Eq.(4).

$$c_j^Q = (e_{new,j})^2 = (x_{new,j} - \hat{x}_{new,j})^2 \quad (4)$$

where  $\hat{x}_{new,j}$  is reconstruction variable corresponding to a new measurement  $x_{new,j}$ .

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Contribution to  $D$ -statistic ( $T^2$ -statistic) for continuous processes is described in Eq.(5).

$$c_j^D = \mathbf{t}_{new}^T \Lambda^{-1} [x_{new,j} \mathbf{p}_j (\mathbf{P}^T \mathbf{P})^{-1}]^T \quad (5)$$

where  $\mathbf{P}^T \mathbf{P} = \mathbf{I}$  for PCA method,  $\mathbf{t}_{new}$  is scores corresponding to new measurement  $x_{new}$ ,  $\Lambda$  is the diagonal matrix of the eigenvalues associated with score vectors  $\mathbf{t}_{new}$ ,  $\mathbf{p}_j$  is the  $j$ th row of  $\mathbf{P}$ .

The existing work has made a lot of discussions on contribution plots and displayed their effectiveness in some fault scenarios. However, deep theory explanations and generalization to nonlinear PCA are still needed. So this paper is to make further study of contribution calculation in the next section.

## 2.2 New contribution plots

For simplification the statistics  $T^2$  and  $Q$  are replaced with a variable symbol  $f$  as Eq. (6).

$$f = \mathbf{x} \Sigma \mathbf{x}^T \quad (6)$$

where  $\Sigma = \mathbf{P} \Lambda^{-1} \mathbf{P}^T$  for  $T^2$  statistic and  $\Sigma = \mathbf{I} - \mathbf{P} \mathbf{P}^T$  for  $Q$  statistic.

Variable  $f$  is a function of measured variables  $\mathbf{x} = [x_1, x_2, \dots, x_m]$  expressed using Eq.(7)

$$f = f(x_1, x_2, \dots, x_m) \quad (7)$$

Where  $x_j$  is the  $j$ th variable.

From Lagrange's mean value theorem, Eq. (8) is obtained.

$$\begin{aligned} & f(x_1, \dots, x_m) - f(x_{10}, \dots, x_{m0}) \\ &= \left( (x_1 - x_{10}) \frac{\partial}{\partial x_1} + \dots + (x_m - x_{m0}) \frac{\partial}{\partial x_m} \right) f(x_{10}, \dots, x_{m0}) \\ &+ \theta (x_1 - x_{10}), \dots, x_{m0} + \theta (x_m - x_{m0}) \quad (0 < \theta < 1) \end{aligned} \quad (8)$$

Given  $x_{10} = 0, \dots, x_{m0} = 0$ , the above equation can be formulated as

$$\begin{aligned} & f(x_1, \dots, x_m) = \\ & f(0, \dots, 0) + \left( x_1 \frac{\partial}{\partial x_1} + \dots + x_m \frac{\partial}{\partial x_m} \right) f(\theta x_1, \dots, \theta x_m) \quad (9) \end{aligned}$$

From Eq.(9), it is seen that each statistic can be decomposed as a sum of each variable's derivative which can be viewed as a variable contribution. So  $j$ th variable contribution to PCA-based monitoring statistic is defined by Eq.(10).

$$C_{-}f(x_j) = x_j \frac{\partial}{\partial x_j} f(\theta x_1, \dots, \theta x_m) \quad (10)$$

PCA-based monitoring statistics  $T^2$  and  $Q$  have some similar interesting characteristics: statistics are zero when the normalized variable  $\mathbf{x}$  equals vector zero and two statistics have similar structure. According to these property, Equation (11)(12) are given as

$$f(0, \dots, 0) = 0 \quad (11)$$

$$\frac{\partial}{\partial x_j} f(\theta x_1, \dots, \theta x_m) = \theta^2 \frac{\partial}{\partial x_j} f(x_1, \dots, x_m) \quad (12)$$

According to Eq.(9), it can be concluded that the monitoring statistic is the sum of all variables' contribution.

In Eq.(12)  $\theta = \frac{1}{\sqrt{2}}$  can be proved easily for PCA-based

process monitoring, so the variable contribution can be calculated as

$$\begin{aligned} C_{-}T^2(x_j)_{new} &= \frac{1}{2} x_j \frac{\partial}{\partial x_j} (\mathbf{x} \mathbf{P} \Lambda^{-1} \mathbf{P}^T \mathbf{x}^T) \\ &= \mathbf{x} \mathbf{P} \Lambda^{-1} \mathbf{p}_j^T x_j = \mathbf{t} \Lambda^{-1} (x_j \mathbf{p}_j^T) \end{aligned} \quad (13)$$

$$\begin{aligned} C_{-}Q(x_j)_{new} &= \frac{1}{2} x_j \frac{\partial}{\partial x_j} (\mathbf{x} \mathbf{P}_r \mathbf{P}_r^T \mathbf{x}^T) \\ &= x_j \mathbf{x} \mathbf{P}_r \mathbf{p}_{rj}^T = x_j (x_j - \hat{x}_j) = x_j e_j \end{aligned} \quad (14)$$

where  $\mathbf{p}_j$  represents the  $j$ th row of  $\mathbf{P}$ ,  $\mathbf{p}_{rj}$  represents the  $j$ th row of  $\mathbf{P}_r$ .

Compared to traditional methods in Eq.(4)(5), Eq.(13)(14) are called new contribution plots methods. It is noted that in both methods contribution to  $T^2$  is essentially same but contribution to  $Q$  in the new method makes important modification.

## 3 Contribution Plots for Nonlinear PCA

Recently nonlinear PCA has become a hot research topic. Kernel PCA(KPCA) was proved to be simple and effective as a nonlinear PCA method whose nonlinear mapping is accomplished by the kernel function. Originally Kernel PCA was developed by Schölkopf et al. [9] and has been applied in fault diagnosis and process monitoring by Lee et al.[10] and Sun et al.[11]. The studies on KPCA show that it can detect fault effectively but it is hard to compute the contributions of original process variables in KPCA-based monitoring because it is difficult or even impossible to find an inverse mapping function from the feature space to the original space. In this paper, we can give contribution plots for KPCA method using the new contribution framework.

KPCA is to map the input space into a feature space by nonlinear transformation and extract the principal components in feature space. It is assumed that  $\Phi(\cdot)$  is a nonlinear mapping function that projects the data in input space to feature space and the covariance matrix in feature space can be expressed as:

$$\text{cov}(\Phi(\mathbf{X})) = \frac{1}{n-1} \sum_{j=1}^n \Phi(\mathbf{x}_j)^T \Phi(\mathbf{x}_j) \quad (15)$$

where  $\mathbf{x}_j$  ( $j=1, \dots, n$ ) is the  $j$ th row of  $\mathbf{X}$ . In the feature space the eigenvalue problem must be solved for KPCA decomposition.

$$\text{cov}(\Phi(\mathbf{X})) \mathbf{p}_i = \lambda_i \mathbf{p}_i \quad (16)$$

It should be pointed out that it is difficult to solve the problem of Eq. (16) as  $\Phi(\cdot)$  can not be obtained in most cases. However, there exist coefficients  $\alpha_{ij}$  ( $j=1, 2, \dots, n$ ) such that

$$\mathbf{p}_i = \sum_{j=1}^n \alpha_{ij} \Phi(\mathbf{x}_j)^T \quad (17)$$

Combining Eqs.(15), (16) and (17), the following equation can be obtained

$$(n-1) \lambda_i \alpha_i = \mathbf{K} \alpha_i \quad (18)$$

where  $\mathbf{K}$  is defined as  $[\mathbf{K}]_{ij} = k(\mathbf{x}_i, \mathbf{x}_j) = \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle$ .

One can avoid nonlinear mapping by defining kernel function  $k(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle$ . With the use of kernel function, the score vectors are expressed as:

$$\mathbf{t}_i = \langle \mathbf{p}_i, \Phi(\mathbf{x}) \rangle = \sum_{j=1}^n \alpha_{ij} \langle \Phi(\mathbf{x}_j), \Phi(\mathbf{x}) \rangle \quad (19)$$

Two statistics used in KPCA-based process monitoring are  $T^2$  and  $Q$ :

$$T^2 = \mathbf{t} \Lambda^{-1} \mathbf{t}^T = \mathbf{K}_t^T \mathbf{a} \Lambda^{-1} \mathbf{a}^T \mathbf{K}_t \quad (20)$$

$$C_{-}T^2(x_{tj}) = x_{tj} \frac{\partial}{\partial x_{tj}} (\mathbf{K}_t^T \mathbf{a} \Lambda^{-1} \mathbf{a}^T \mathbf{K}_t) \bigg|_{\theta \mathbf{x}_t} = 2x_{tj} \frac{\partial \mathbf{K}_t^T}{\partial x_{tj}} \mathbf{a} \Lambda^{-1} \mathbf{a}^T \mathbf{K}_t \bigg|_{\theta \mathbf{x}_t} \quad (22)$$

$$C_{-}Q(x_{tj}) = x_{tj} \frac{\partial}{\partial x_{tj}} (k(\mathbf{x}_t, \mathbf{x}_t) - \mathbf{K}_t^T \mathbf{a} \mathbf{a}^T \mathbf{K}_t) \bigg|_{\theta \mathbf{x}_t} = x_{tj} \left( \frac{\partial k(\mathbf{x}_t, \mathbf{x}_t)}{\partial x_{tj}} - 2 \frac{\partial \mathbf{K}_t^T}{\partial x_{tj}} \mathbf{a} \mathbf{a}^T \mathbf{K}_t \bigg|_{\theta \mathbf{x}_t} \right) \quad (23)$$

where

$$\frac{\partial \mathbf{K}_t^T}{\partial x_{tj}} \bigg|_{\theta \mathbf{x}_t} = \left[ \frac{\partial k(\theta \mathbf{x}_t, \mathbf{x}_1)}{\partial x_{tj}} \frac{\partial k(\theta \mathbf{x}_t, \mathbf{x}_2)}{\partial x_{tj}} \dots \frac{\partial k(\theta \mathbf{x}_t, \mathbf{x}_n)}{\partial x_{tj}} \right] \quad (24)$$

$$k(\theta \mathbf{x}_t, \theta \mathbf{x}_t) = 1 - \frac{2}{n} \sum_{l=1}^n \exp(-\|\theta \mathbf{x}_t - \mathbf{x}_l\|^2 / \sigma) + \frac{1}{n^2} \sum_{l=1}^n \sum_{k=1}^n \exp(-\|\mathbf{x}_l - \mathbf{x}_k\|^2 / \sigma) \quad (25)$$

$$\frac{\partial k(\theta \mathbf{x}_t, \theta \mathbf{x}_t)}{\partial x_{tj}} = \frac{2}{n} \sum_{l=1}^n \frac{1}{\sigma} 2\theta(x_{tj} - x_{lj}) \exp(-\|\theta \mathbf{x}_t - \mathbf{x}_l\|^2 / \sigma) \quad (26)$$

$$k(\theta \mathbf{x}_t, \mathbf{x}_i) = \exp(-\|\theta \mathbf{x}_t - \mathbf{x}_i\|^2 / \sigma) - \frac{1}{n} \sum_{l=1}^n \exp(-\|\theta \mathbf{x}_t - \mathbf{x}_l\|^2 / \sigma) - \frac{1}{n} \sum_{l=1}^n \exp(-\|\mathbf{x}_l - \mathbf{x}_i\|^2 / \sigma) + \frac{1}{n^2} \sum_{l=1}^n \sum_{k=1}^n \exp(-\|\mathbf{x}_l - \mathbf{x}_k\|^2 / \sigma) \quad (27)$$

$$\frac{\partial k(\theta \mathbf{x}_t, \mathbf{x}_i)}{\partial x_{tj}} = -\frac{1}{\sigma} 2\theta(x_{tj} - x_{ij}) \exp(-\|\theta \mathbf{x}_t - \mathbf{x}_i\|^2 / \sigma) + \frac{1}{n} \sum_{l=1}^n \frac{1}{\sigma} 2\theta(x_{tj} - x_{lj}) \exp(-\|\theta \mathbf{x}_t - \mathbf{x}_l\|^2 / \sigma) \quad (28)$$

In Eq.(22)(23),  $\theta$  is required for contribution calculation. There are two calculating methods: one is to calculate  $\theta$  according to Eq.(9), by which a precise value of  $\theta$  can be available. But we think this is not necessary because it is complex and time-consuming to compute a different  $\theta$  for each sample. So another substituted method is to use an approximation of  $\theta$  which can be obtained by some normal behavior data sets.

#### 4 A Unified Framework and Some Issues

In the above analysis a new method to calculate variable contribution has been discussed for both PCA and KPCA. Analogously, the proposed method can be generalized to other similar MSPM methods, so a unified framework for MSPM contribution plots can be built for fault isolation. For any statistics expressed by  $f$ , variable contribution to  $f$  can be given using Eq.(29)

$$C_{-}f(x_j) = x_j \frac{\partial}{\partial x_j} f(\theta \mathbf{x}_1, \dots, \theta \mathbf{x}_m), (0 < \theta < 1) \quad (29)$$

where  $\theta$  can be approximately estimated by some normal behavior data sets for the purpose of fault variable isolation.

There are some issues to be discussed about new contribution plots. The first topic is about negative contributions. The contribution of process variables in Eq.(29) can be positive or negative. We think the sign of the contributions is not important and the absolute value indicates the affections of process variables to statistics. So the absolute value of contributions is used in a contribution

$$Q = (k(\mathbf{x}_t, \mathbf{x}_t) - \mathbf{t} \mathbf{t}^T) = (k(\mathbf{x}_t, \mathbf{x}_t) - \mathbf{K}_t^T \mathbf{a} \mathbf{a}^T \mathbf{K}_t) \quad (21)$$

where  $\mathbf{K}_t$  is normalized kernel matrix,  $\mathbf{a}$  is transformation matrix,  $\Lambda$  is weighted matrix.

According to Eq.(10), variable contribution to statistics can be calculated by Eq.(22)(23). In this study, radial basis kernel function  $k(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|^2 / c)$  is chosen, so Eqs.(26)-(28) can be available.

graphic. Another issue is a contribution's confidence limit. Currently the contribution plots are a graphical representation of the original absolute contributions and confidence limits are not used to identify the bounds of normal behavior for individual multivariate statistical contributions. Colin et al.[12] has given three methods to calculate the derivation in confidence limits which in instinct make use of the standard derivation of the contribution. Considering each variable's contribution with a different confidence limit, so relative contribution is built for more accurate fault isolation. Its expression is shown in Eq.(30).

$$C_{-}^R f = \frac{C_{-}f - \text{mean}(C_{-}f_{\text{normal}})}{\text{std}(C_{-}f_{\text{normal}})} \quad (30)$$

where  $C_{-}f_{\text{normal}}$  is variable contribution under normal operation condition.

#### 5 Case Study

The proposed fault isolation strategy is tested with a simulated process, a non-isothermal continuous stirred tank reactor (CSTR) system. A schematic diagram of the CSTR with feedback control system is shown in Fig. 1. It is assumed that the classic first order irreversible reaction happens in CSTR. The flow of solvent and reactant A into a reactor produces a single component B as an outlet stream. Heat from the exothermic reaction is removed through cooling flow of jacket. The reactor temperature is controlled to set-point by manipulating the coolant flow. The level is controlled by manipulating the outlet flow.

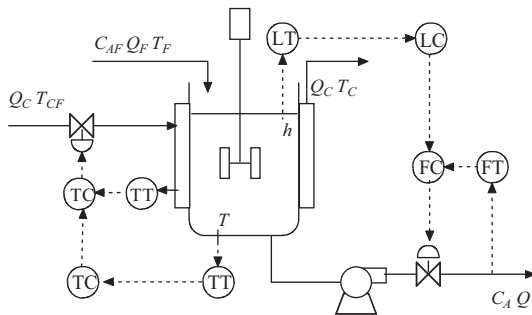


Fig.1. A diagram of the CSTR system

The process data sets including normal operating situation and ten kinds of fault pattern are generated by simulating the CSTR process. The applied fault pattern (Fault F1~F10) can be seen in Table 1. These faults contain process change, sensor malfunction and valve faults. In order to test data-driven process monitoring methods, some important variables should be measured and stored in simulation procedure. Gaussian noise is added to all measured variables in simulation procedure. The simulation interval is set to 2 seconds but in our study database records one sample every 12 seconds to store long time period data sets. By simulating normal situation and fault patterns, 500 samples are collected for algorithm study and every fault is introduced at the 200th sample.

Fault F3 is illustrated for fault detection and isolation, which means the feed concentration change corresponding to variable 7. PCA is performed for process monitoring and the monitoring statistics alarm threshold is set to a 99% confidence limit. According to the fault detection results in Fig.2,  $T^2$  statistic exceeds the confidence limit clearly at the 287th sample.

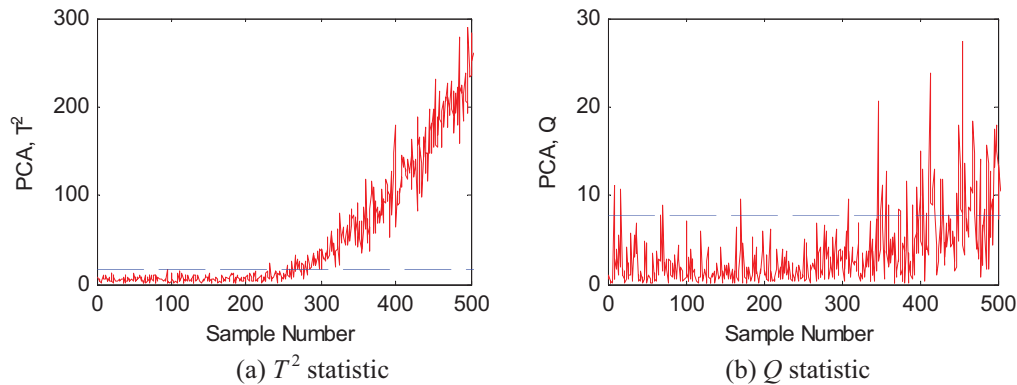


Fig.2. PCA monitoring with 99% confidence limit for Fault F3 traditional method

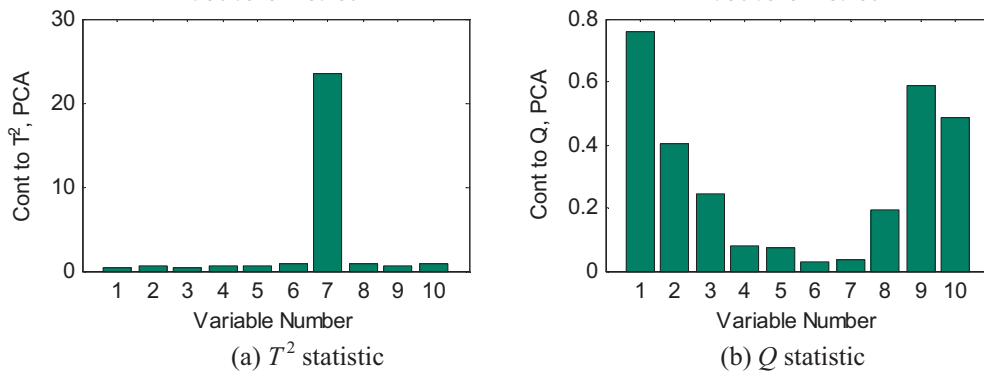


Fig.3. Average contribution plot for Fault F3 (traditional method)

Table 1 Process faults for CSTR system

Fault	Description
F1	Step change in feed flow rate.
F2	The feed temperature ramps up or down.
F3	The feed concentration ramps up or down.
F4	The hear transfer coefficient ramps down.
F5	Catalyst deactivation.
F6	The coolant feed temperature ramps up or down.
F7	Set point change for the reactor temperature.
F8	The feed temperature measurement has a bias
F9	The reactor temperature measurement has a bias
F10	The coolant valve was fixed at the steady value.

Variable contributions are plotted to identify fault variables for early remedy. To avoid accident error at some specific sample, 20 samples from a fault detection sample are used to calculate the average contributions. When traditional contribution plot method is applied, Fig.3 indicates that contribution plots for  $T^2$  are more apparent to isolate fault while contribution plots to  $Q$  still cannot isolate accurate variables. But if the new contribution plots method is applied without considering of relative contribution, it is concluded that contributions to  $T^2$  and  $Q$  both list variable 7 as the maximum contribution in Fig.4. However, in Fig.4(b) the difference between variable contribution is not obvious. With the application of relative contribution, the isolation plots in Fig.5 find the right abnormal variables more clearly.

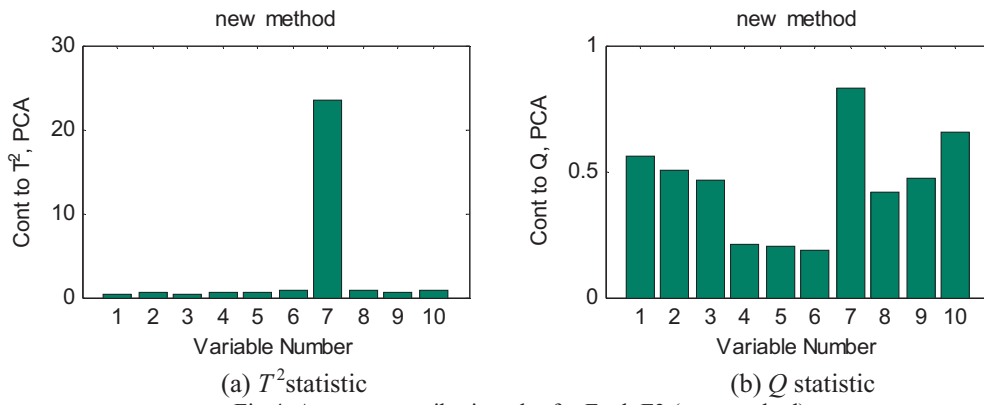


Fig.4. Average contribution plot for Fault F3 (new method)

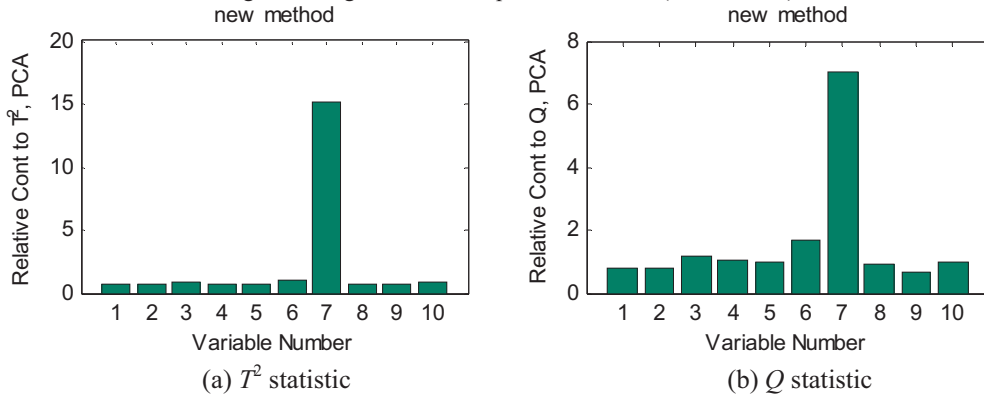


Fig.5. Relative contribution plot for Fault F3 (new method)

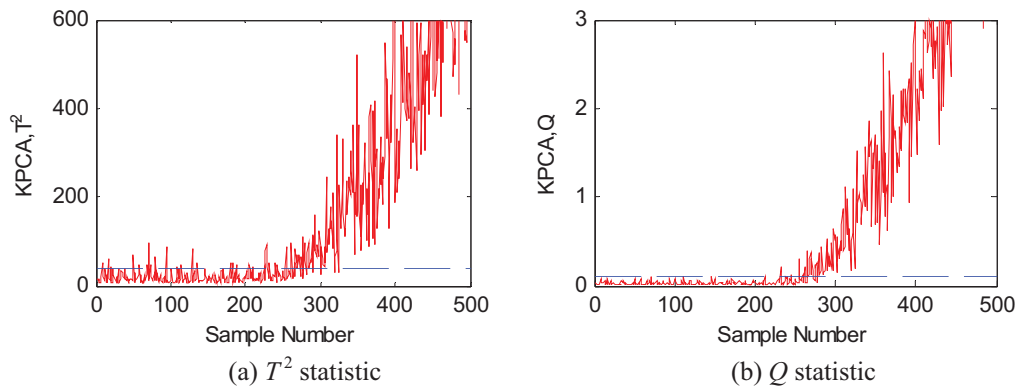


Fig.6. KPCA monitoring with 99% confidence limit for Fault F3

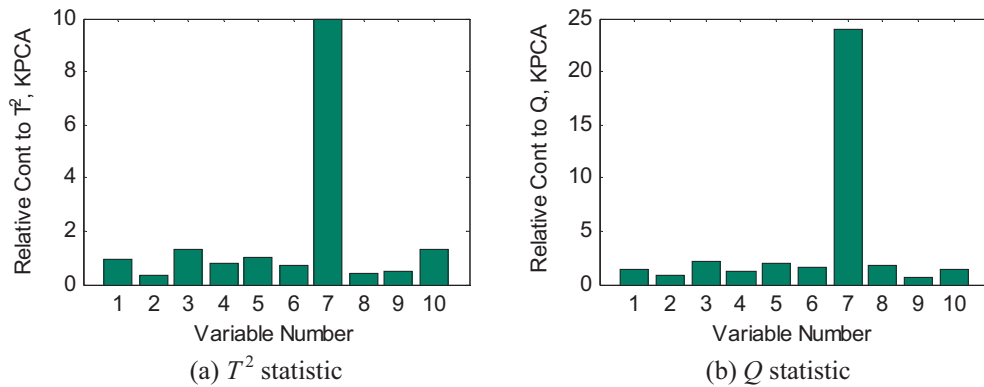


Fig.7. Relative contribution plot for Fault F3 when KPCA is applied

If KPCA is applied to monitor the CSTR process, it has better detection ability as nonlinear method. From Fig.6, fault F3 is detected at 265th sample in KPCA-based monitoring and then the new contribution method is performed to isolate fault variables. The isolation results for fault F3 are illustrated in Fig. 7 which show that variable 7 is

indicated as the greatest contribution variables. These conclusions are consistent to the process mechanism. So KPCA with new contribution method not only can detect faults more effectively, but can isolate fault variable correctly.



## 6. Conclusions

In this paper a unified contribution calculating framework was built for linear PCA and nonlinear KPCA which provides a clear and straightforward solution for fault variable location. The proposed method can also be generalized to some classical MSPM methods such as canonical variate analysis and independent component analysis. In fact, many other linear and nonlinear statistical monitoring methods can be also discussed in this framework which is a topic for future study. The issues of negative contributions and confidence limits provide a more reasonable interpretation of contribution plots and lead to relative contribution. The simulation results on the CSTR system reveal that the application of the new method can give more accurate contribution plots than traditional method.

However, it should not be overestimated that contribution plots can make a perfect solution for fault source identification in data-driven process monitoring. Contribution plots can only be viewed as first step of fault identification and provide some important help on initial fault location, and it can not diagnose complex faults which involve many fault variables. More deep study about fault isolation methods and fault propagation process analysis should be developed.

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